

Mantyl tagged oligo α (1- \rightarrow 2) mannosides as *Candida albicans* β -mannosyltransferases substrates: a comparison between synthetic strategies

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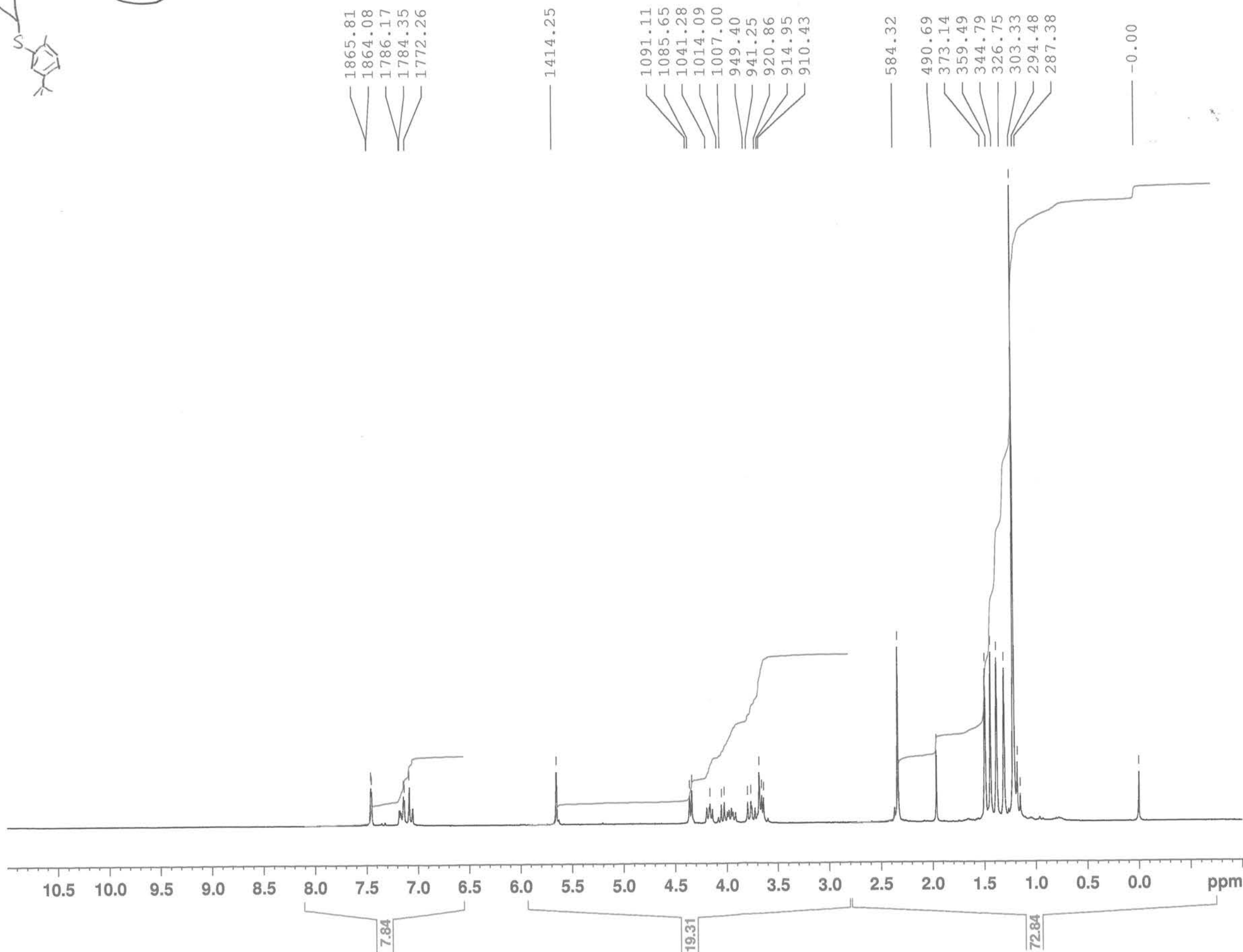
RSC Advances, 2013

Supplementary information:

^1H and ^{13}C NMR spectra of synthesized compounds

MP1/14

2



Current Data Parameters
NAME May27-2011-JMM
EXPNO 60
PROCNO 1

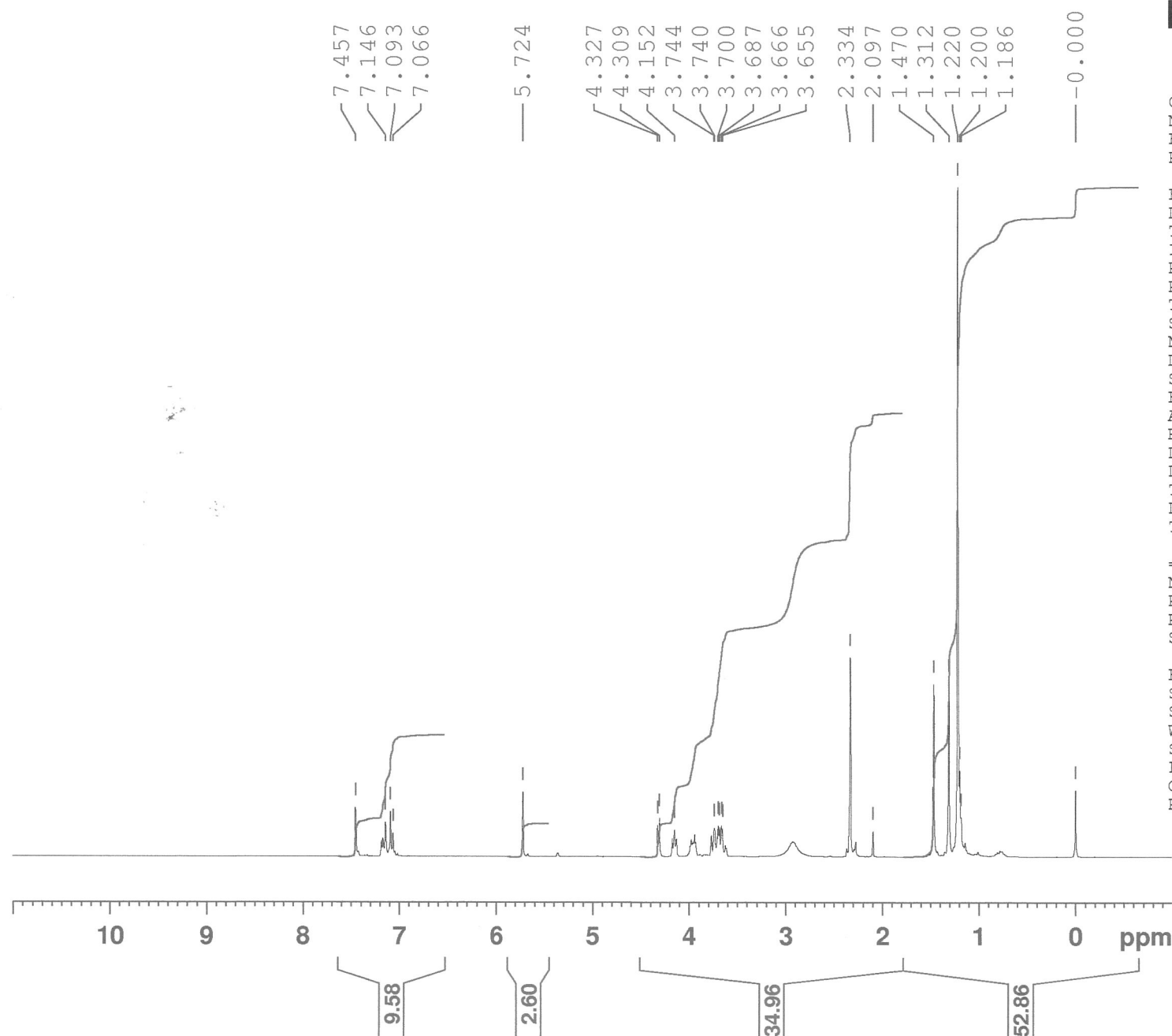
F2 - Acquisition Parameters
Date_ 20110527
Time 13.47
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 64
DS 2
SWH 5175.983 Hz
FIDRES 0.315917 Hz
AQ 1.5827444 sec
RG 114
DW 96.600 usec
DE 8.00 usec
TE 300.0 K
D1 0.20000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 250.1315446 MHz

F2 - Processing parameters
SI 8192
SF 250.1300270 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

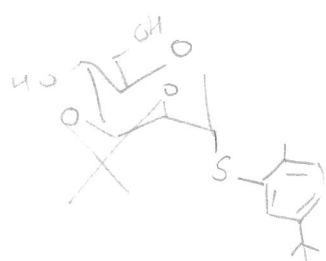
3

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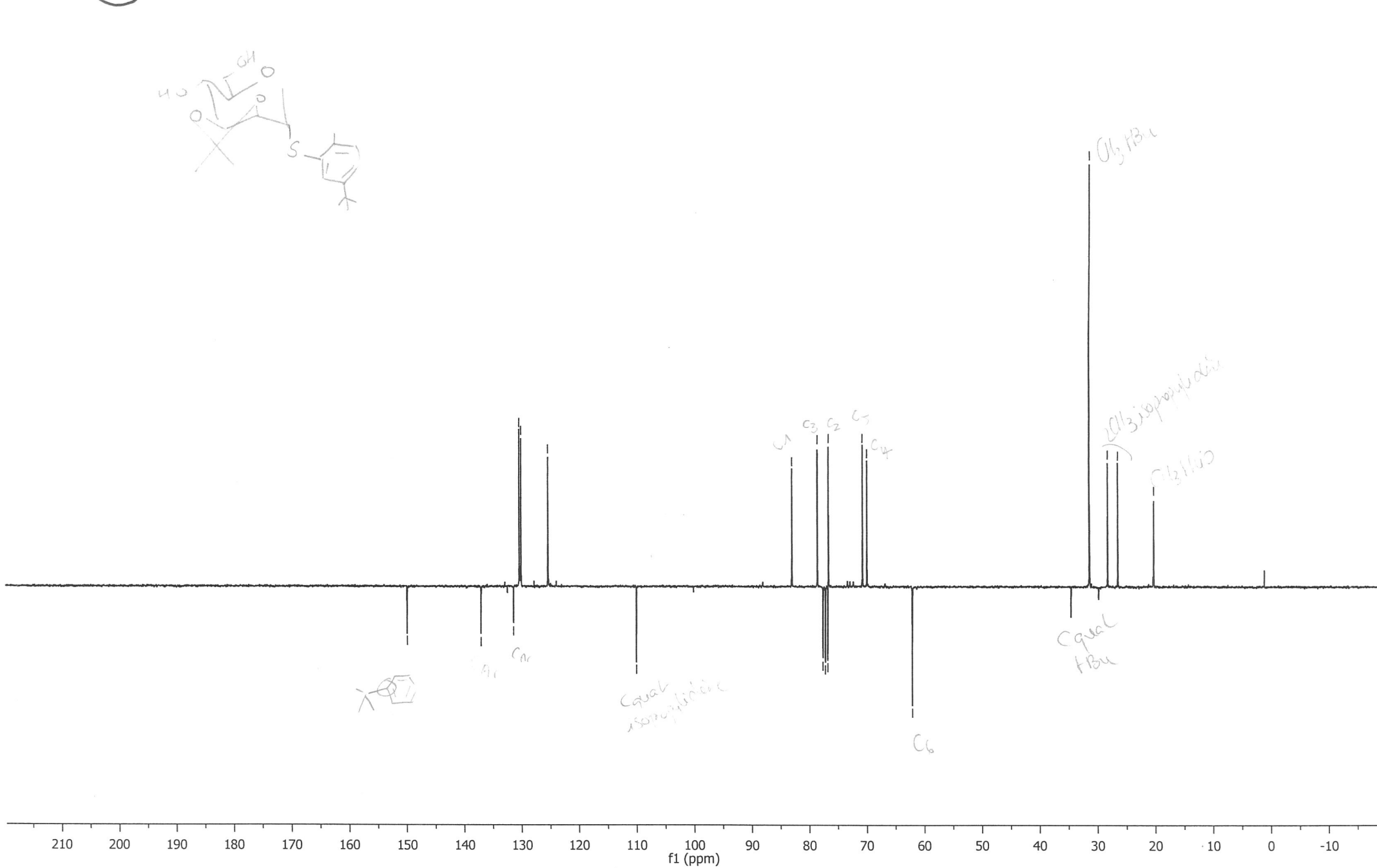


Jun06-2012-JMM
 MP1/21

3

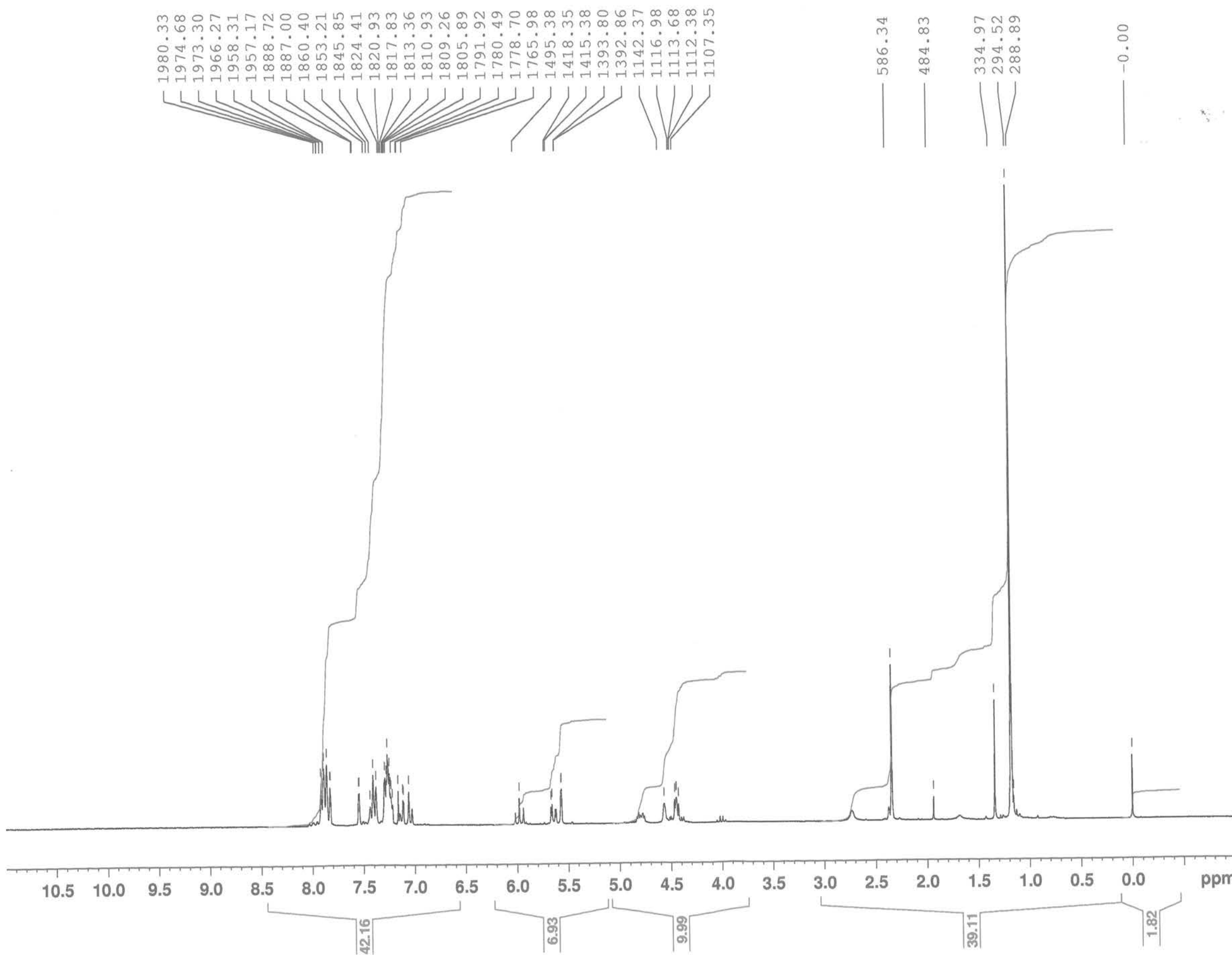


149.91, 137.08, 131.41, 130.41, 130.09, 125.40, 110.05, 83.09, 78.63, 77.65, 77.23, 76.81, 76.70, 70.84, 70.05, 62.15, 34.66, 31.50, 28.33, 26.58, 20.34



MP1/19

6



Current Data Parameters
NAME Jun07-2011-JMM
EXPNO 60
PROCNO 1

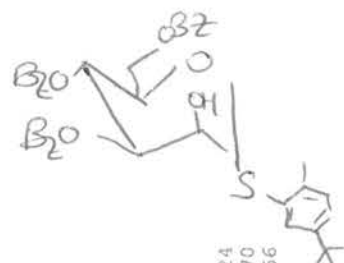
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Time 12.21
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 64
DS 2
SWH 5175.983 Hz
FIDRES 0.315917 Hz
AQ 1.5827444 sec
RG 228.1
DW 96.600 usec
DE 8.00 usec
TE 300.0 K
D1 0.20000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 250.1315446 MHz

F2 - Processing parameters
SI 8192
SF 250.1300318 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

MP1/19

6



166.24
165.70
165.56

150.08
136.41
133.49
133.41
132.97
132.12
130.14
129.87
129.78
129.68
129.07
129.01
128.51
128.44
128.31
125.08

87.69

77.58
77.07
76.56
72.98
71.23
70.18
67.07
63.44

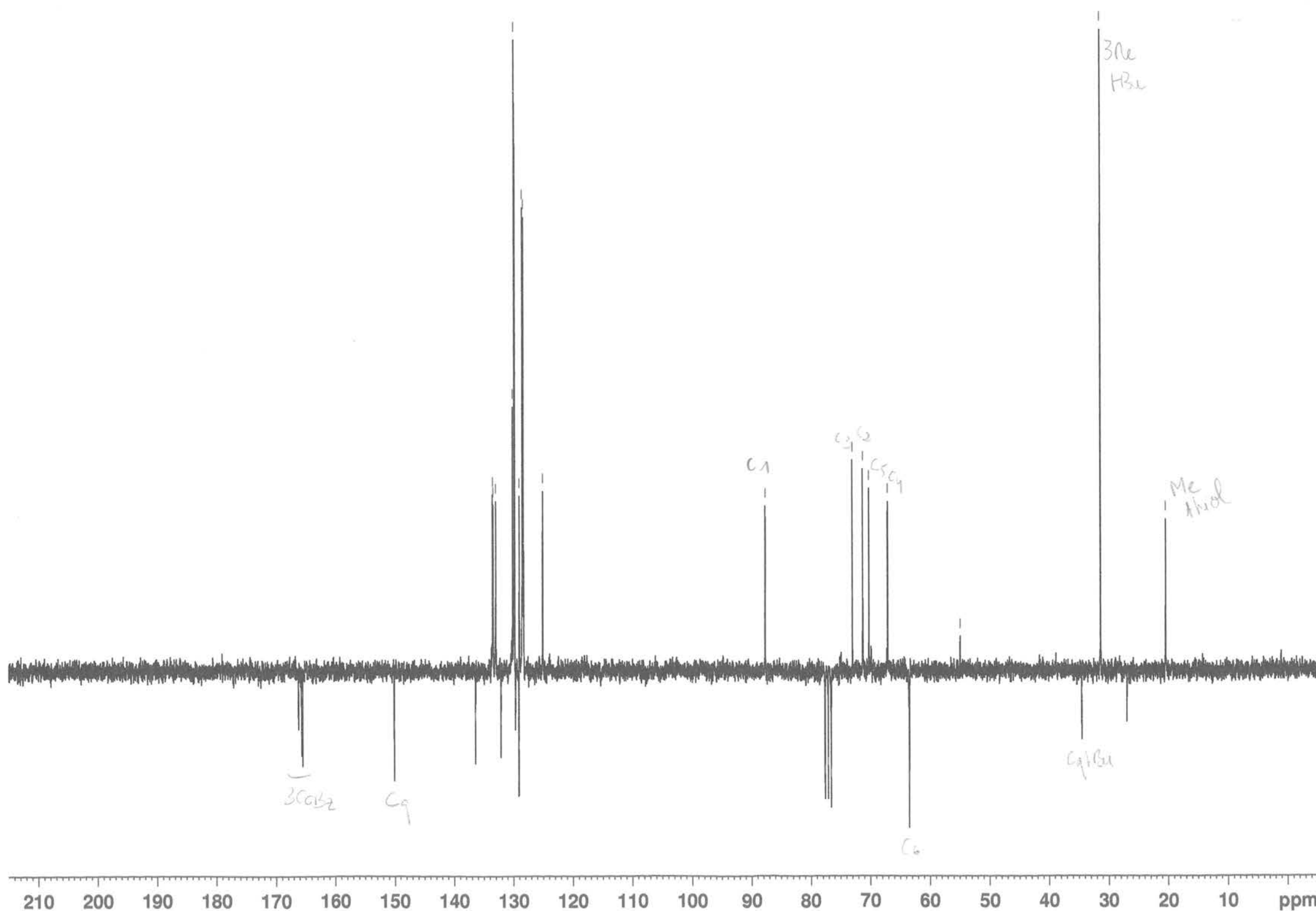
54.90

34.51

31.31

26.94

20.38



Current Data Parameters
 NAME Jun07-2011-JMM
 EXPNO 70
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110607
 Time 12.40
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 15060.241 Hz
 FIDRES 0.229801 Hz
 AQ 2.1758451 sec
 RG 16384
 DW 33.200 usec
 DE 8.00 usec
 TE 300.0 K
 CNST2 145.000000
 CNST11 1.000000
 D1 2.0000000 sec
 d20 0.00689655 sec
 DELTA 0.00001019 sec
 TD0 1

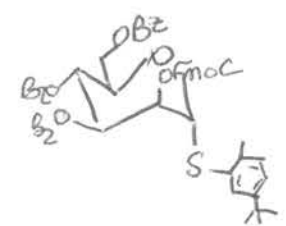
==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 p2 16.00 usec
 PL1 -3.00 dB
 SFO1 62.9015280 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -3.00 dB
 PL12 19.00 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952390 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

MP1/27

7



Current Data Parameters
NAME Jun22-2011-JMM
EXPNO 40
PROCNO 1

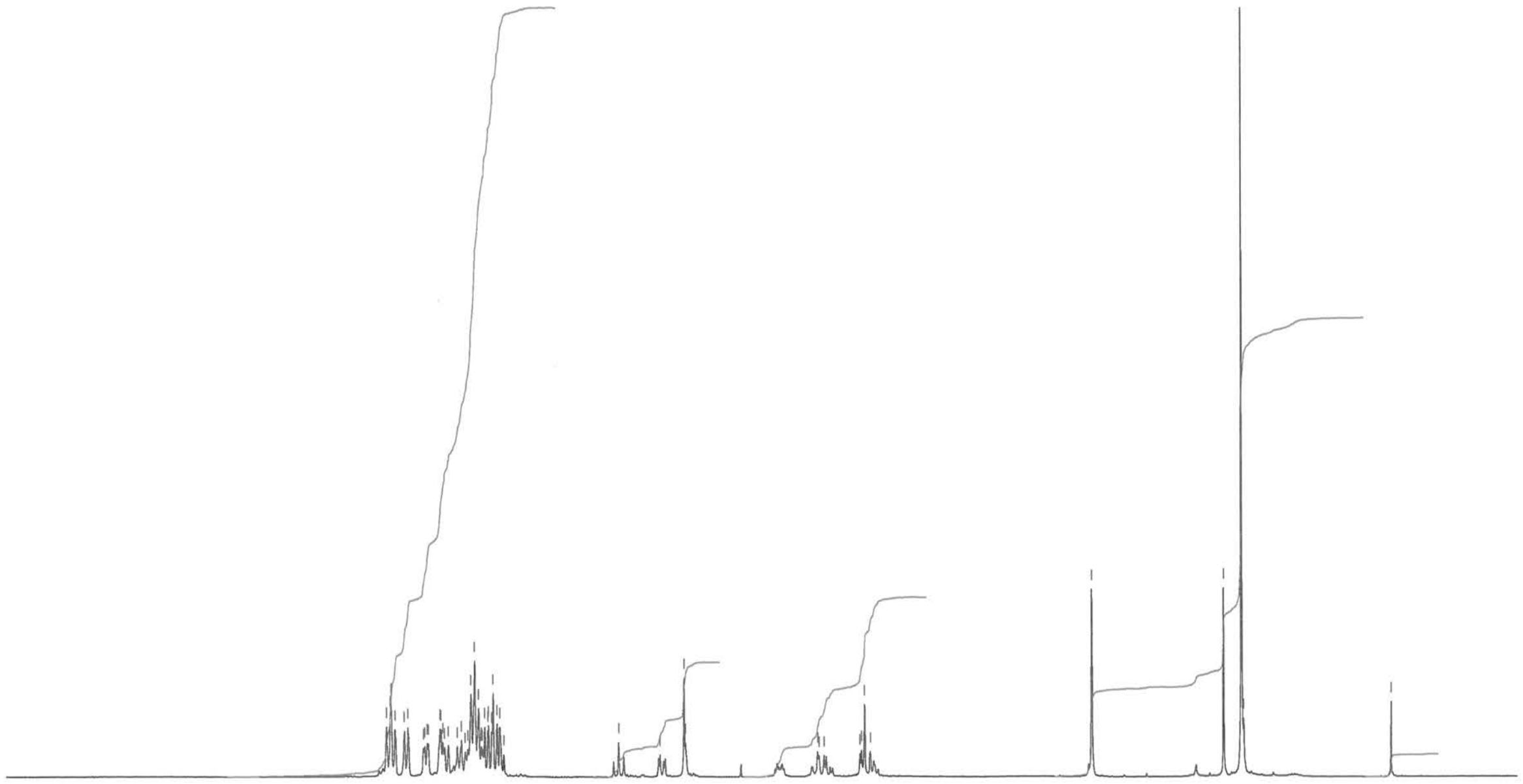
F2 - Acquisition Parameters
Date_ 20110622
Time 12.30
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 64
DS 2
SWH 5175.983 Hz
FIDRES 0.315917 Hz
AQ 1.5827444 sec
RG 161.3
DW 96.600 usec
DE 8.00 usec
TE 300.0 K
D1 0.20000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 250.1315446 MHz

F2 - Processing parameters
SI 8192
SF 250.1300409 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1994.78
1987.41
1985.90
1977.91
1959.40
1952.13
1921.67
1918.92
1914.26
1911.48
1888.55
1886.62
1883.21
1879.56
1872.10
1854.56
1846.05
1838.53
1833.48
1827.29
1819.68
1811.61
1807.28
1806.35
1804.24
1799.96
1793.38
1792.52
1785.85
1783.04
1775.12
1769.39
1761.49
1532.77
1450.66
1402.72
1400.08
1138.34
1135.69
1125.82
1054.37
1051.31
1045.31
1033.66

593.04
331.67
296.79
292.19
-0.00



10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

49.80

7.41

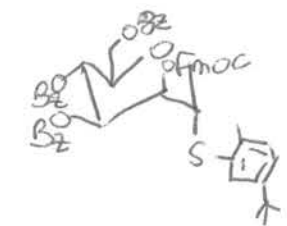
11.61

29.71

1.46

(+)

MP1/27



165.16
164.43
164.27
153.31
149.10
142.21
141.97
140.18
136.01
132.42
132.34
131.97
130.51
129.24
129.00
128.85
128.76
128.68
127.94
127.82
127.42
127.31
126.92
126.35
126.25
124.61
124.23
118.99

84.69
76.52
76.01
75.51
74.33
69.54
69.37
69.25
65.80
62.16

45.45

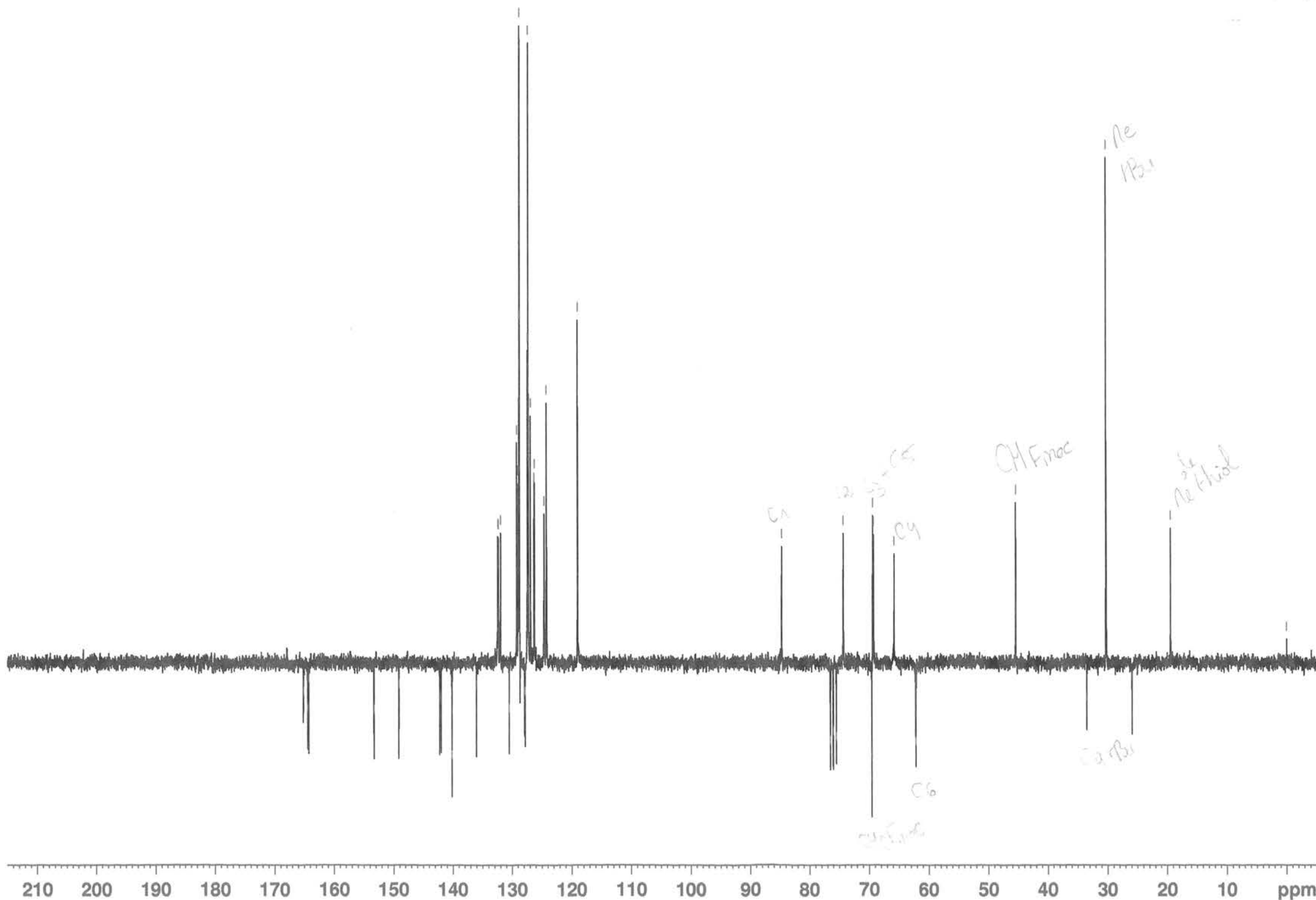
33.45

30.25

25.88

19.44

0.00



Current Data Parameters
 NAME Jun22-2011-JMM
 EXPNO 41
 PROCNO 1

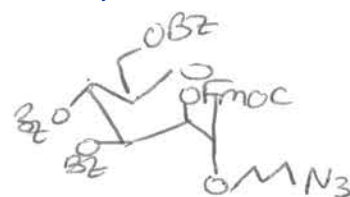
F2 - Acquisition Parameters
 Date_ 20110622
 Time 12.49
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 15060.241 Hz
 FIDRES 0.229801 Hz
 AQ 2.1758451 sec
 RG 16384
 DW 33.200 usec
 DE 8.00 usec
 TE 300.0 K
 CNST2 145.000000
 CNST11 1.000000
 D1 2.0000000 sec
 d20 0.00689655 sec
 DELTA 0.00001019 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 p2 16.00 usec
 PL1 -3.00 dB
 SFO1 62.9015280 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -3.00 dB
 PL12 19.00 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8953078 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

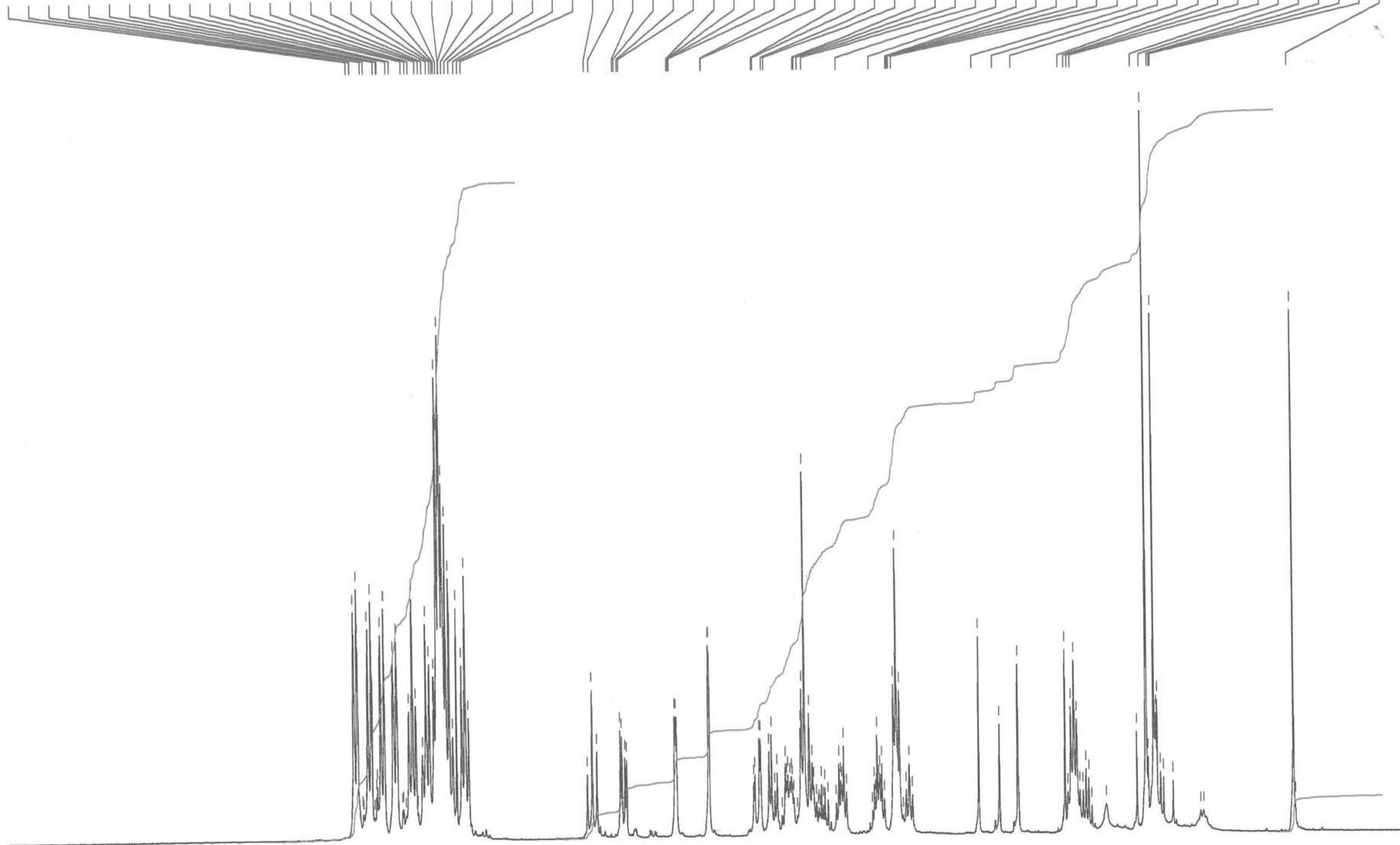
MP1/17



8



2010.80
2003.67
2002.09
1980.53
1973.36
1952.81
1945.64
1944.61
1926.08
1918.60
1892.90
1885.51
1878.11
1863.54
1856.25
1848.95
1839.17
1832.37
1827.82
1824.96
1820.08
1814.00
1813.04
1806.53
1798.99
1790.82
1780.17
1772.47
1764.83
1501.03
1490.97
1440.79
1437.53
1430.67
1427.42
1324.55
1322.86
1321.50
1319.70
1252.19
1250.80
1144.02
1141.36
1123.09
1117.94
1055.74
1053.38
1047.04
1037.04
963.21
891.63
856.33
854.24
852.44
849.87
843.32
672.48
628.29
588.64
488.11
475.72
469.39
463.12
334.34
314.80
298.35
293.81
291.46
0.00



10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

46.47

51.03

2.49

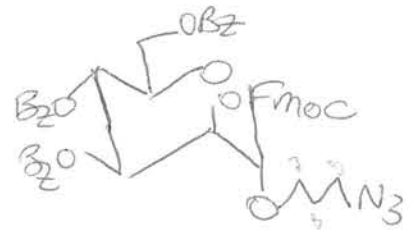
Current Data Parameters
NAME May27-2011-JMM
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110527
Time 12.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 64
DS 2
SWH 5175.983 Hz
FIDRES 0.315917 Hz
AQ 1.5827444 sec
RG 203.2
DW 96.600 usec
DE 8.00 usec
TE 300.0 K
D1 0.20000000 sec
TD0 1

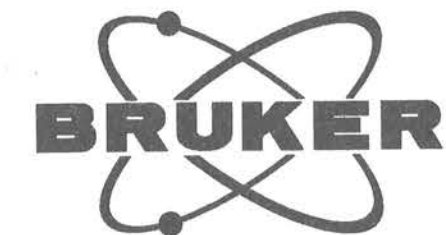
==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 250.1315446 MHz

F2 - Processing parameters
SI 8192
SF 250.1300330 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

MP1/17



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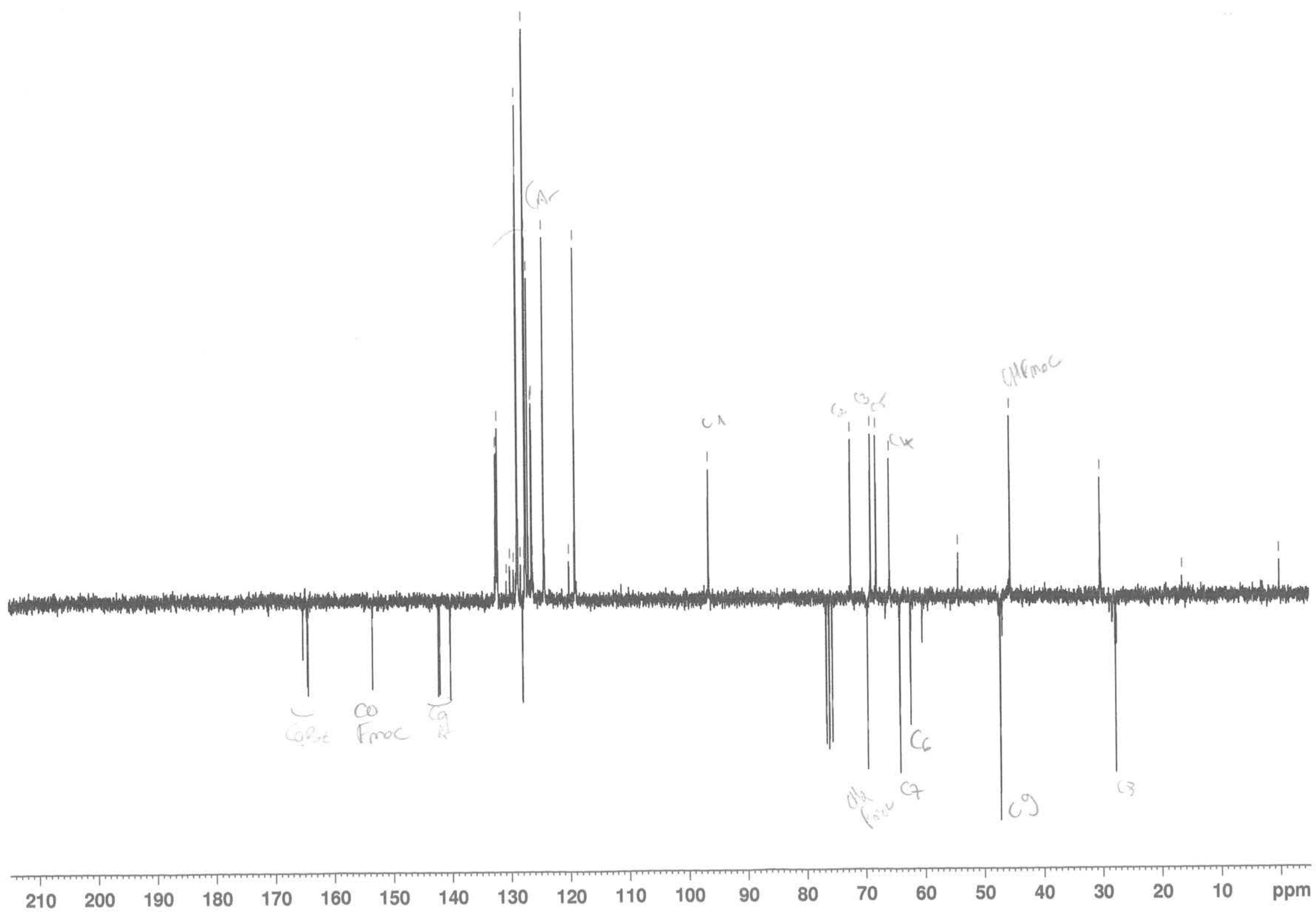
165.17
164.45
164.34
153.40
142.23
142.00
140.20
132.56
132.40
132.26
132.08
130.62
130.03
129.41
128.82
128.72
128.69
128.22
127.94
127.92
127.57
127.39
127.27
126.93
126.36
126.27
126.15
124.25
124.15
119.99
119.01
96.45

76.54
76.03
75.52
72.31
69.54
68.95
68.03
66.51
65.77
64.10
62.26
60.30
54.20
47.43
47.17
46.81
45.45

30.21
30.15
28.24
28.12
27.69
27.55

16.39

-0.00



Current Data Parameters
 NAME May27-2011-JMM
 EXPNO 41
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110527
 Time 12.53
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 15060.241 Hz
 FIDRES 0.229801 Hz
 AQ 2.1758451 sec
 RG 16384
 DW 33.200 usec
 DE 8.00 usec
 TE 300.0 K
 CNST2 145.000000
 CNST11 1.000000
 D1 2.0000000 sec
 d20 0.00689655 sec
 DELTA 0.00001019 sec
 TD0 1

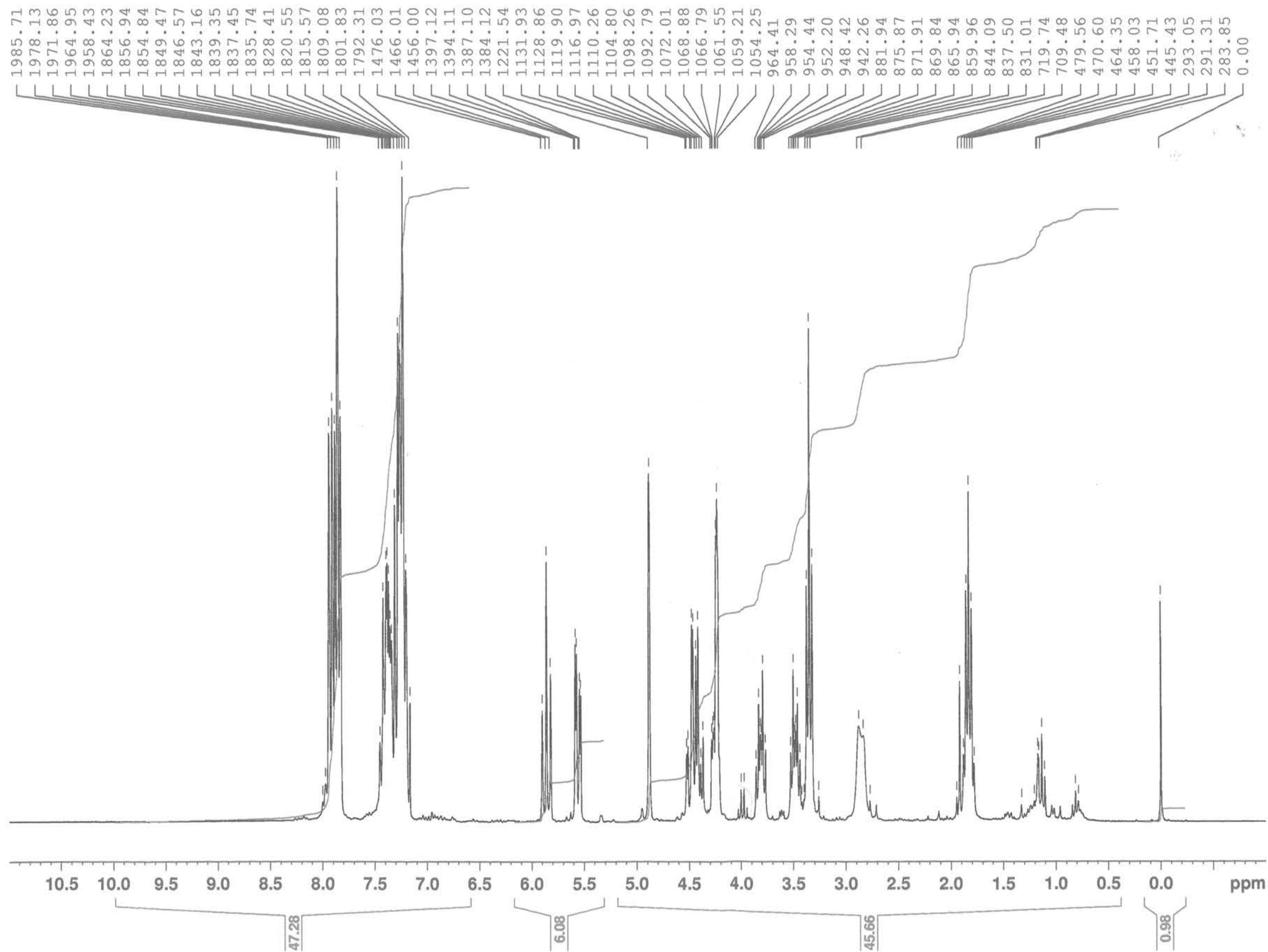
==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 p2 16.00 usec
 PL1 -3.00 dB
 SFO1 62.9015280 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -3.00 dB
 PL12 19.00 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8953060 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

MP1/23C

9a



Current Data Parameters
NAME Jun16-2011-JMM
EXPNO 30
PROCNO 1

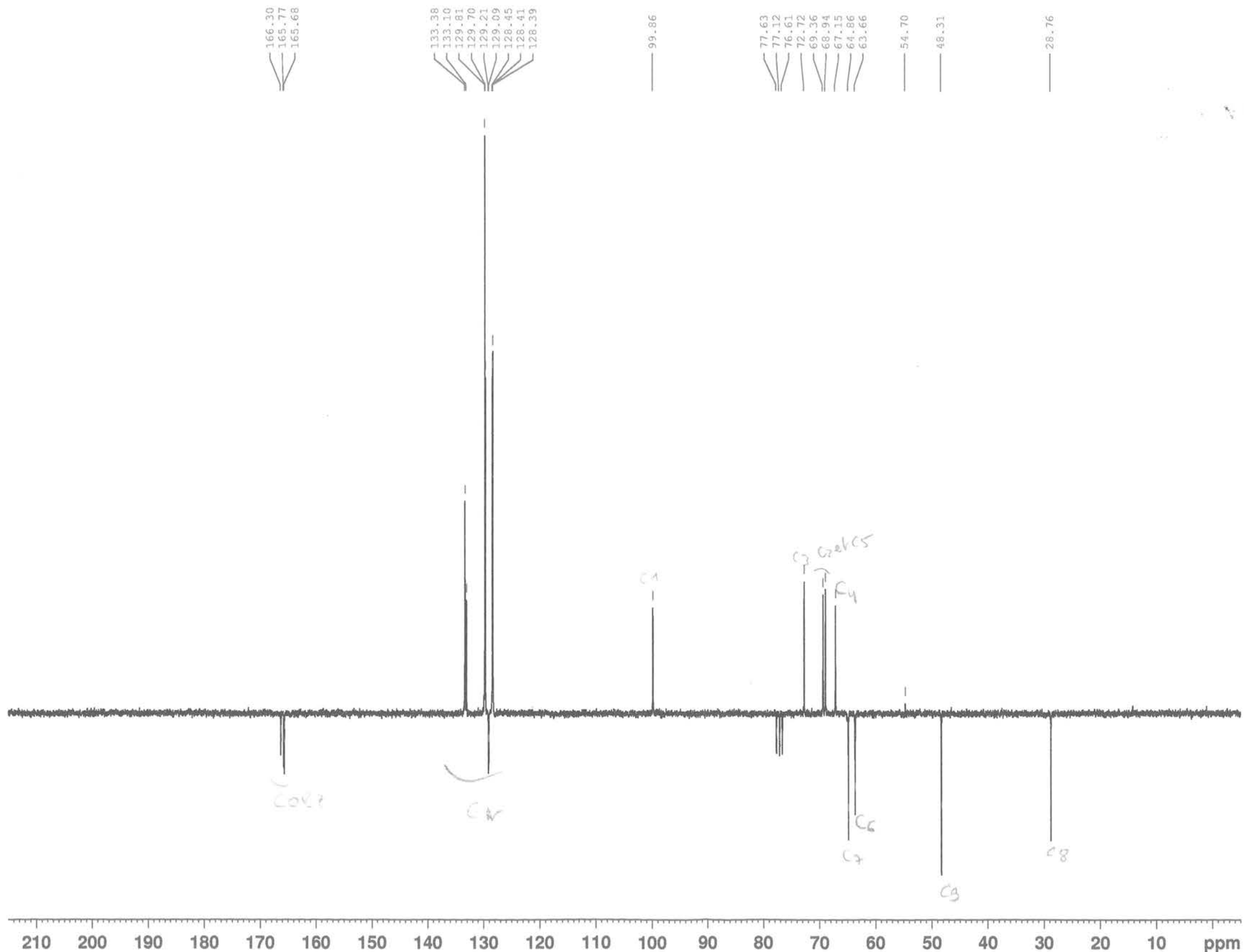
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Date_ 20110616
Time 11.54
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 64
DS 2
SWH 5175.983 Hz
FIDRES 0.315917 Hz
AQ 1.5827444 sec
RG 203.2
DW 96.600 usec
DE 8.00 usec
TE 300.0 K
D1 0.20000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 250.1315446 MHz

F2 - Processing parameters
SI 8192
SF 250.1300312 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

MP1/23C

9a



Current Data Parameters
NAME Jun16-2011-JMM
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110616
Time 12.13
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 15060.241 Hz
FIDRES 0.229801 Hz
AQ 2.1758451 sec
RG 16384
DW 33.200 usec
DE 8.00 usec
TE 300.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
d20 0.00689655 sec
DELTA 0.00001019 sec
TDO 1

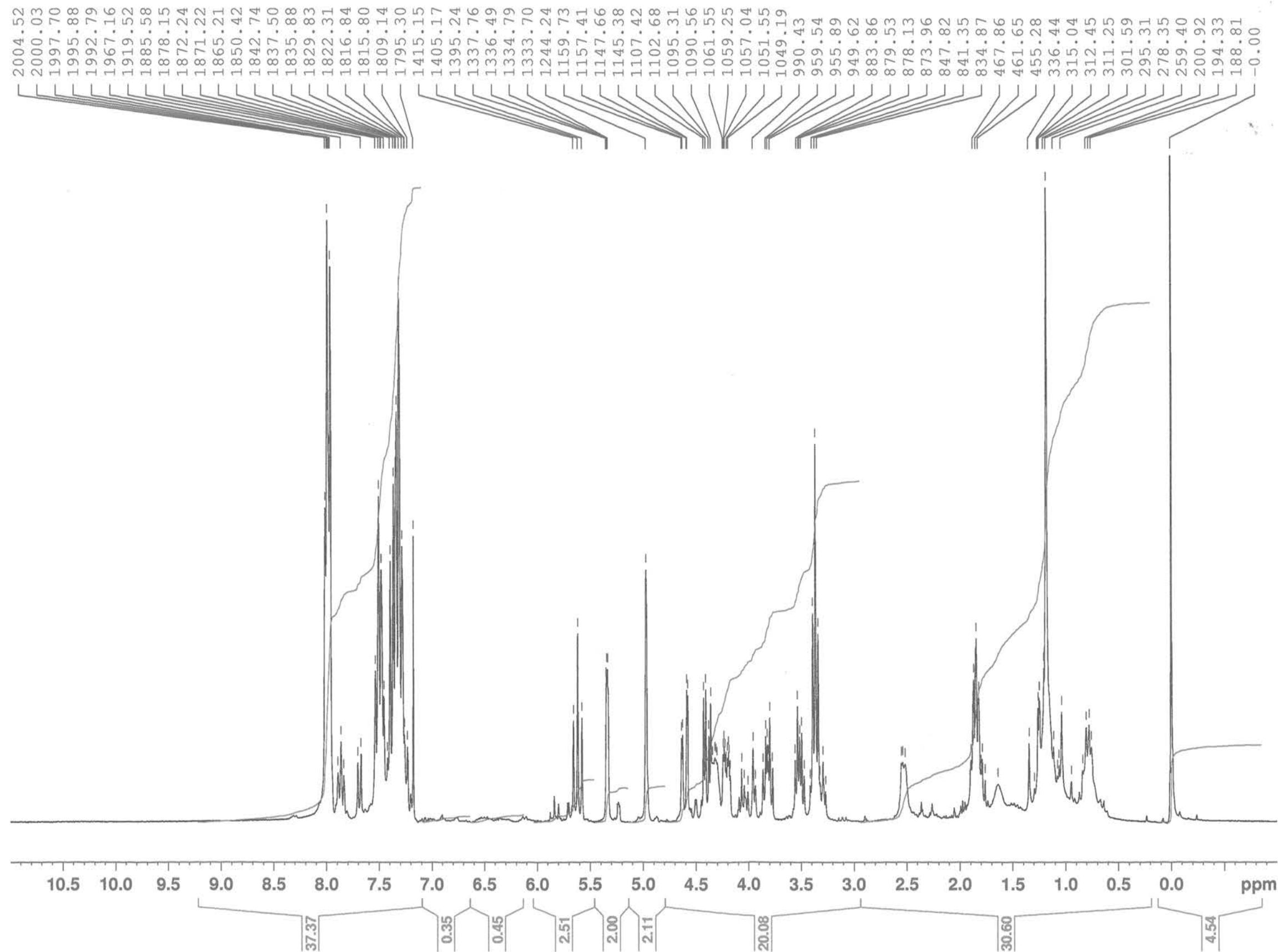
==== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
p2 16.00 usec
PL1 -3.00 dB
SFO1 62.9015280 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 19.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

9b

MP1/23A



Current Data Parameters
NAME Jun16-2011-JMM
EXPNO 40
PROCNO 1

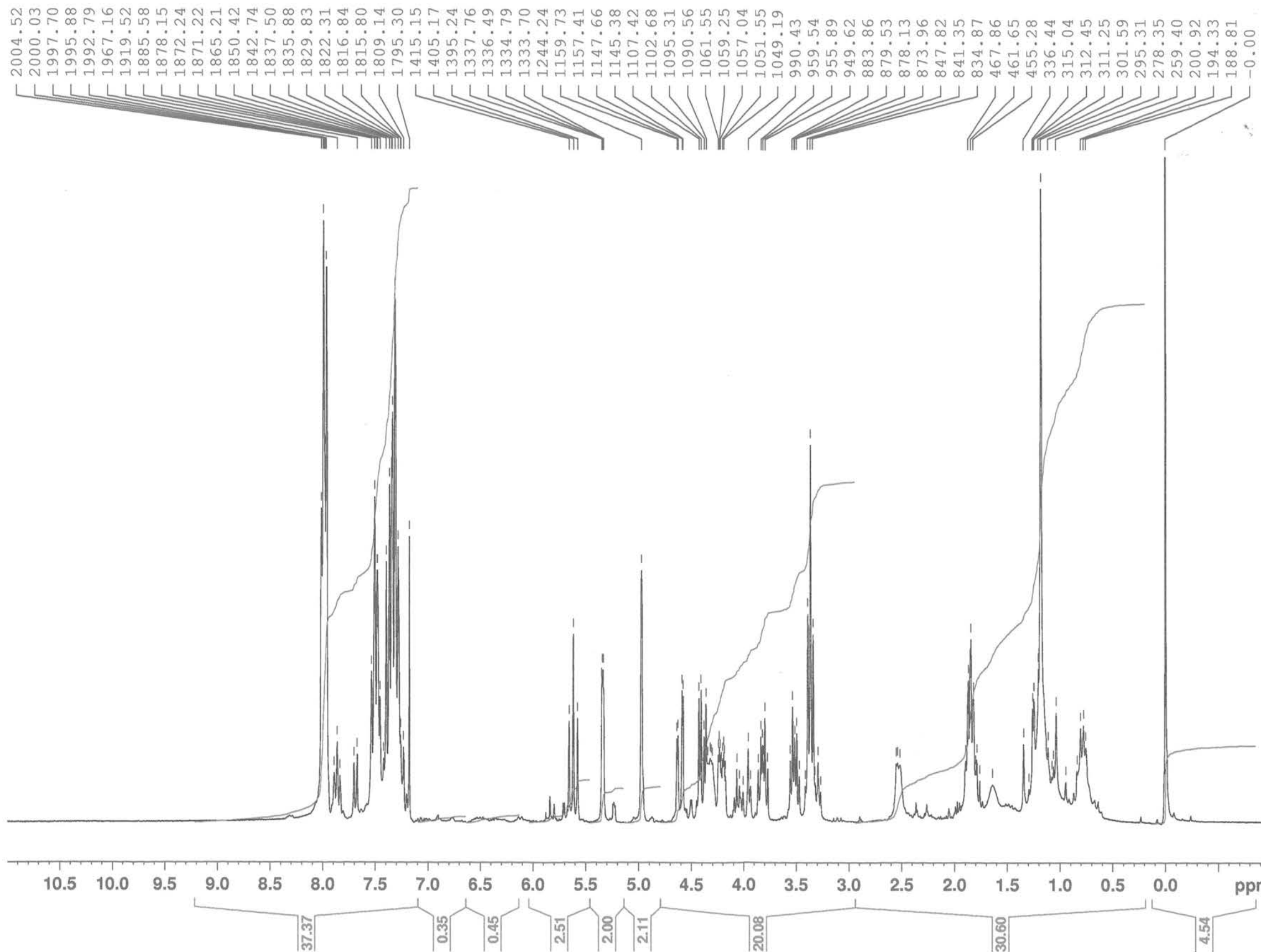
F2 - Acquisition Parameters
Date_ 20110616
Time 12.22
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 64
DS 2
SWH 5175.983 Hz
FIDRES 0.315917 Hz
AQ 1.5827444 sec
RG 406.4
DW 96.600 usec
DE 8.00 usec
TE 300.0 K
D1 0.20000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 250.1315446 MHz

F2 - Processing parameters
SI 8192
SF 250.1300285 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

9b

MP1/23A



Current Data Parameters
NAME Jun16-2011-JMM
EXPNO 40
PROCNO 1

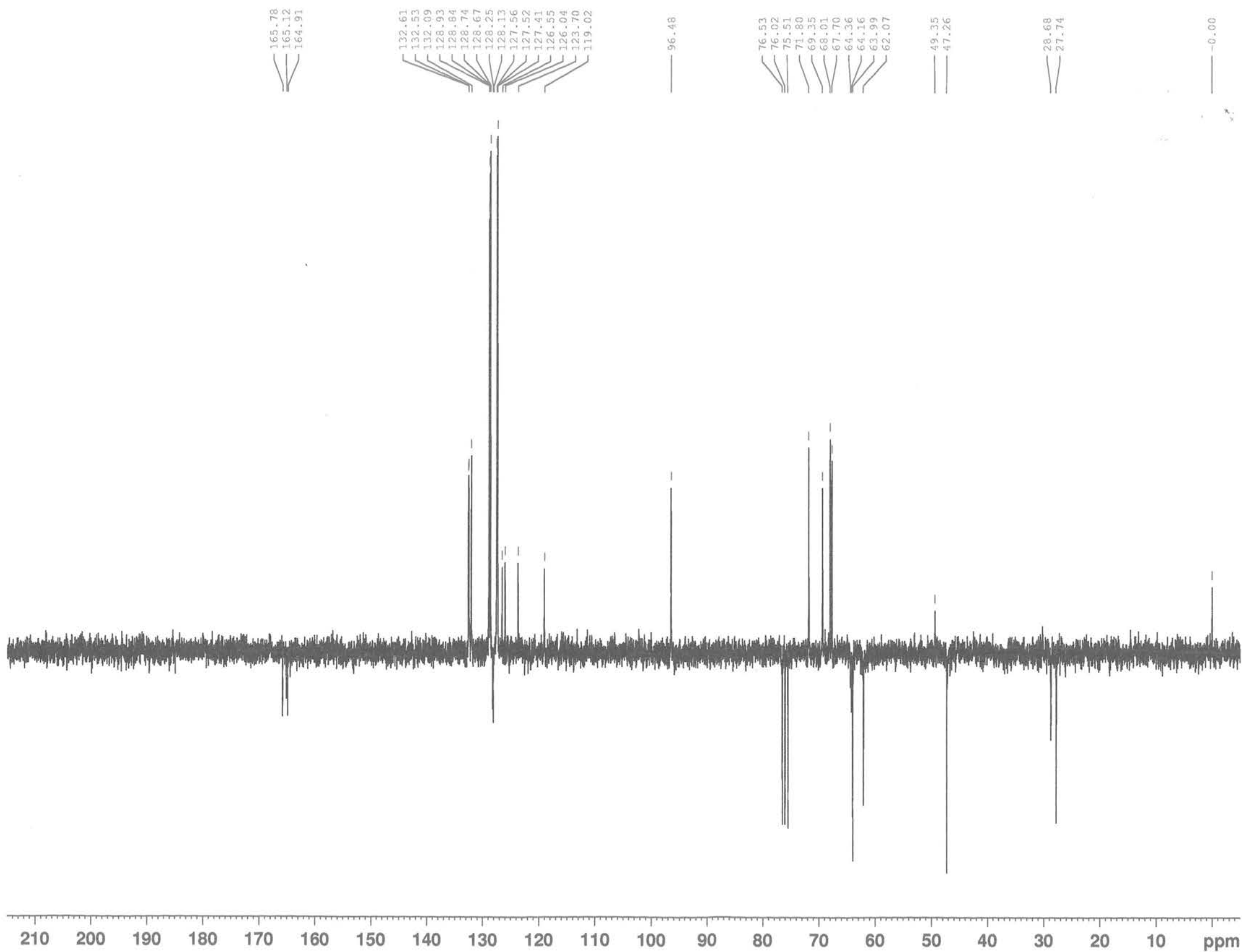
F2 - Acquisition Parameters
Date_ 20110616
Time 12.22
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT CDC13
NS 64
DS 2
SWH 5175.983 Hz
FIDRES 0.315917 Hz
AQ 1.5827444 sec
RG 406.4
DW 96.600 usec
DE 8.00 usec
TE 300.0 K
D1 0.20000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SF01 250.1315446 MHz

F2 - Processing parameters
SI 8192
SF 250.1300285 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

gb

MP1/23A



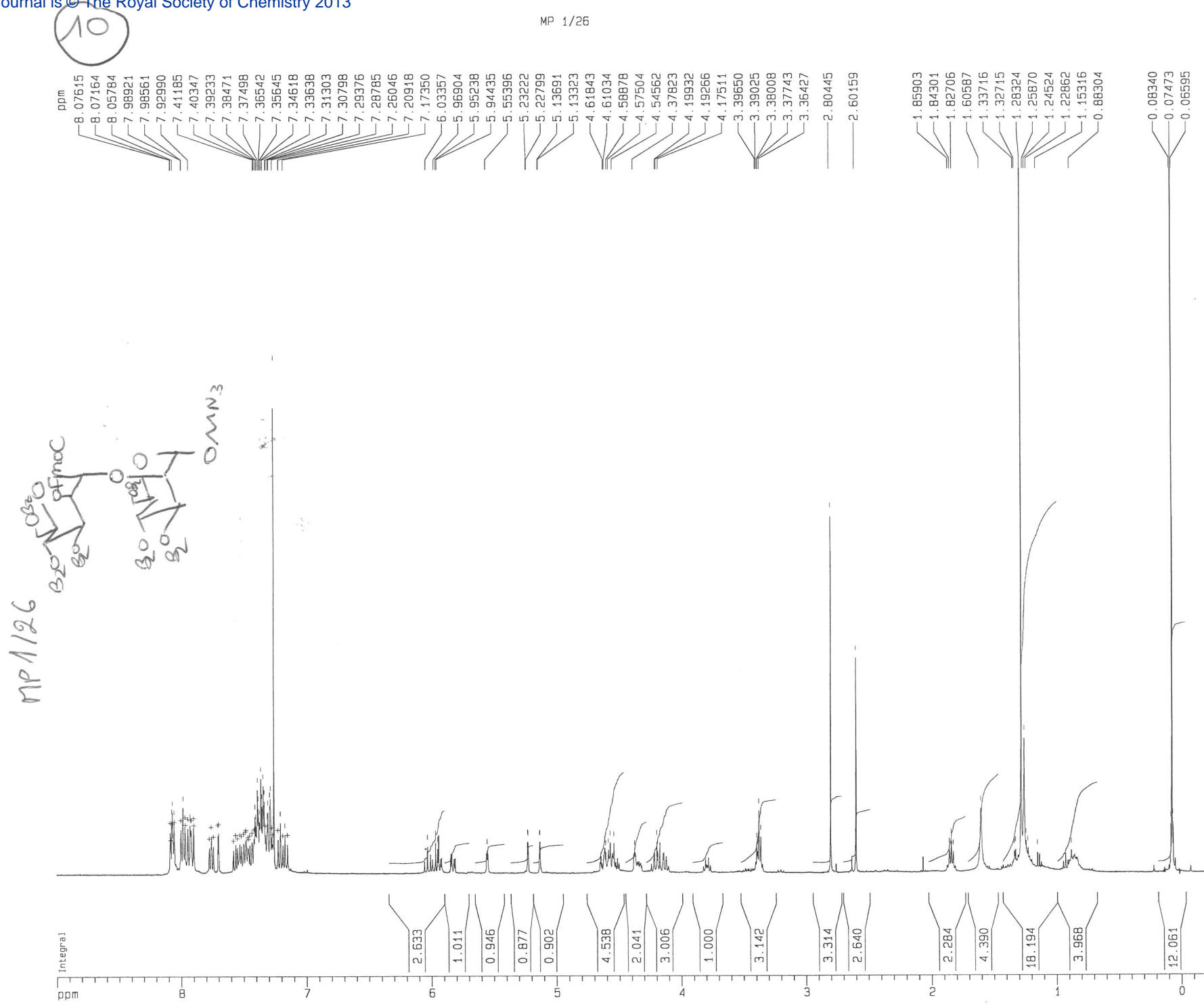
Current Data Parameters
NAME Jun16-2011-JMM
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110616
Time 12.41
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 15060.241 Hz
FIDRES 0.229801 Hz
AQ 2.1758451 sec
RG 16384
DW 33.200 usec
DE 8.00 usec
TE 300.0 K
CNST2 145.000000
CNST11 1.000000
D1 2.0000000 sec
d20 0.00689655 sec
DELTA 0.00001019 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
p2 16.00 usec
PL1 -3.00 dB
SFO1 62.9015280 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 19.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8953041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



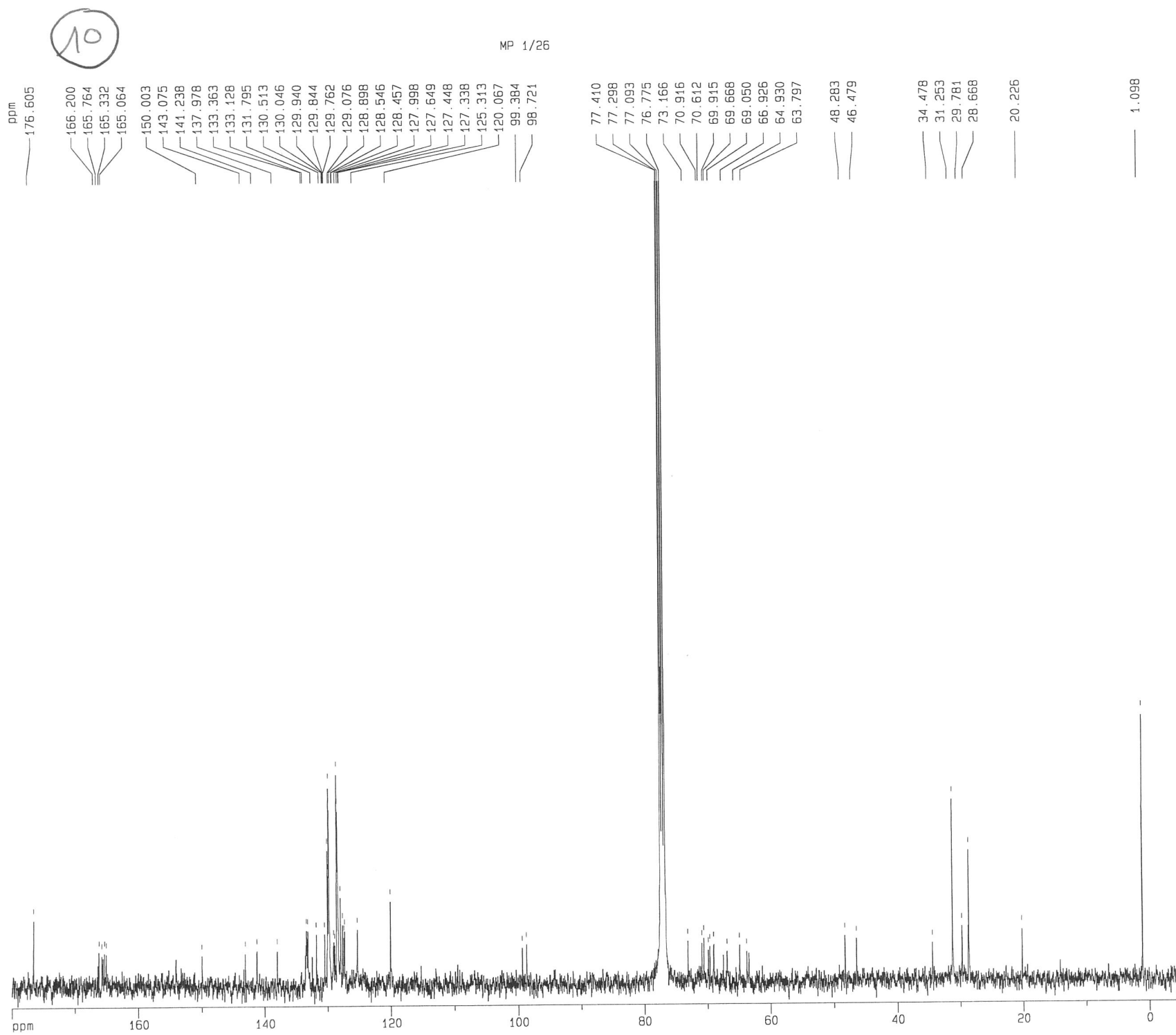
Current Data Parameters
 NAME swmp0507
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110705
 Time 12.40
 INSTRUM spect
 PROBHD 5 mm GNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 181
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SF01 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300092 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 F1P 9.000 ppm
 F1 3601.17 Hz
 F2P -0.200 ppm
 F2 -80.03 Hz
 PPMCM 0.40889 ppm/cm
 HZCM 163.60870 Hz/cm



Current Data Parameters
 NAME swmp0507
 EXPNO 5
 PROCNO 1

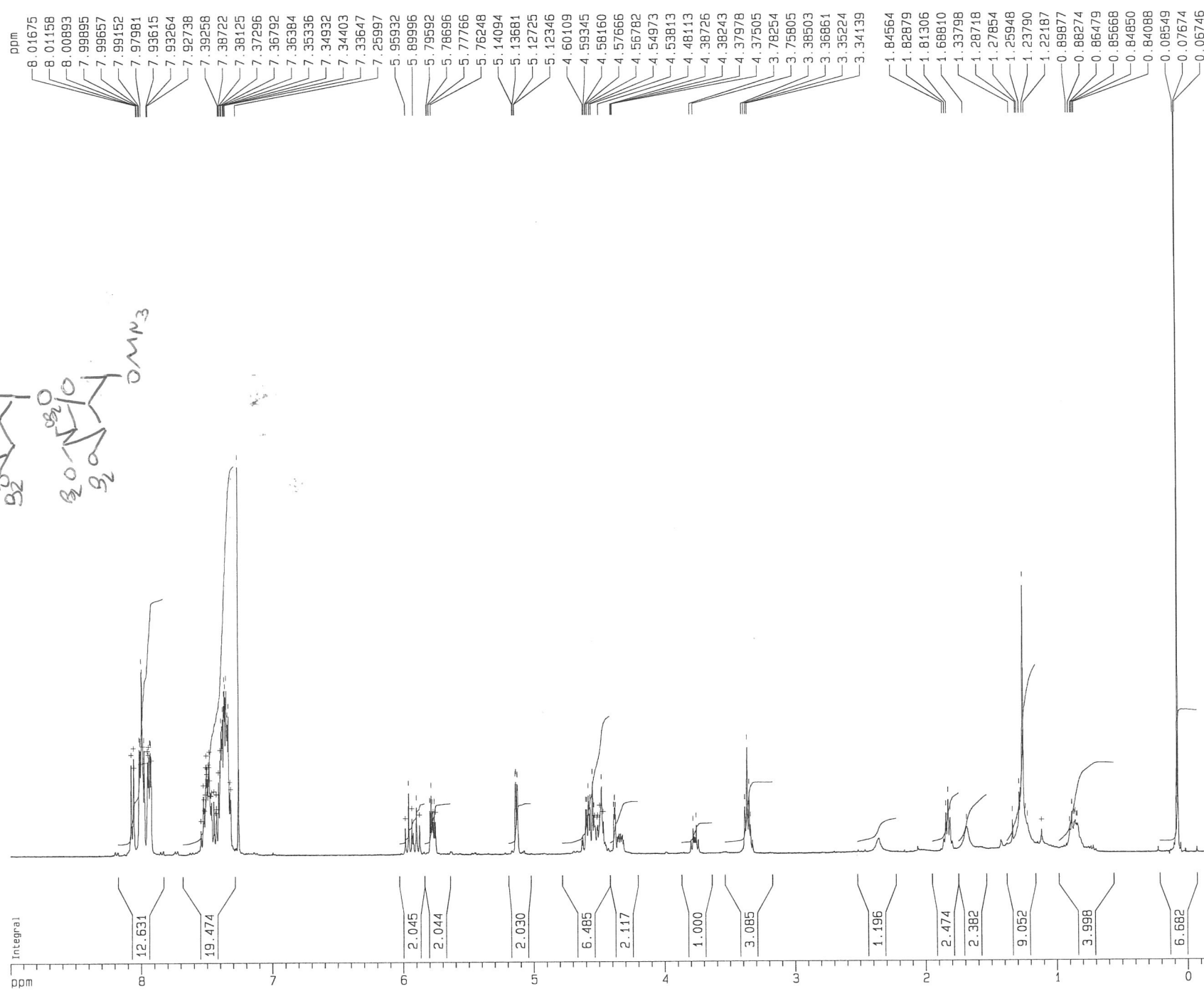
F2 - Acquisition Parameters
 Date_ 20110705
 Time 15.08
 INSTRUM spect
 PROBHD 5 mm GNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2400
 DS 0
 SWH 25000.000 Hz
 FIDRES 0.381470 Hz
 AQ 1.3107700 sec
 RG 6502
 DW 20.000 usec
 DE 25.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.50 usec
 PL1 -6.00 dB
 SF01 100.6237964 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 20.00 dB
 PL13 26.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127631 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 F1P 180.000 ppm
 F1 18110.30 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 8.22222 ppm/cm
 HZCM 827.26050 Hz/cm



Current Data Parameters
 NAME swmp0507
 EXPNO 1
 PROCNO 1

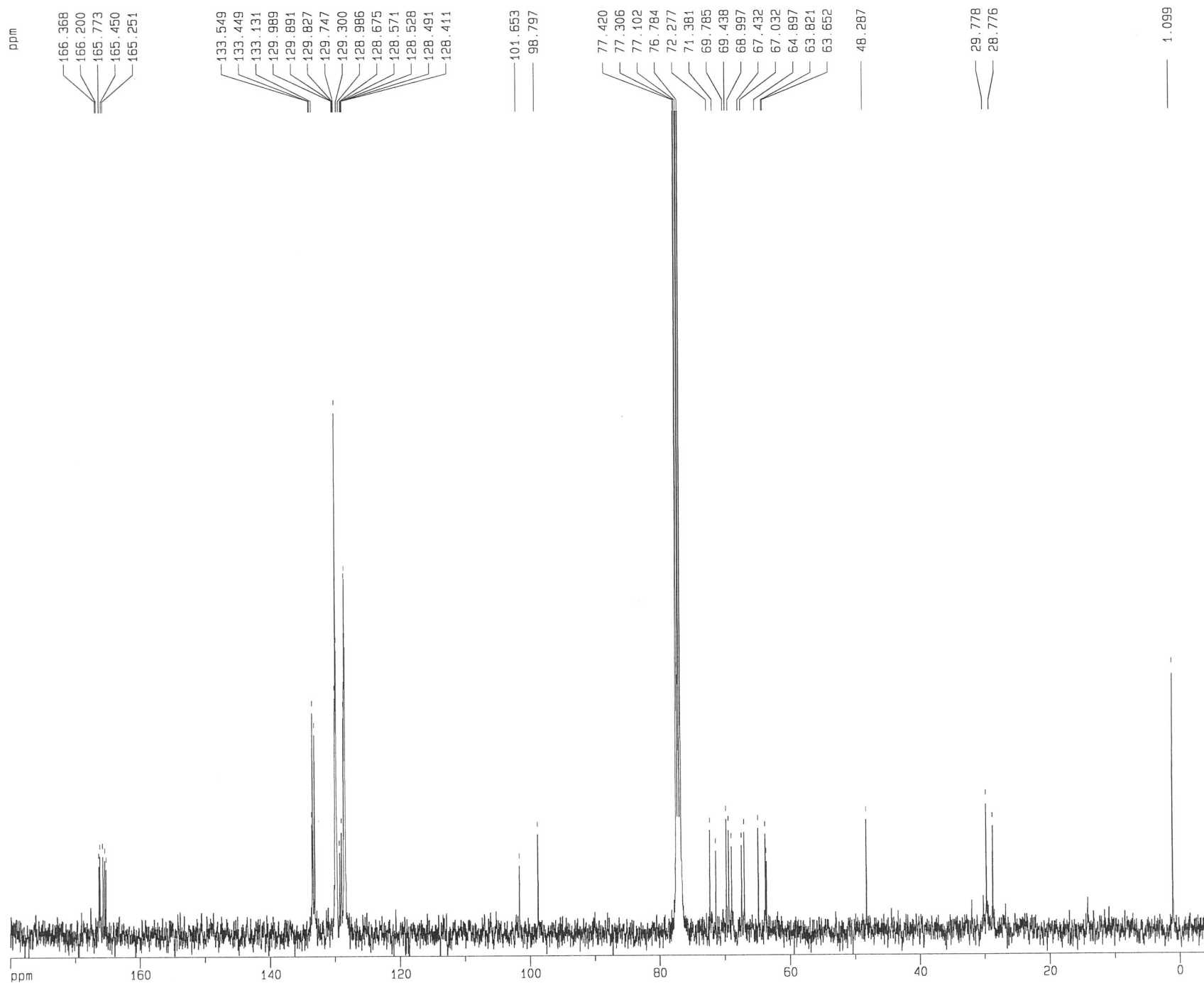
F2 - Acquisition Parameters
 Date_ 20110705
 Time 11.25
 INSTRUM spect
 PROBHD 5 mm GNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 203.2
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SF01 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300095 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 F1P 9.000 ppm
 F1 3601.17 Hz
 F2P -0.200 ppm
 F2 -80.03 Hz
 PPMCM 0.40889 ppm/cm
 HZCM 163.60870 Hz/cm

Ma



Current Data Parameters
 NAME swmp0507
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110705
 Time 11.49
 INSTRUM spect
 PROBHD 5 mm GNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 800
 DS 0
 SWH 25000.000 Hz
 FIDRES 0.381470 Hz
 AQ 1.3107700 sec
 RG 6502
 DW 20.000 usec
 DE 25.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.50 usec
 PL1 -6.00 dB
 SF01 100.6237964 MHz

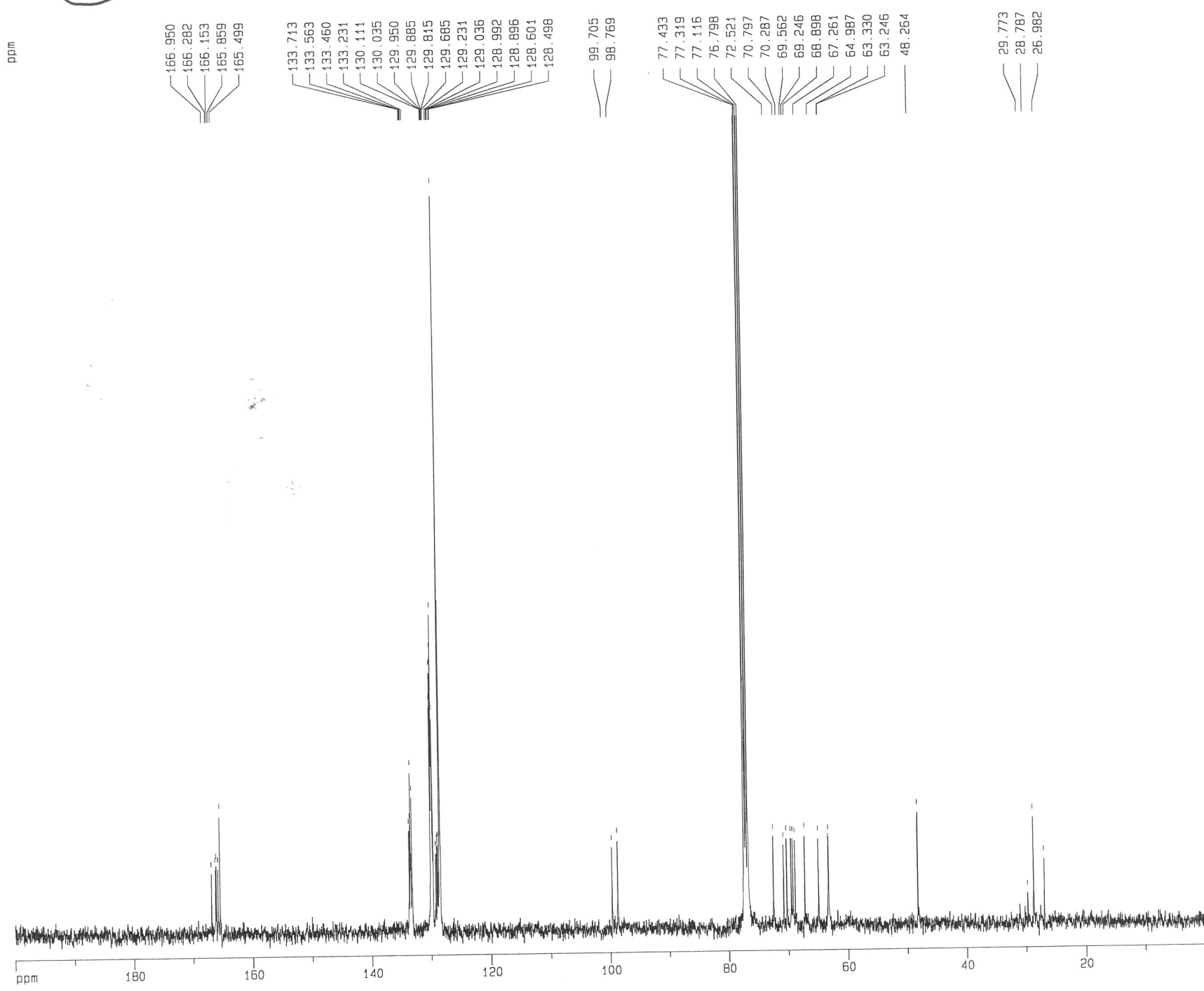
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL13 20.00 dB
 PL12 26.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127631 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 F1P 180.000 ppm
 F1 18110.30 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 8.22222 ppm/cm
 HZCM 827.26050 Hz/cm

11b

MP 1/32 A2



Current Data Parameters
 NAME swmp0507
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110705
 Time 17.07
 INSTRUM spect
 PROBHD 5 mm GNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 800
 DS 0
 SWH 25000.000 Hz
 FIDRES 0.381470 Hz
 AQ 1.3107700 sec
 RG 6502
 DW 20.000 usec
 DE 25.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 7.50 usec
 PL1 -6.00 dB
 SFO1 100.6237964 MHz

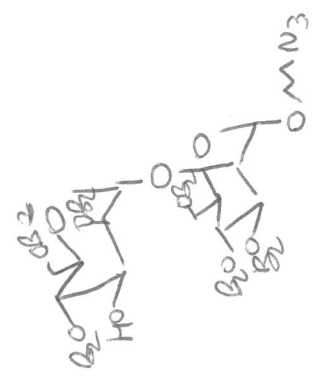
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 20.00 dB
 PL13 26.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127631 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

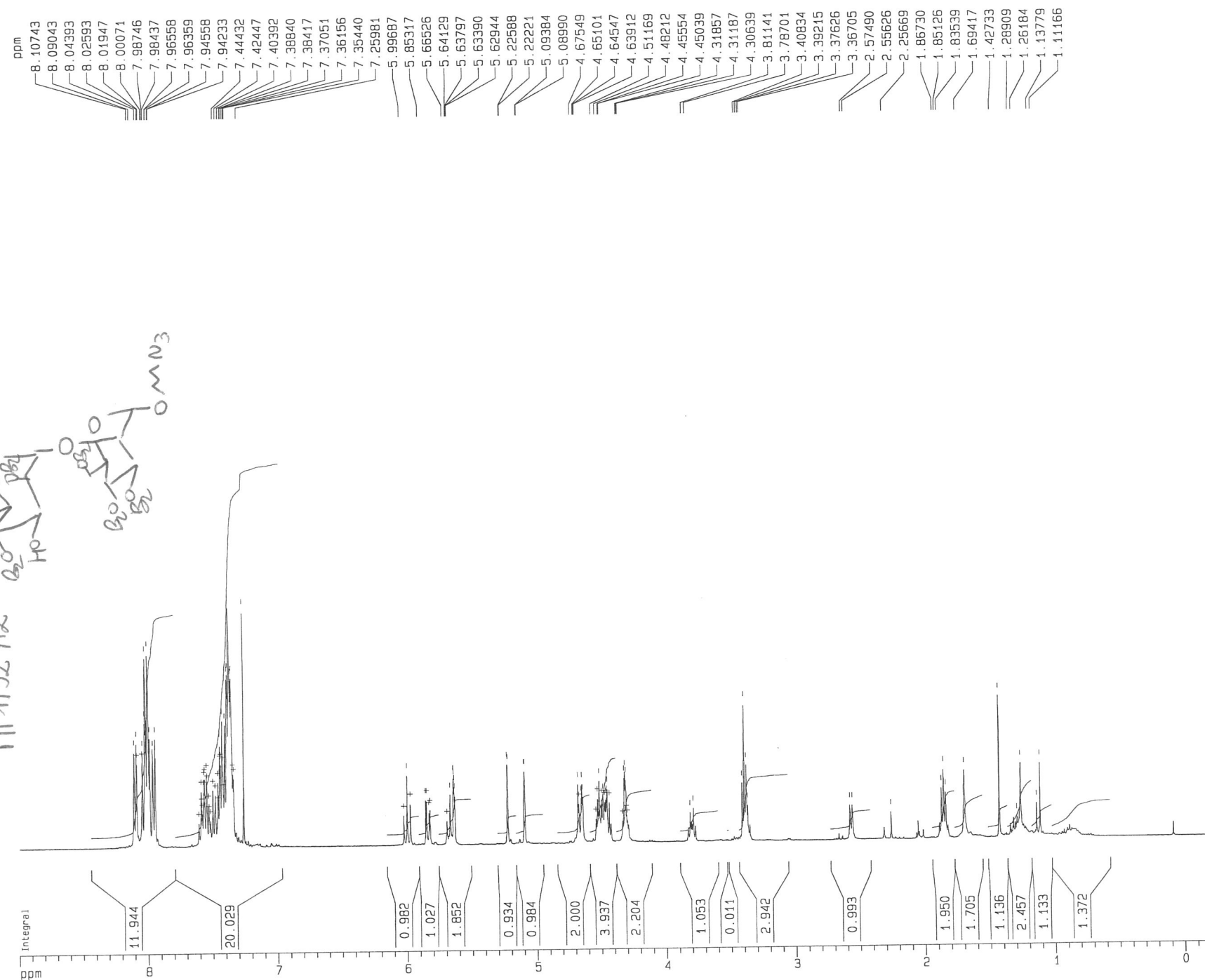
1D NMR plot parameters
 CX 22.50 cm
 F1P 200.000 ppm
 F1 20122.55 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 8.88889 ppm/cm
 HZCM 894.33569 Hz/cm

11b

MP 1/32 A2



MP1/32 A2



Current Data Parameters
 NAME swmp0507
 EXPNO 7
 PROCNO 1

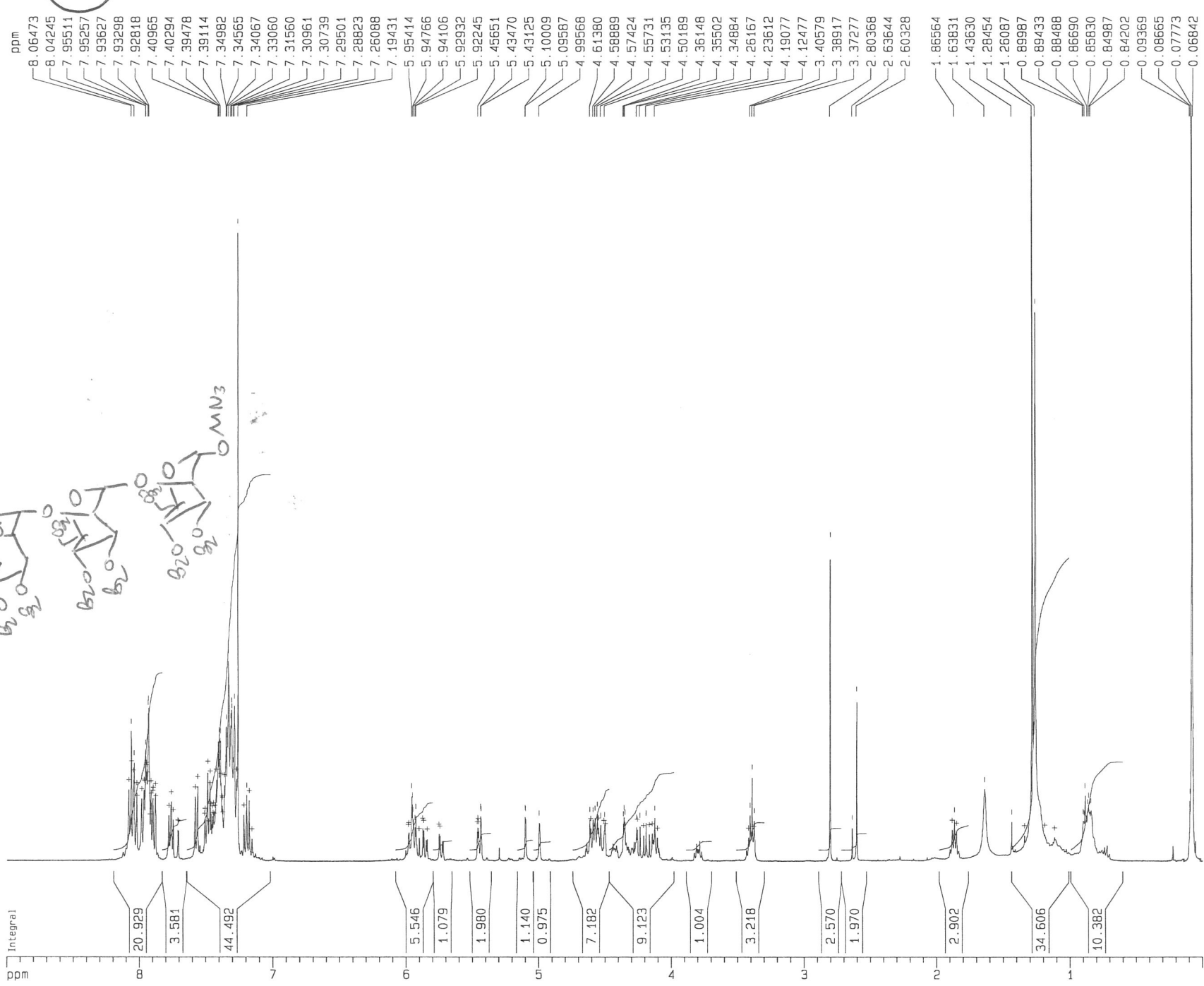
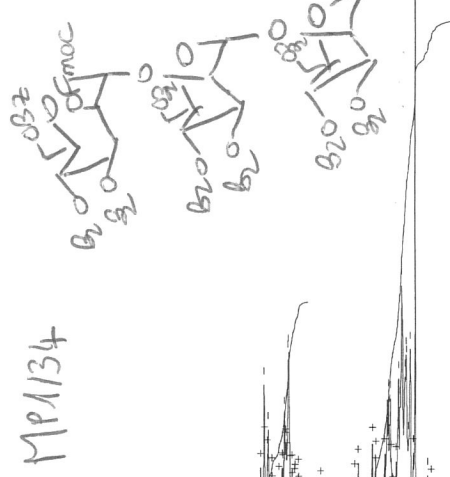
F2 - Acquisition Parameters
 Date_ 20110705
 Time 16.20
 INSTRUM spect
 PROBHD 5 mm GNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 90.5
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300095 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 F1P 9.000 ppm
 F1 3601.17 Hz
 F2P -0.200 ppm
 F2 -80.03 Hz
 PPMCM 0.40889 ppm/cm
 HZCM 163.60870 Hz/cm

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Current Data Parameters
 NAME mrm1907
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110719
 Time 12.29
 INSTRUM spect
 PROBHD 5 mm BBI 1H-B
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 90.5
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.0000000 sec

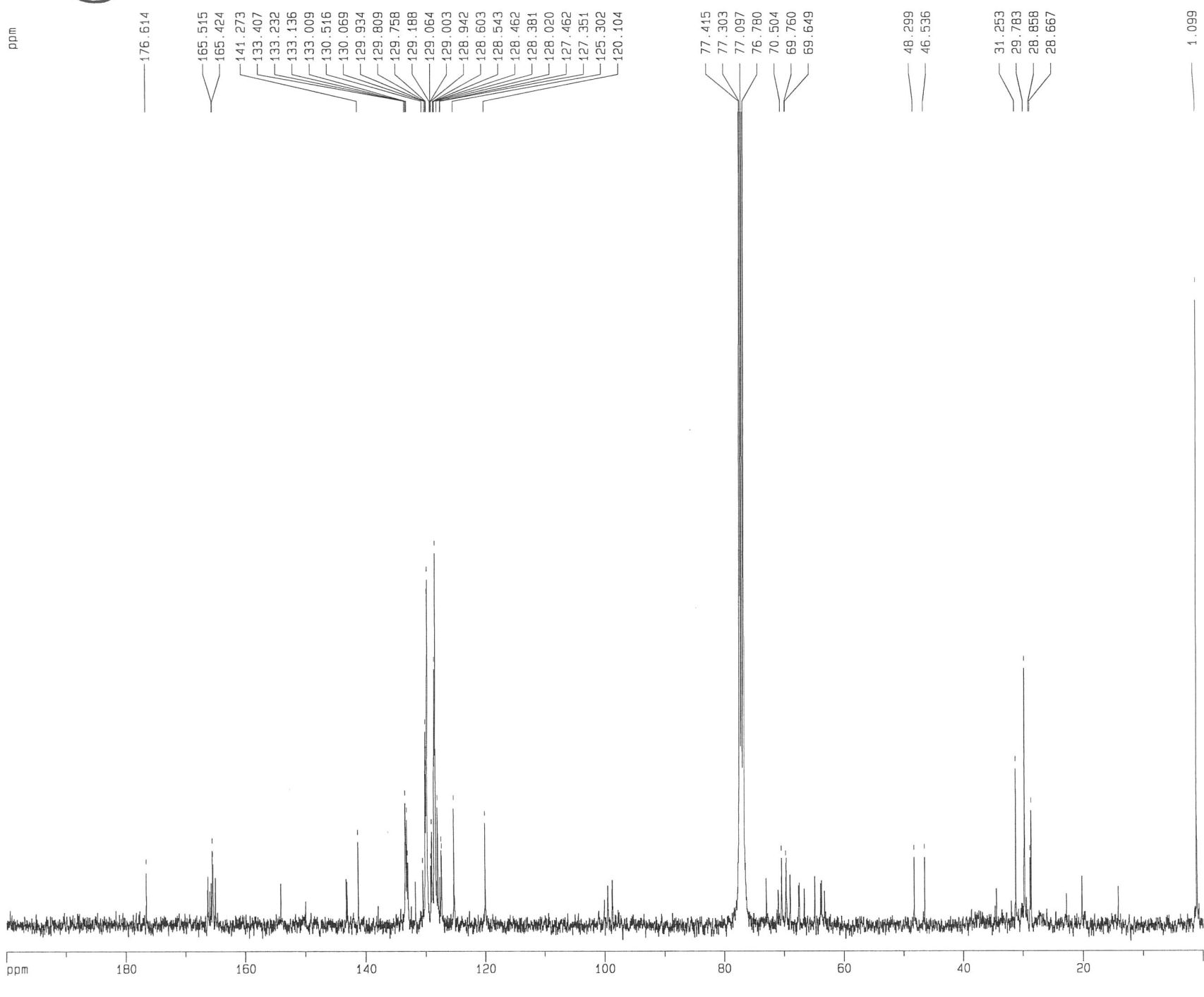
===== CHANNEL f1 =====
 NUC1 1H
 P1 7.00 usec
 PL1 0.00 dB
 SF01 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300092 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 F1P 9.000 ppm
 F1 3601.17 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.40000 ppm/cm
 HZCM 160.05200 Hz/cm

12

mp1/34



Current Data Parameters
 NAME mrm1907
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110722
 Time 17.10
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4200
 DS 0
 SWH 25000.000 Hz
 FIDRES 0.381470 Hz
 AQ 1.3107700 sec
 RG 13004
 DW 20.000 usec
 DE 25.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 D12 0.0000200 sec

===== CHANNEL f1 =====
 NUC1 13C
 PL1 -6.00 dB
 SF01 100.6237964 MHz

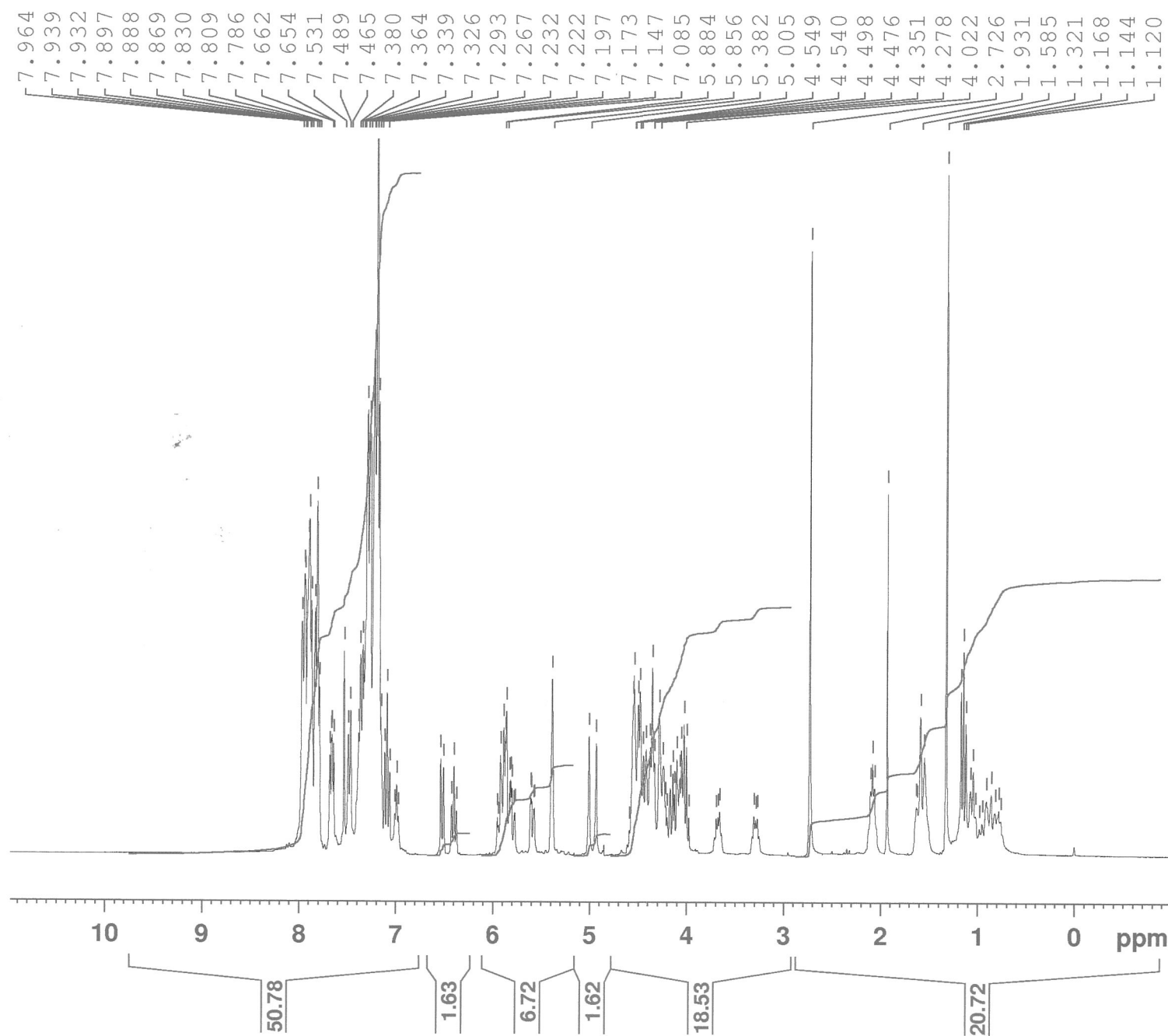
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 20.00 dB
 PL13 26.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127631 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 F1P 200.000 ppm
 F1 20122.55 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 8.88889 ppm/cm
 HZCM 894.33569 Hz/cm

16

MP2/67



Current Data Parameters
NAME Oct19-2012-JMM
EXPNO 170
PROCNO 1

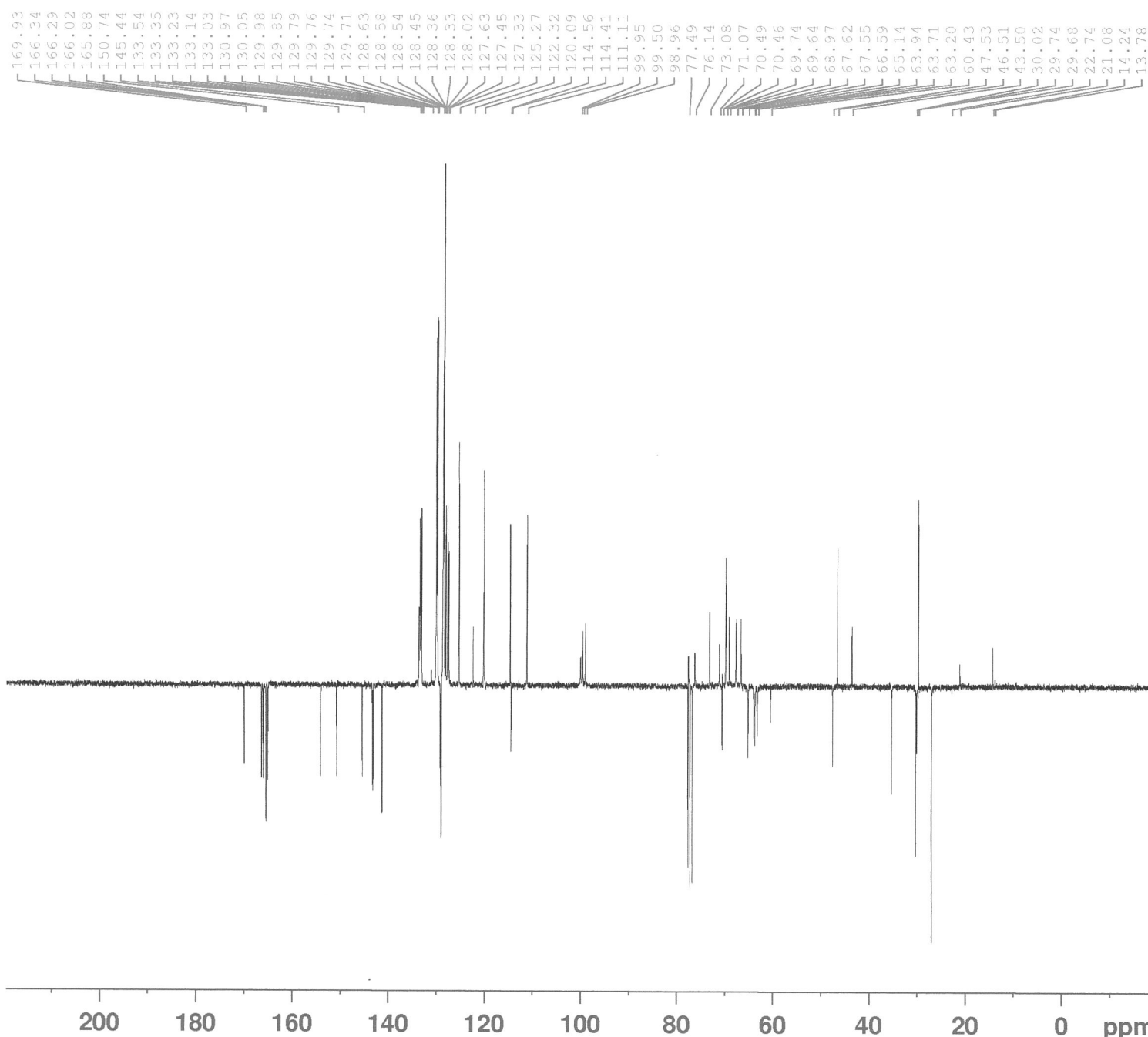
F2 - Acquisition Parameters
Date_ 20121019
Time 19.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 43268
SOLVENT CDCl3
NS 32
DS 2
SWH 6009.615 Hz
FIDRES 0.138893 Hz
AQ 3.5998976 sec
RG 28.5
DW 83.200 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 300.1815009 MHz
NUC1 1H
P1 13.60 usec
PLW1 7.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800442 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

16

MP2/67



Current Data Parameters
NAME Oct19-2012-JMM
EXPNO 175
PROCNO 1

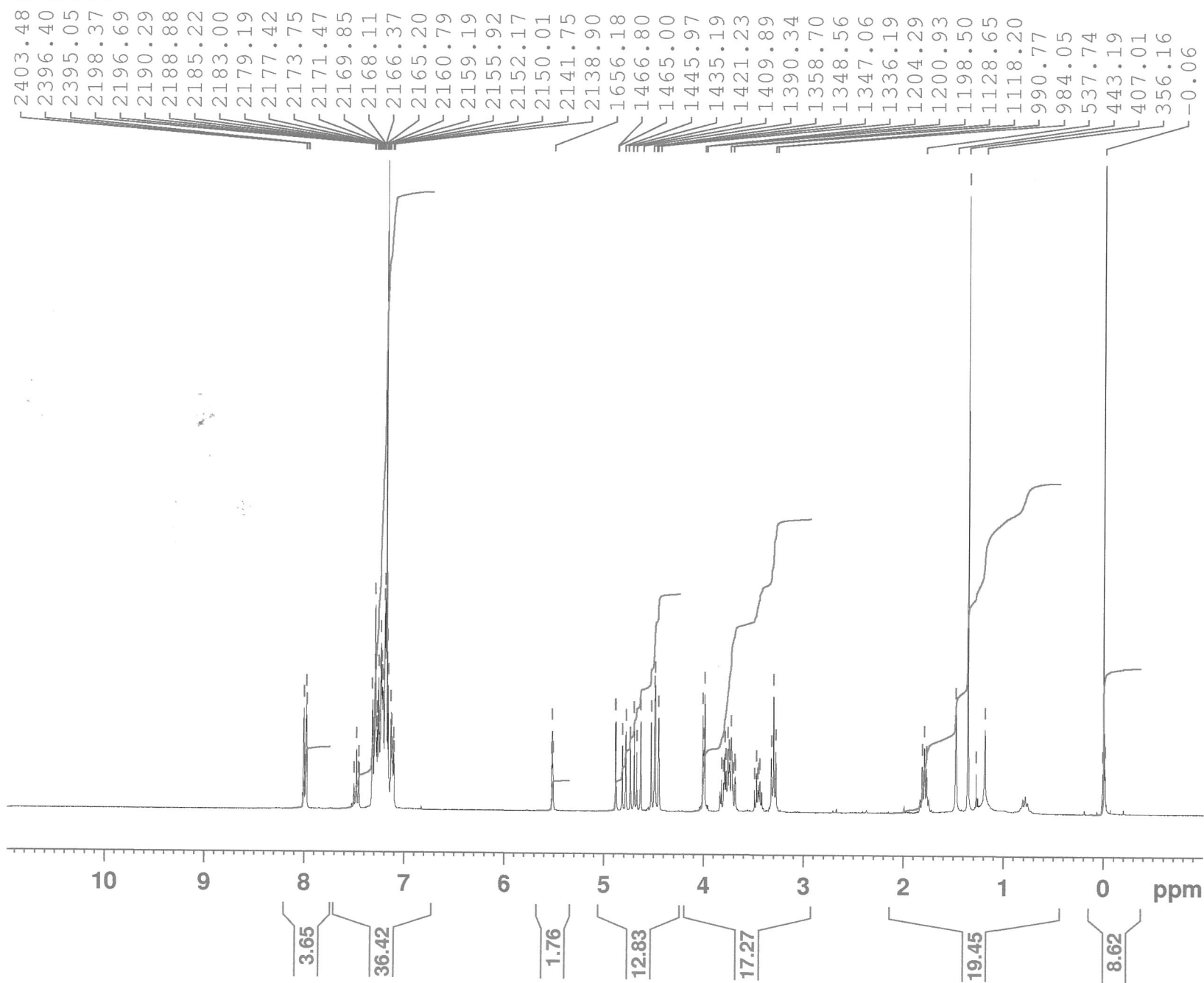
F2 - Acquisition Parameters
Date_ 20121020
Time 3.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 6.50 usec
TE 297.6 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

==== CHANNEL f1 =====
SFO1 75.4878691 MHz
NUC1 13C
P1 9.00 usec
P2 18.00 usec
PLW1 38.00000000 W

==== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 100.00 usec
PLW2 7.00000000 W
PLW12 0.13964000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

MP1/104



BRUKER

Current Data Parameters
 NAME Nov22-2011-JMM
 EXPNO 100
 PROCNO 1

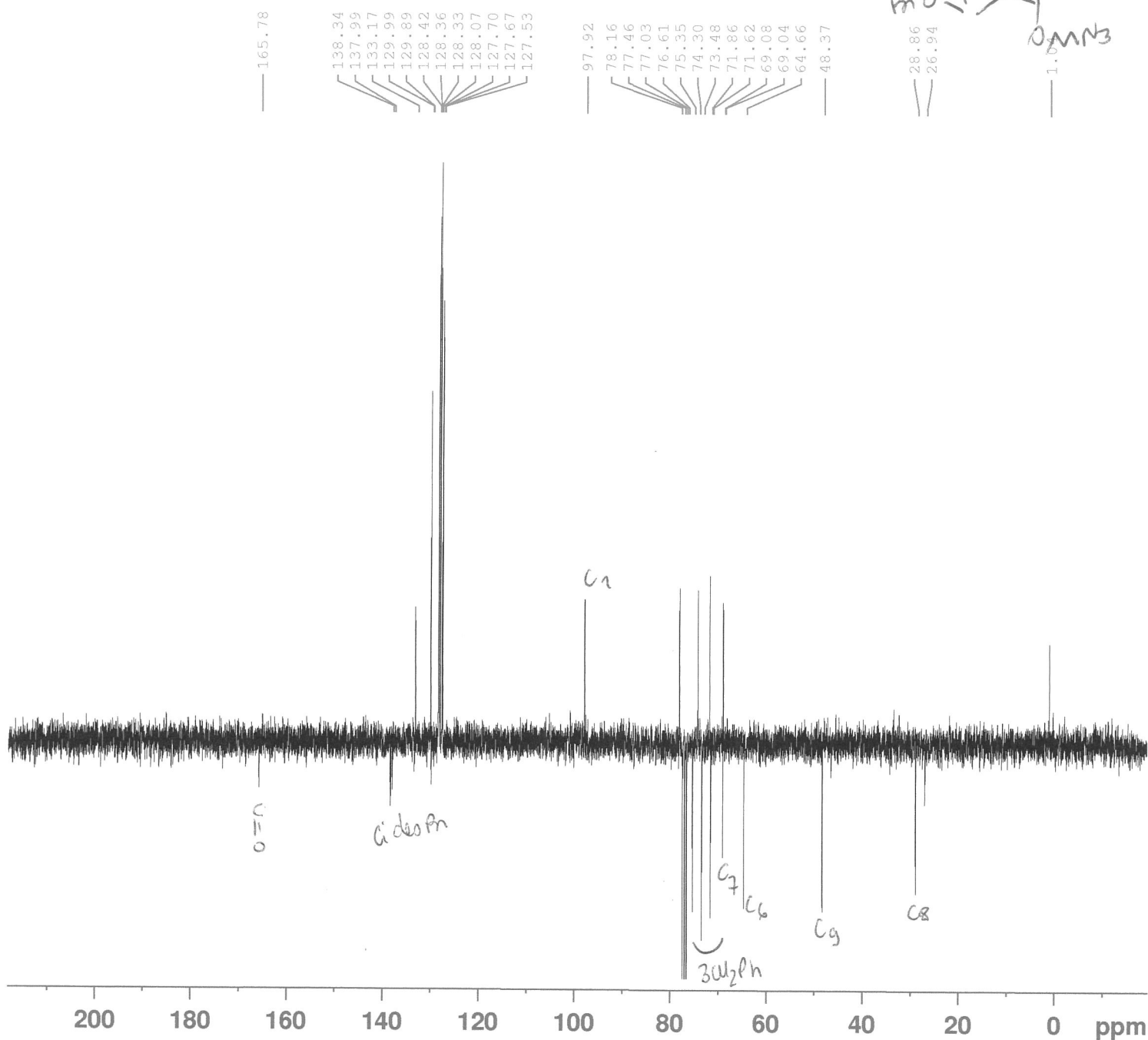
F2 - Acquisition Parameters
 Date_ 20111122
 Time 16.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 43268
 SOLVENT CDC13
 NS 32
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.138893 Hz
 AQ 3.5999477 sec
 RG 161
 DW 83.200 use
 DE 6.50 use
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.60 use
 PLW1 7.0000000 W
 SFO1 300.1815009 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1800338 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

18

MP1/104



Current Data Parameters
 NAME Nov22-2011-JMM
 EXPNO 101
 PROCNO 1

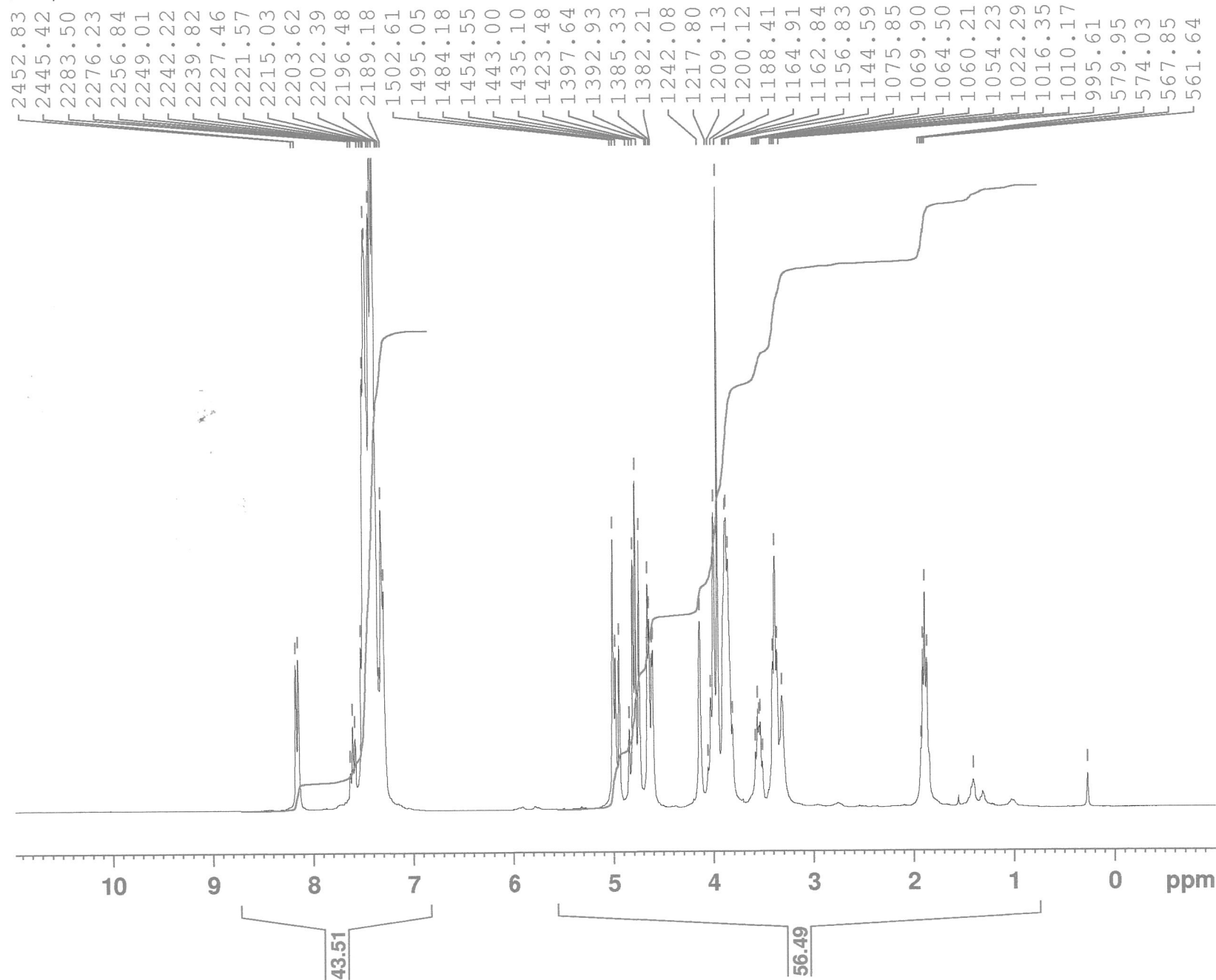
F2 - Acquisition Parameters
 Date_ 20111122
 Time 17.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 6.50 usec
 TE 300.0 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 38.00000000 W
 SFO1 75.4878691 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PLW2 7.00000000 W
 PLW12 0.13964000 W
 SFO2 300.1812007 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

MP1/126



Current Data Parameters
 NAME Jan12-2012-JMM
 EXPNO 50
 PROCNO 1

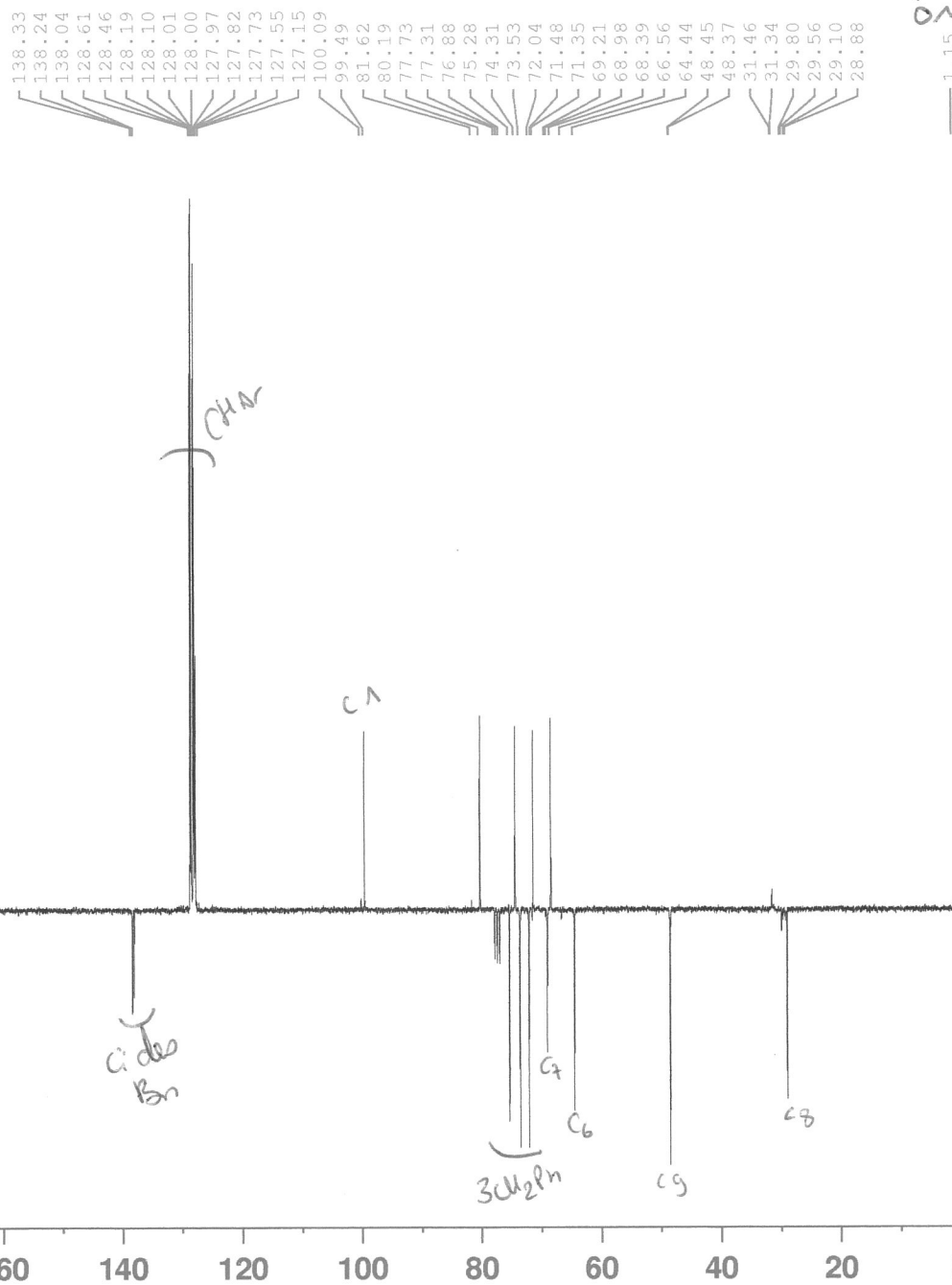
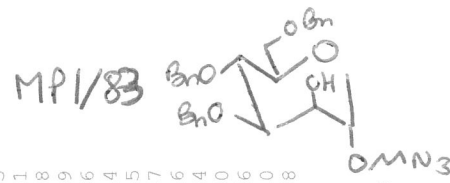
F2 - Acquisition Parameters
 Date_ 20120112
 Time 11.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 43268
 SOLVENT CDC13
 NS 32
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.138893 Hz
 AQ 3.5999477 sec
 RG 11.3
 DW 83.200 usec
 DE 6.50 usec
 TE 294.4 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.60 usec
 PLW1 7.0000000 W
 SFO1 300.1815009 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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MP1/83



Current Data Parameters
 NAME Oct14-2011-JMM
 EXPNO 11
 PROCNO 1

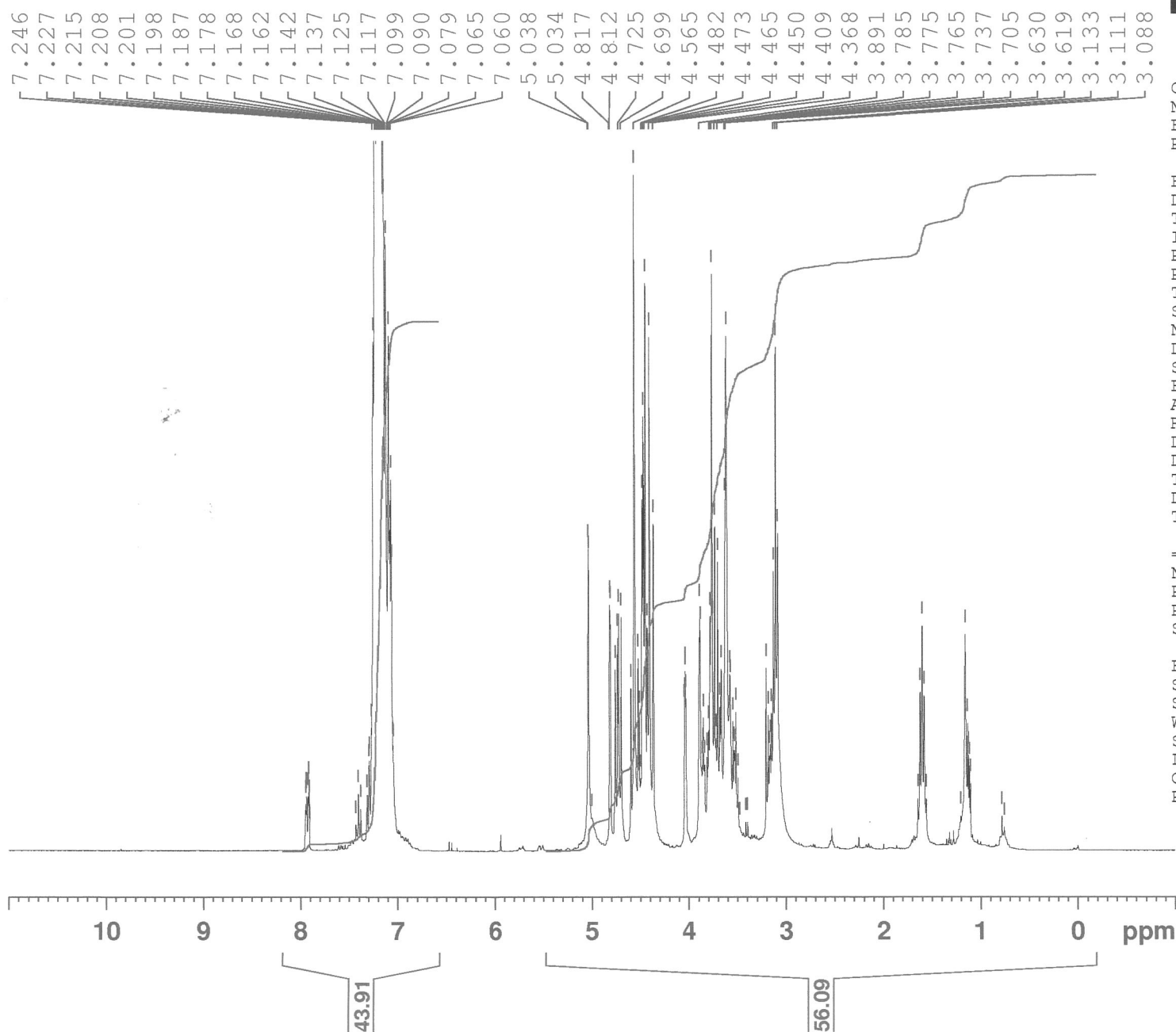
F2 - Acquisition Parameters
 Date_ 20111014
 Time 10.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 100
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 6.50 usec
 TE 294.7 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 38.0000000 W
 SFO1 75.4878691 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PLW2 7.0000000 W
 PLW12 0.13964000 W
 SFO2 300.1812007 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

MP2/14



Current Data Parameters
NAME May16-2012-JMM
EXPNO 40
PROCNO 1

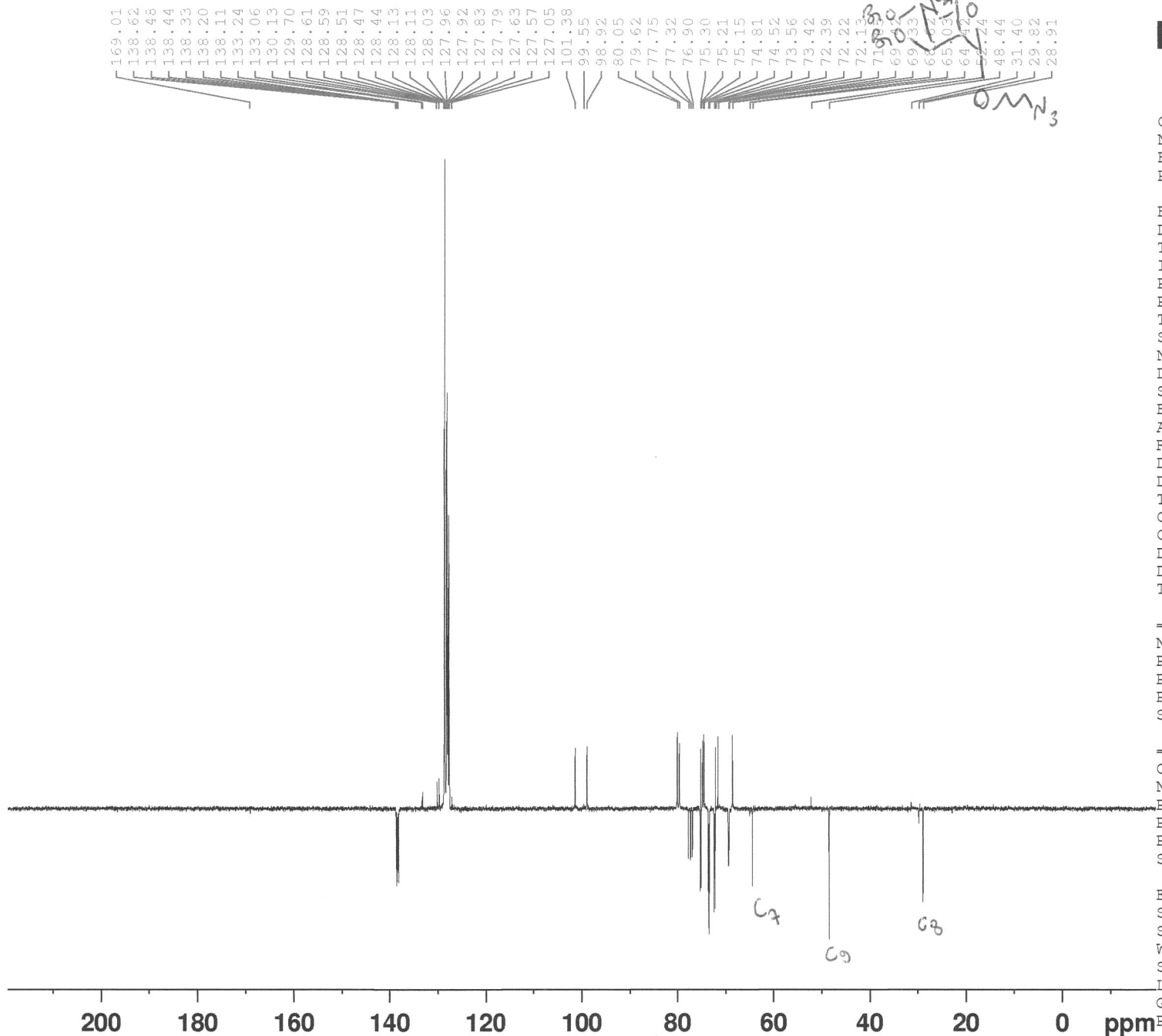
F2 - Acquisition Parameters
Date_ 20120516
Time 11.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 43268
SOLVENT CDC13
NS 32
DS 2
SWH 6009.615 Hz
FIDRES 0.138893 Hz
AQ 3.5999477 sec
RG 18
DW 83.200 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PLW1 7.00000000 W
SFO1 300.1815009 MHz

F2 - Processing parameters
SI 65536
SF 300.1800698 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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MP2/14



Current Data Parameters
NAME May16-2012-JMM
EXPNO 41
PROCNO 1

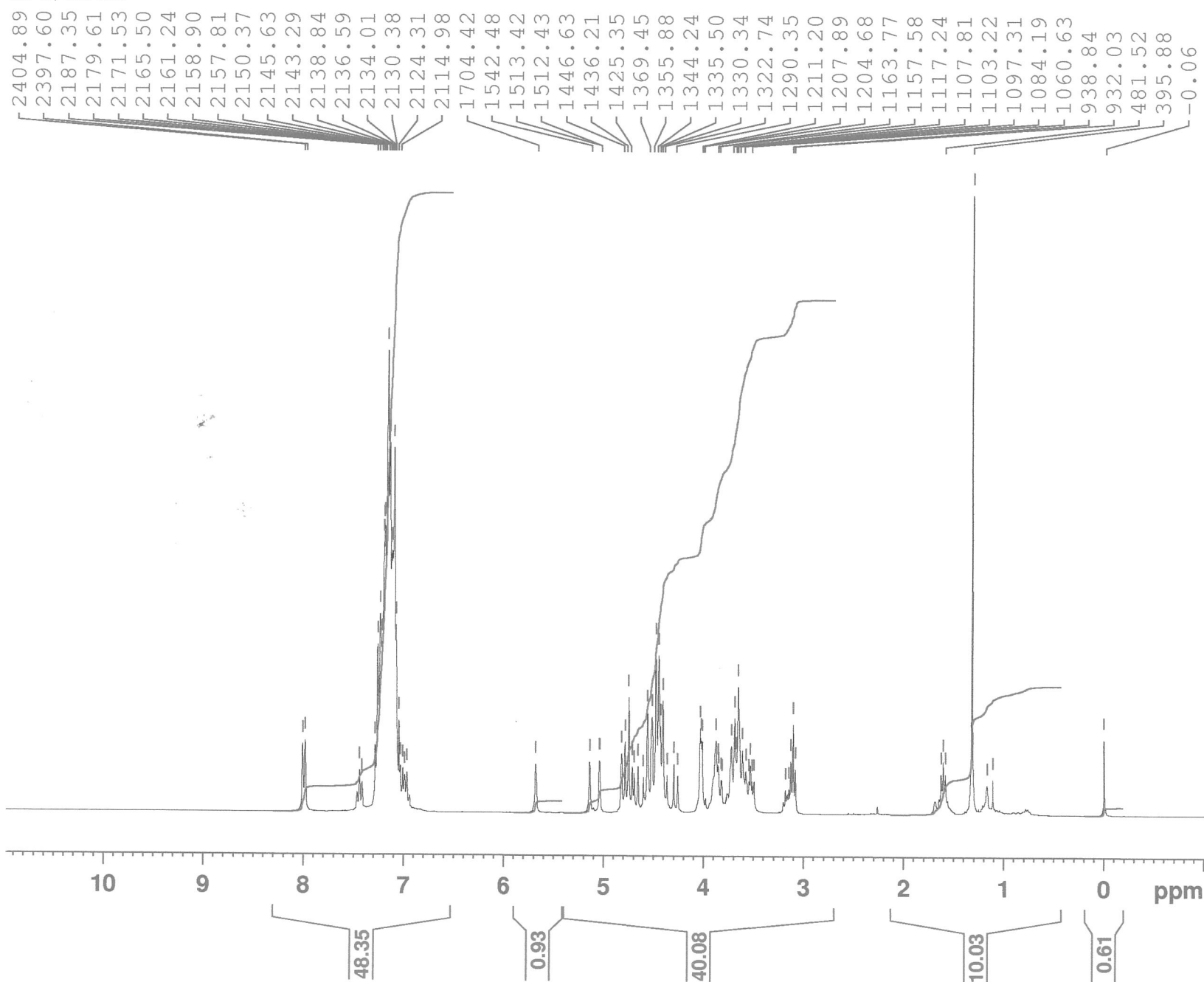
F2 - Acquisition Parameters
Date_ 20120516
Time 11.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 200
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 6.50 usec
TE 295.6 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
P2 18.00 usec
PLW1 38.00000000 W
SFO1 75.4878691 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PLW2 7.00000000 W
PLW12 0.13964000 W
SFO2 300.1812007 MHz

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

MP1/111A



Current Data Parameters
 NAME Dec02-2011-JMM
 EXPNO 20
 PROCNO 1

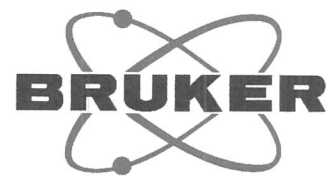
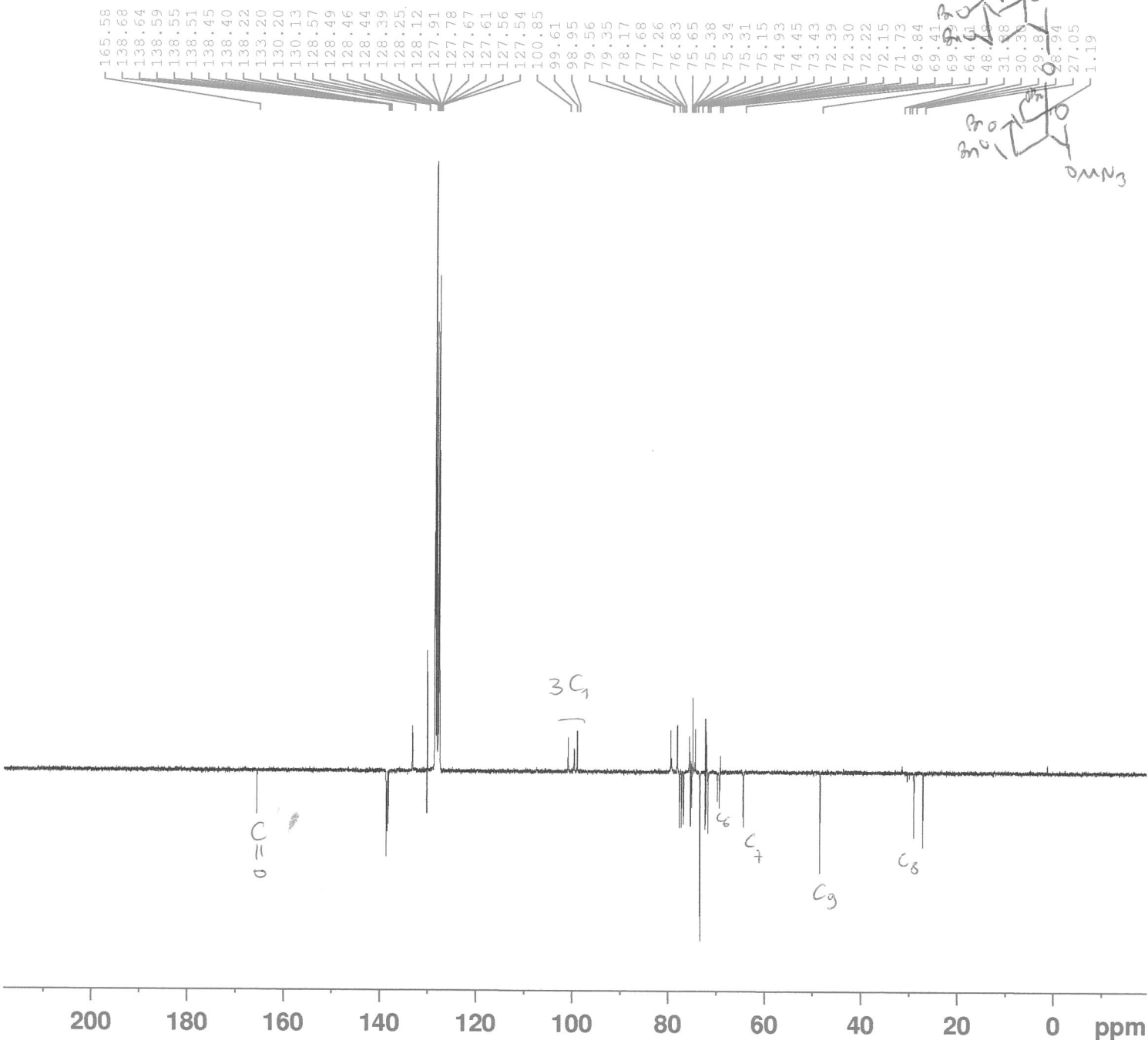
F2 - Acquisition Parameters
 Date_ 20111202
 Time 9.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 43268
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.138893 Hz
 AQ 3.5999477 sec
 RG 20.2
 DW 83.200 use
 DE 6.50 use
 TE 294.5 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.60 use
 PLW1 7.0000000 W
 SFO1 300.1815009 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1800741 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

22

MP1/111A



Current Data Parameters
 NAME Dec02-2011-JMM
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111202
 Time 10.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 6.50 usec
 TE 295.0 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 38.0000000 W
 SFO1 75.4878691 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PLW2 7.0000000 W
 PLW12 0.1396400 W
 SFO2 300.1812007 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

MP1/161

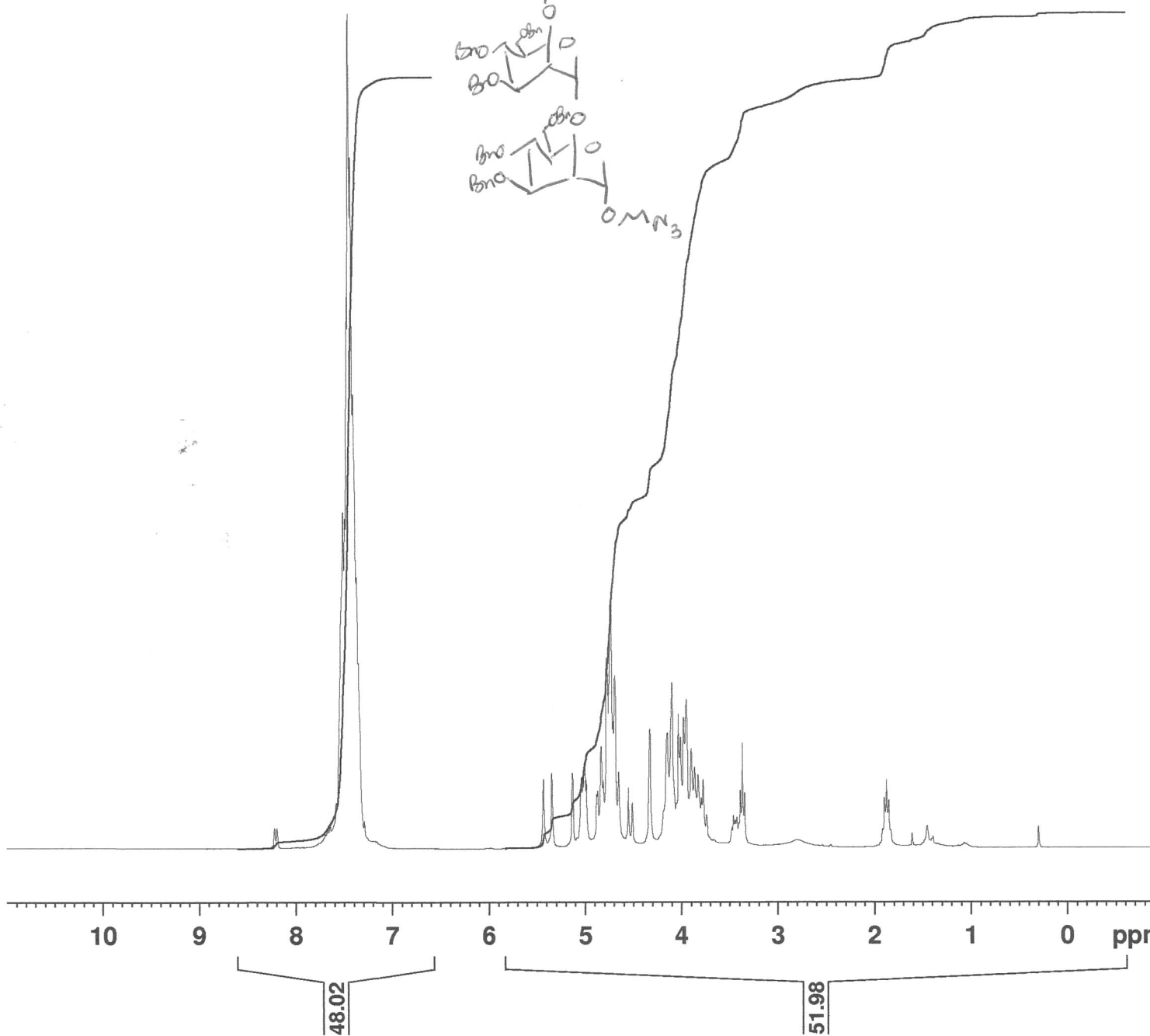


Current Data Parameters
NAME Mar13-2012-JMM
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120313
Time 11.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 43268
SOLVENT CDCl3
NS 32
DS 2
SWH 6009.615 Hz
FIDRES 0.138893 Hz
AQ 3.5999477 sec
RG 14.2
DW 83.200 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PLW1 7.00000000 W
SFO1 300.1815009 MHz

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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MP1/161



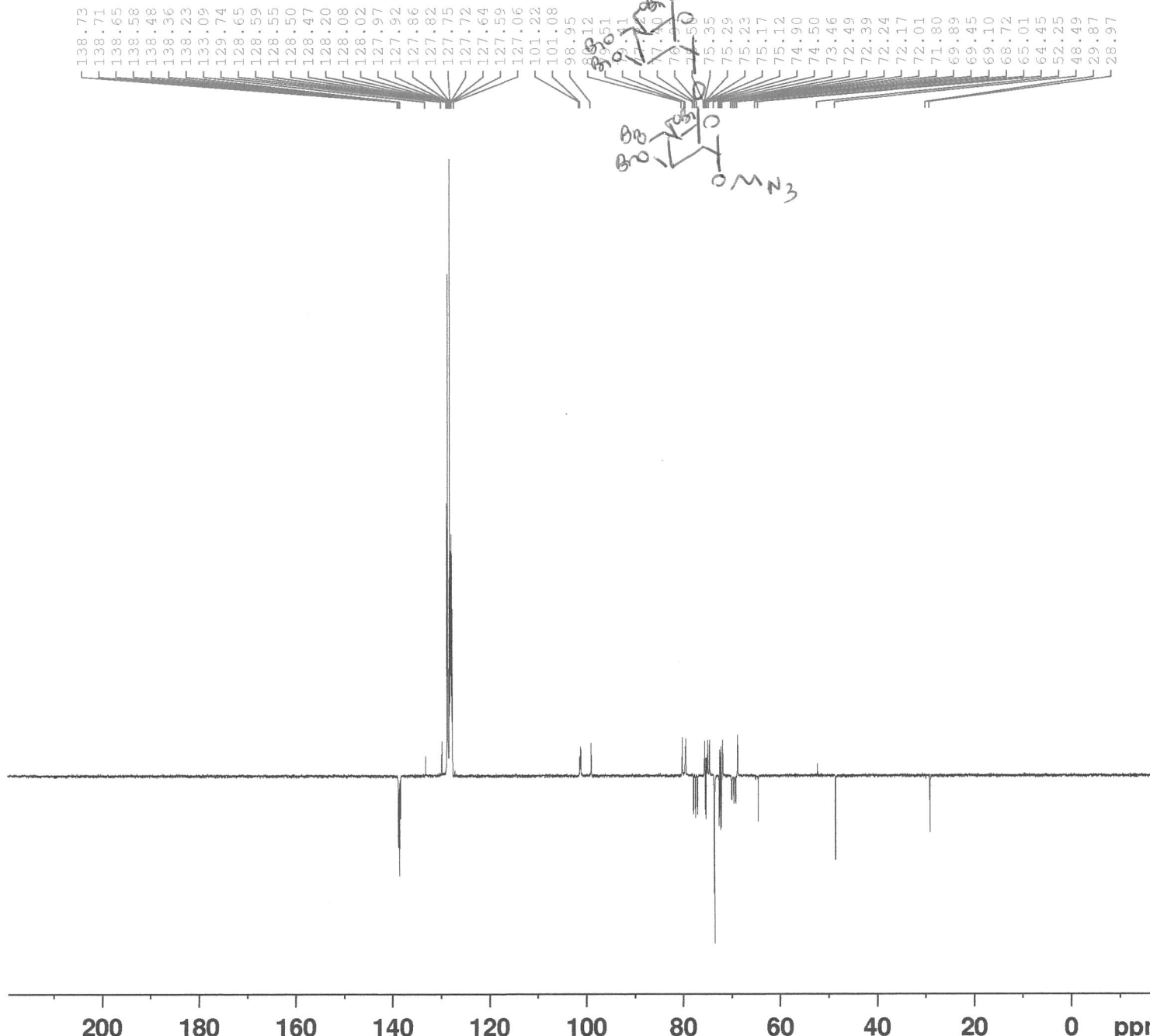
Current Data Parameters
NAME Mar13-2012-JMM
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120313
Time 12.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 6.50 usec
TE 295.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

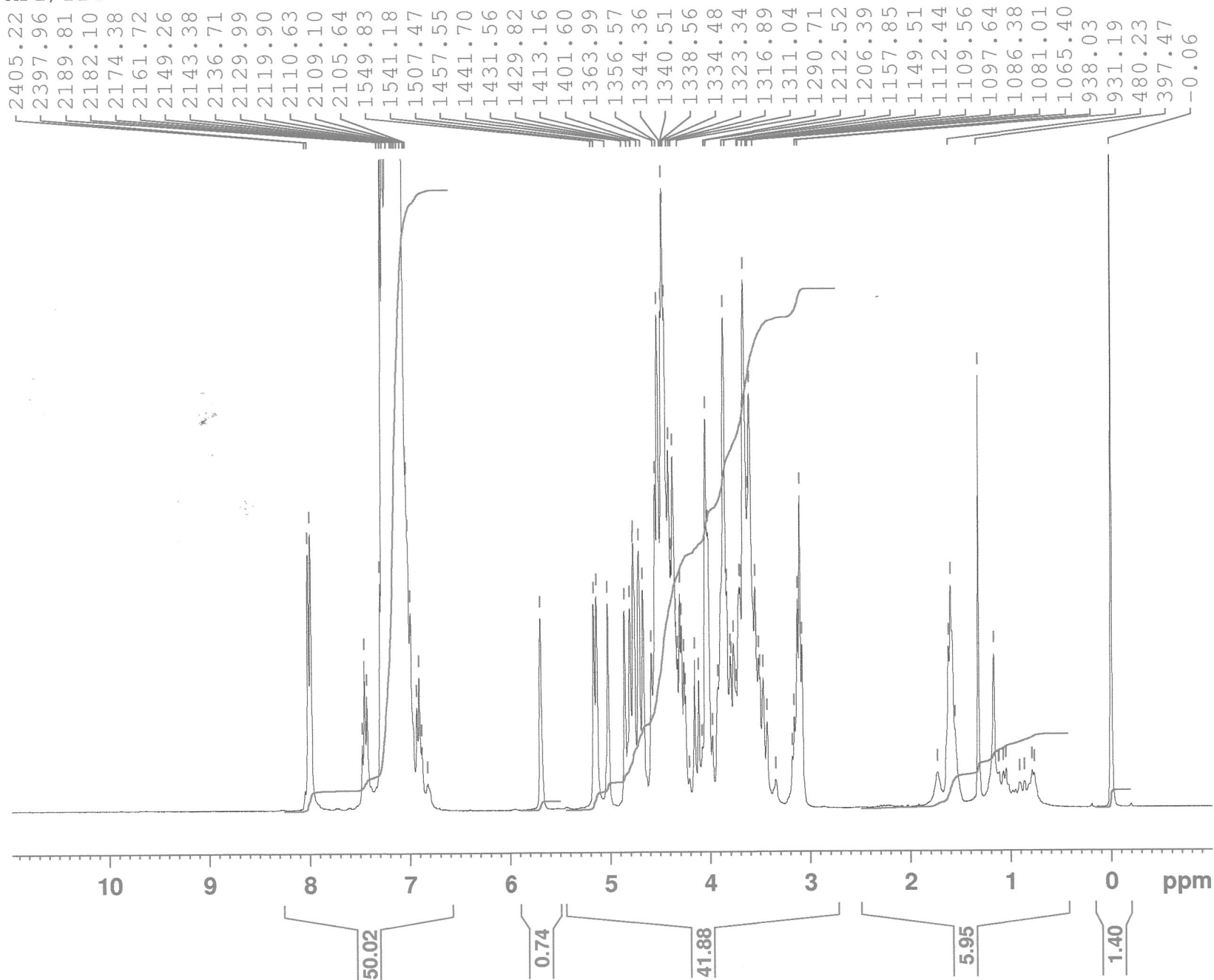
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
P2 18.00 usec
PLW1 38.00000000 W
SFO1 75.4878691 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PLW2 7.00000000 W
PLW12 0.13964000 W
SFO2 300.1812007 MHz

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



MP1/114



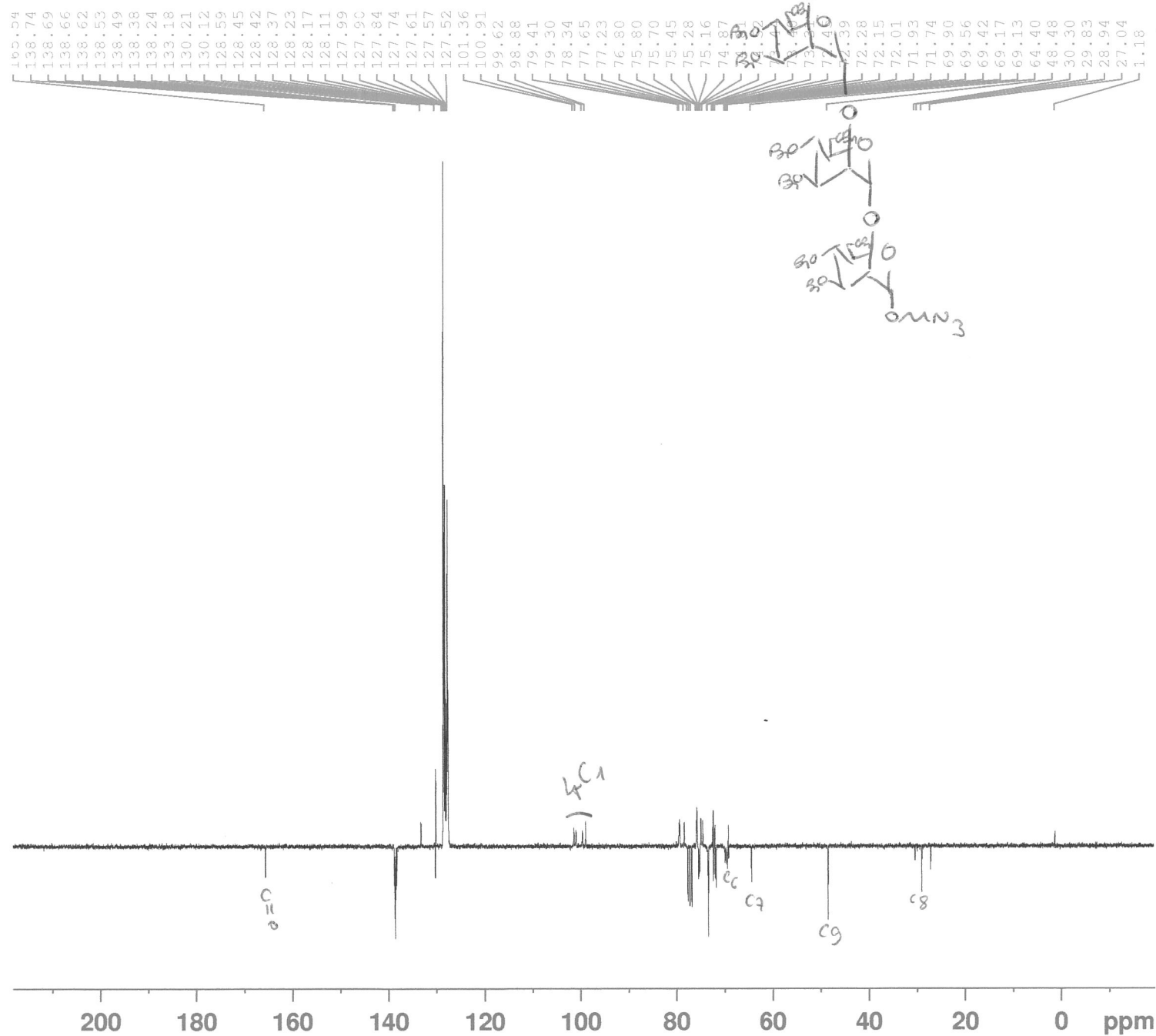
Current Data Parameters
NAME Dec08-2011-JMM
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111208
Time 10.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 43268
SOLVENT CDCl3
NS 32
DS 2
SWH 6009.615 Hz
FIDRES 0.138893 Hz
AQ 3.5999477 sec
RG 32
DW 83.200 use
DE 6.50 use
TE 294.1 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 13.60 use
PLW1 7.0000000 W
SFO1 300.1815009 MHz

F2 - Processing parameters
SI 65536
SF 300.1800693 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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MP1/114



Current Data Parameters
NAME Dec07-2011-JMM
EXPNO 171
PROCNO 1

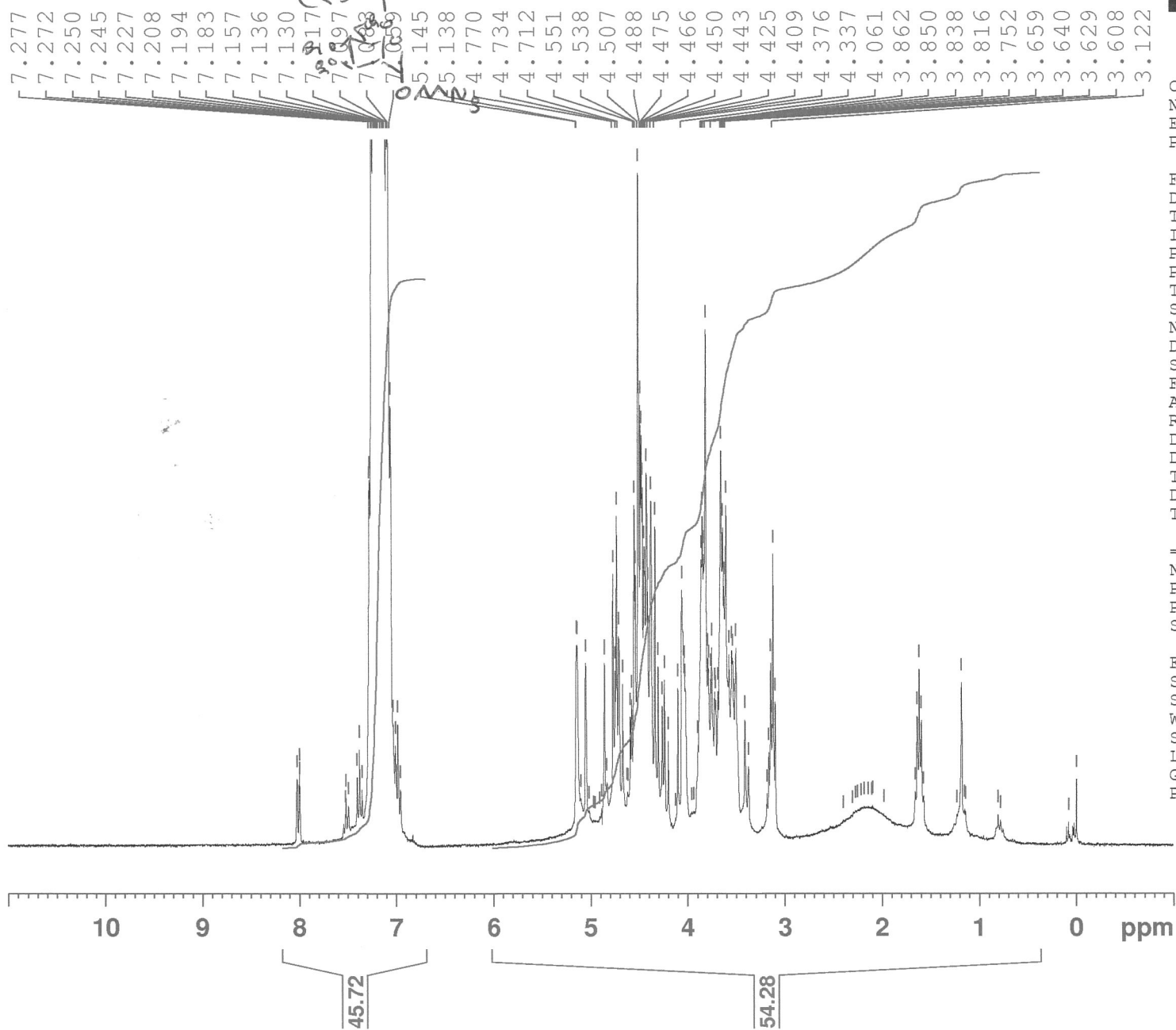
F2 - Acquisition Parameters
Date_ 20111207
Time 18.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 6.50 usec
TE 295.0 K
CNST2 145.000000
CNST11 1.000000
D1 2.0000000 sec
D20 0.00689655 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
P2 18.00 usec
PLW1 38.0000000 W
SFO1 75.4878691 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PLW2 7.0000000 W
PLW12 0.13964000 W
SFO2 300.1812007 MHz

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

MP2/24



Current Data Parameters
 NAME Jun20-2012-JMM
 EXPNO 60
 PROCNO 1

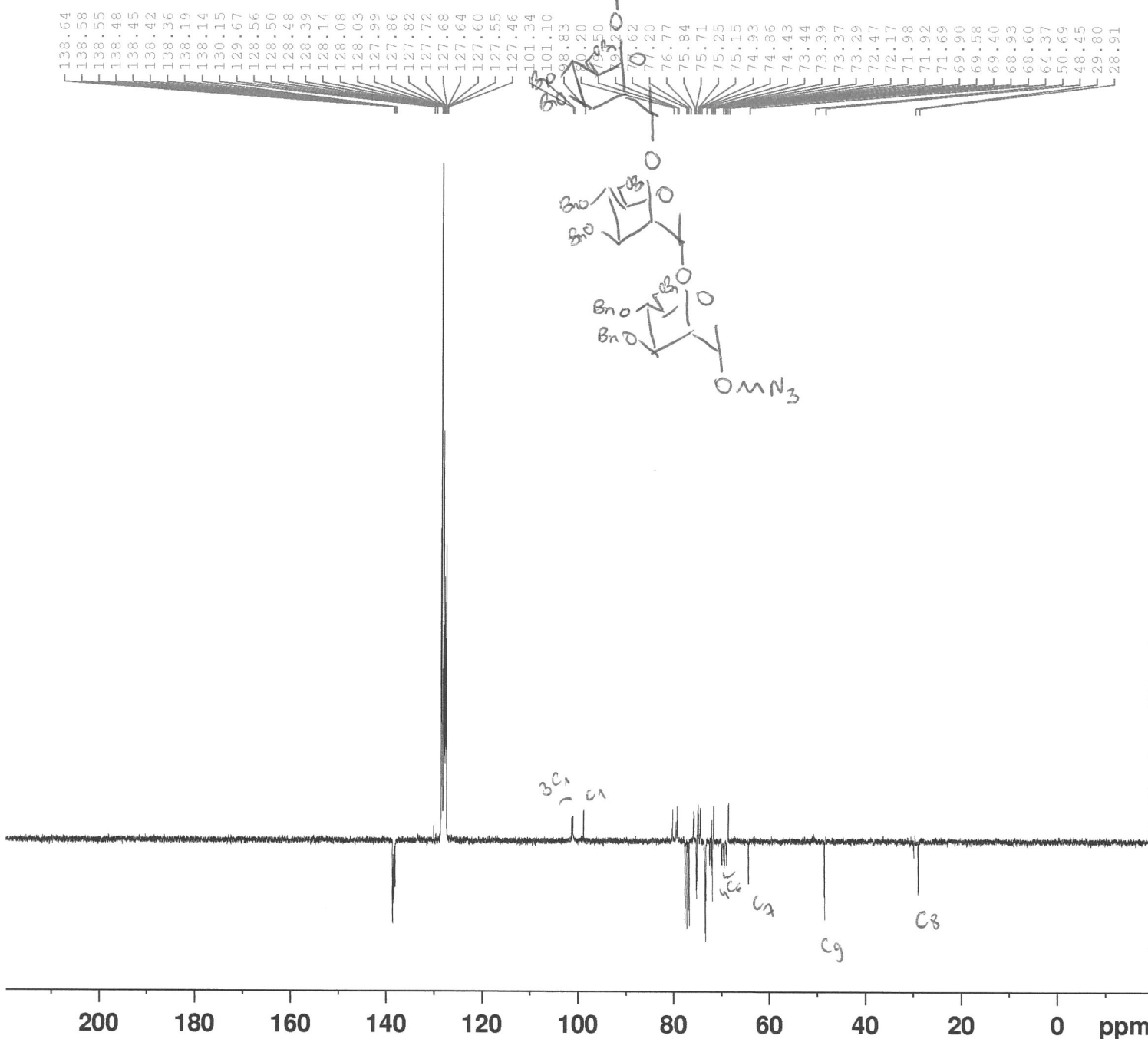
F2 - Acquisition Parameters
 Date_ 20120620
 Time 10.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 43268
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.138893 Hz
 AQ 3.5999477 sec
 RG 161
 DW 83.200 usec
 DE 6.50 usec
 TE 295.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.60 usec
 PLW1 7.00000000 W
 SFO1 300.1815009 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1800336 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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MP1/192



Current Data Parameters
 NAME May16-2012-JMM
 EXPNO 51
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120516
 Time 12.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 6.50 usec
 TE 295.8 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

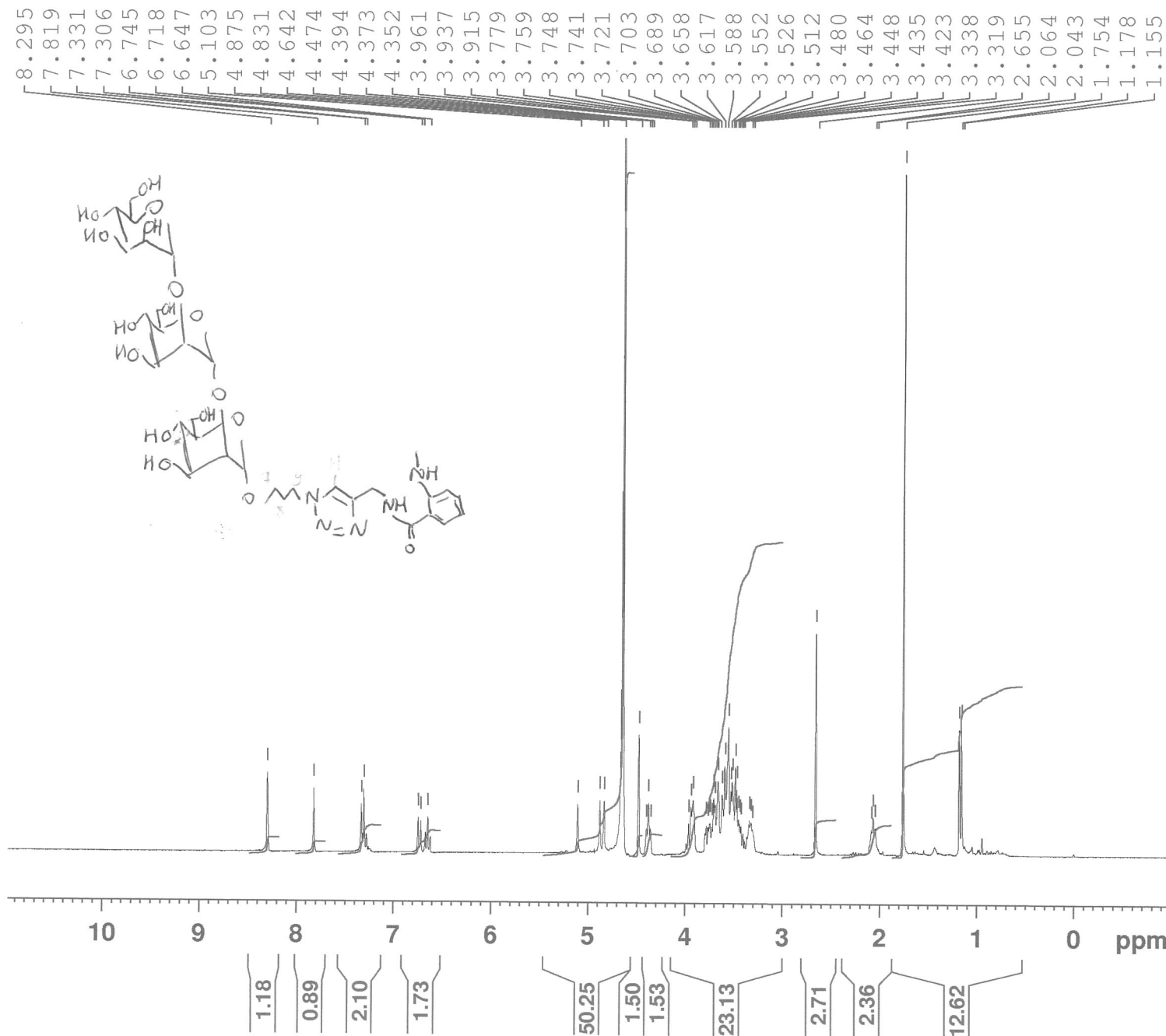
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 38.00000000 W
 SFO1 75.4878691 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PLW2 7.00000000 W
 PLW12 0.13964000 W
 SFO2 300.1812007 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

(A)

MP2/71A



Current Data Parameters
 NAME Oct26-2012-JMM
 EXPNO 100
 PROCNO 1

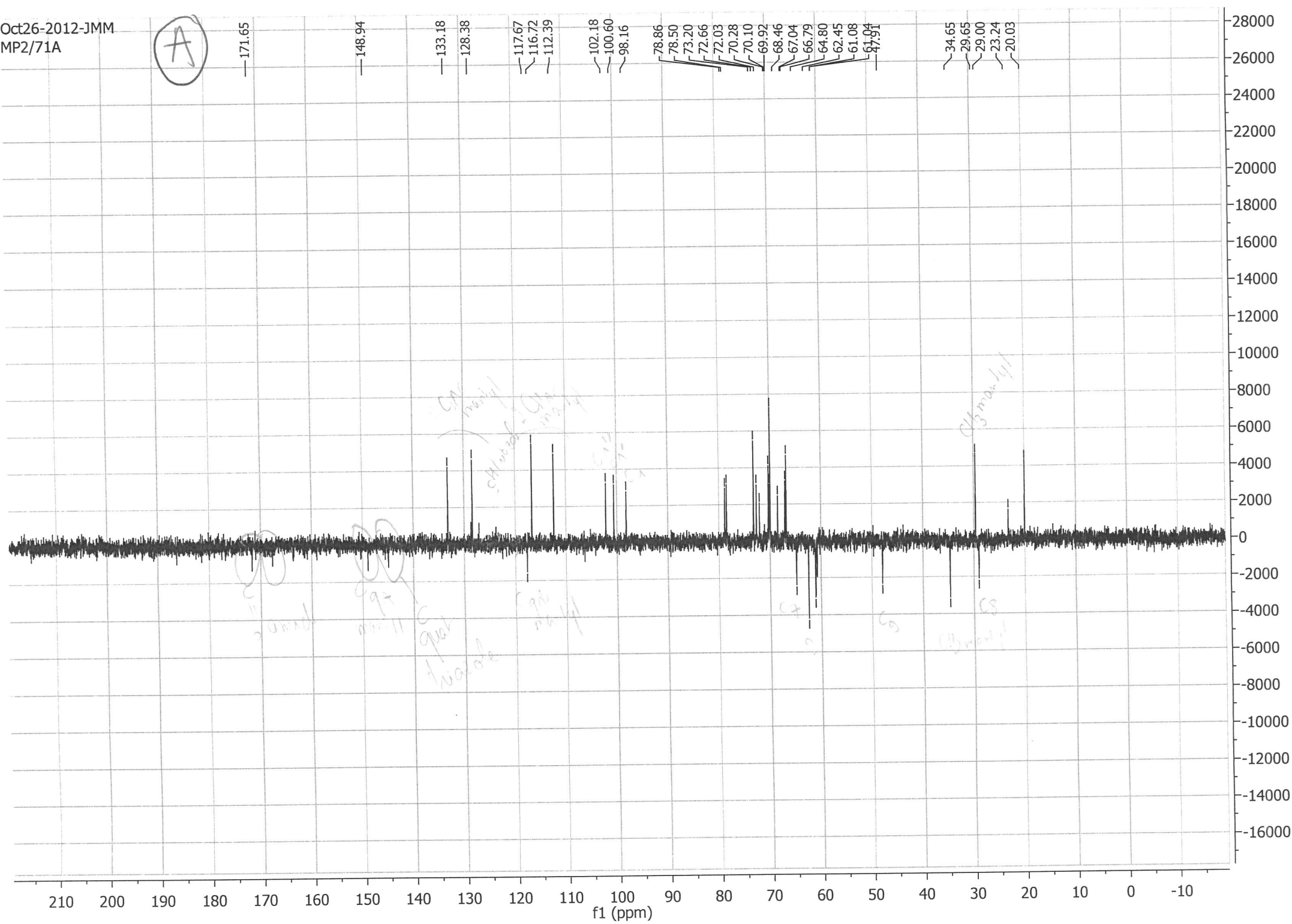
F2 - Acquisition Parameters
 Date_ 20121026
 Time 18.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 43268
 SOLVENT D2O
 NS 32
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.138893 Hz
 AQ 3.5998976 sec
 RG 256
 DW 83.200 usec
 DE 6.50 usec
 TE 296.1 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 300.1815009 MHz
 NUC1 1H
 P1 13.60 usec
 PLW1 7.00000000 W

F2 - Processing parameters
 SI 65536
 SF 300.1800208 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Oct26-2012-JMM
 MP2/71A

(A)



MP2/57A''



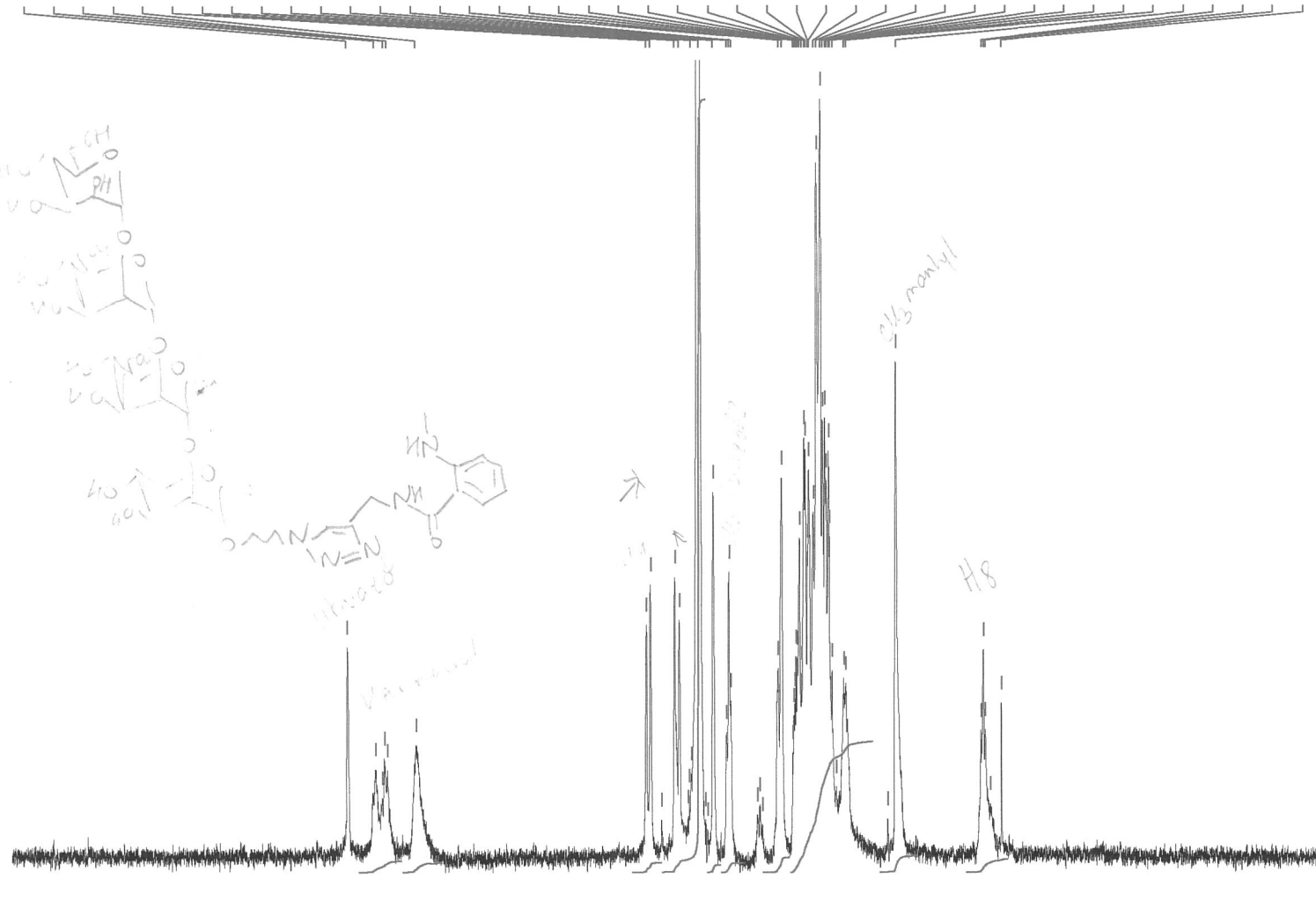
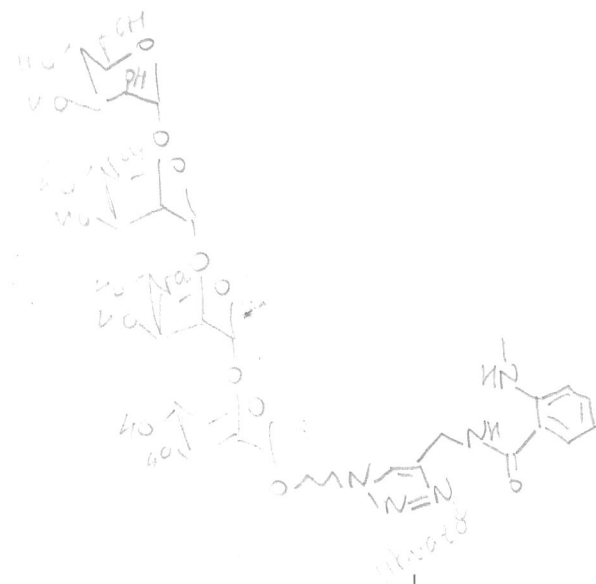
7.910
7.657
7.577
7.548
7.288
5.187
5.149
4.930
4.888
4.781
4.710
4.581
4.455
4.433
4.414
4.414
3.986
3.957
3.853
3.842
3.831
3.822
3.809
3.791
3.772
3.751
3.739
3.717
3.709
3.664
3.639
3.604
3.582
3.560
3.550
3.527
3.518
3.495
3.389
3.369
2.916
2.139
2.117
2.099
1.953

Current Data Parameters
 NAME Nov23-2012-JMM
 EXPNO 70
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121123
 Time 16.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 43268
 SOLVENT D2O
 NS 32
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.138893 Hz
 AQ 3.5998976 sec
 RG 362
 DW 83.200 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 300.1815009 MHz
 NUC1 1H
 P1 13.60 usec
 PLW1 7.00000000 W

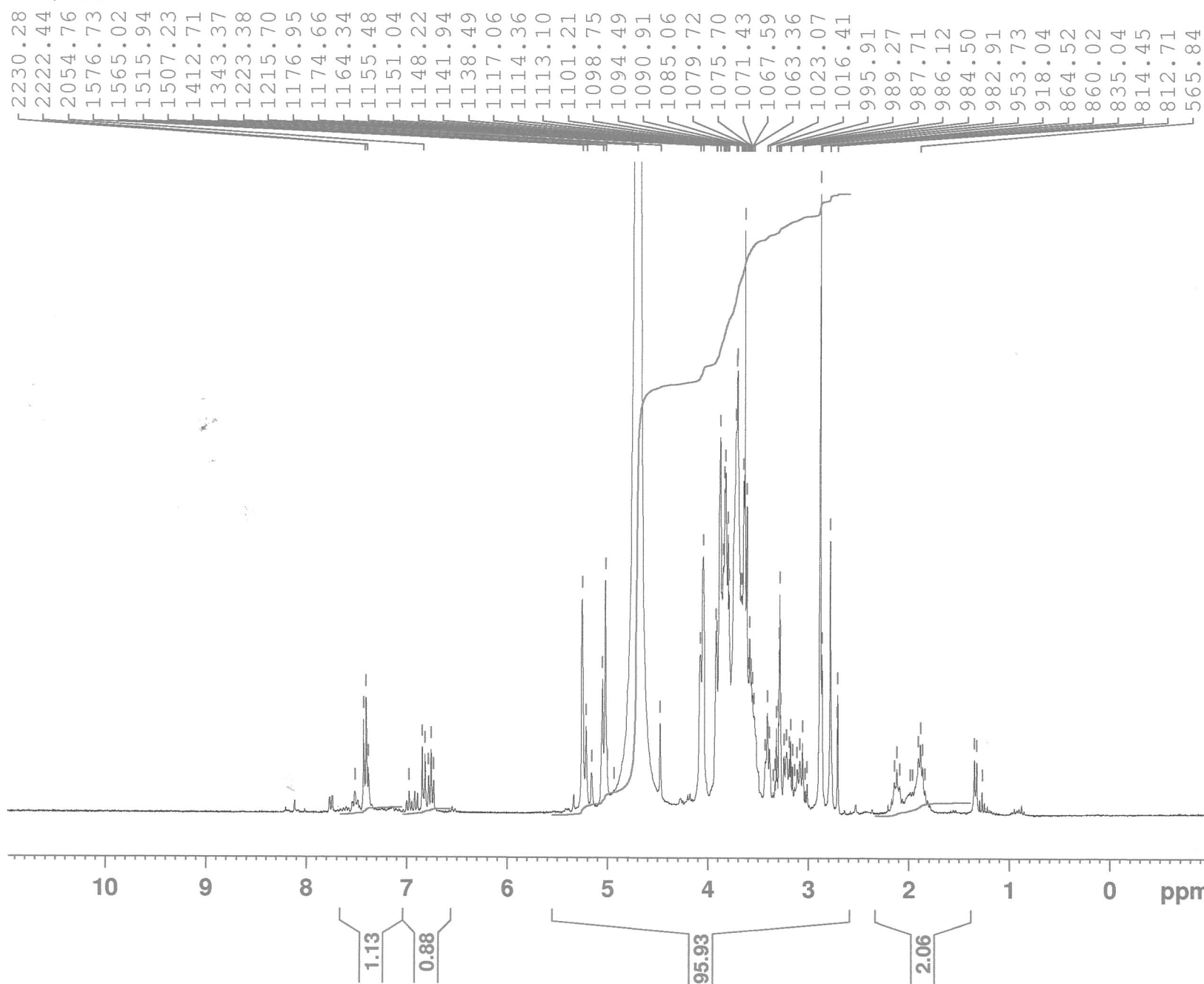
F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



10 9 8 7 6 5 4 3 2 1 0 ppm

1.15
0.98
1.02
77.48
0.77
0.93
1.55
13.11
1.67
1.34

MP1/158



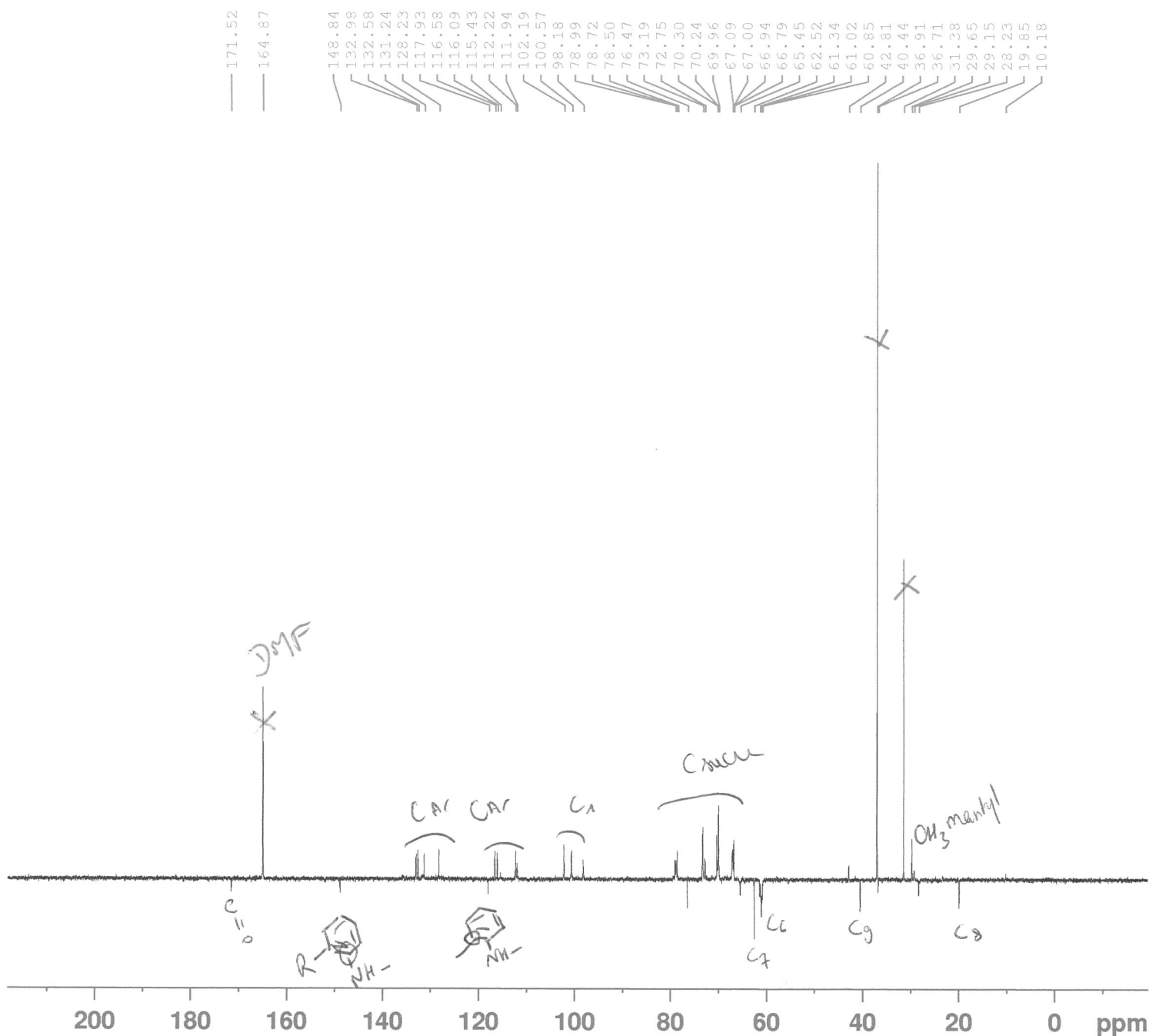
Current Data Parameters
 NAME Mar02-2012-JMM
 EXPNO 120
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120302
 Time 16.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 43268
 SOLVENT D2O
 NS 32
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.138893 Hz
 AQ 3.5999477 sec
 RG 144
 DW 83.200 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.60 usec
 PLW1 7.00000000 W
 SFO1 300.1815009 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1800000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

MP1/153



Current Data Parameters
 NAME Feb24-2012-JMM
 EXPNO 81
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120225
 Time 1.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT D2O
 NS 5000
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 6.50 usec
 TE 295.3 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 P2 18.00 usec
 PLW1 38.00000000 W
 SFO1 75.4878691 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PLW2 7.00000000 W
 PLW12 0.13964000 W
 SFO2 300.1812007 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4803210 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40