

Design, Synthesis, and Structure-activity Relationships for Chimeric Inhibitors of Hsp90

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Supporting Information

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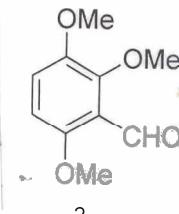
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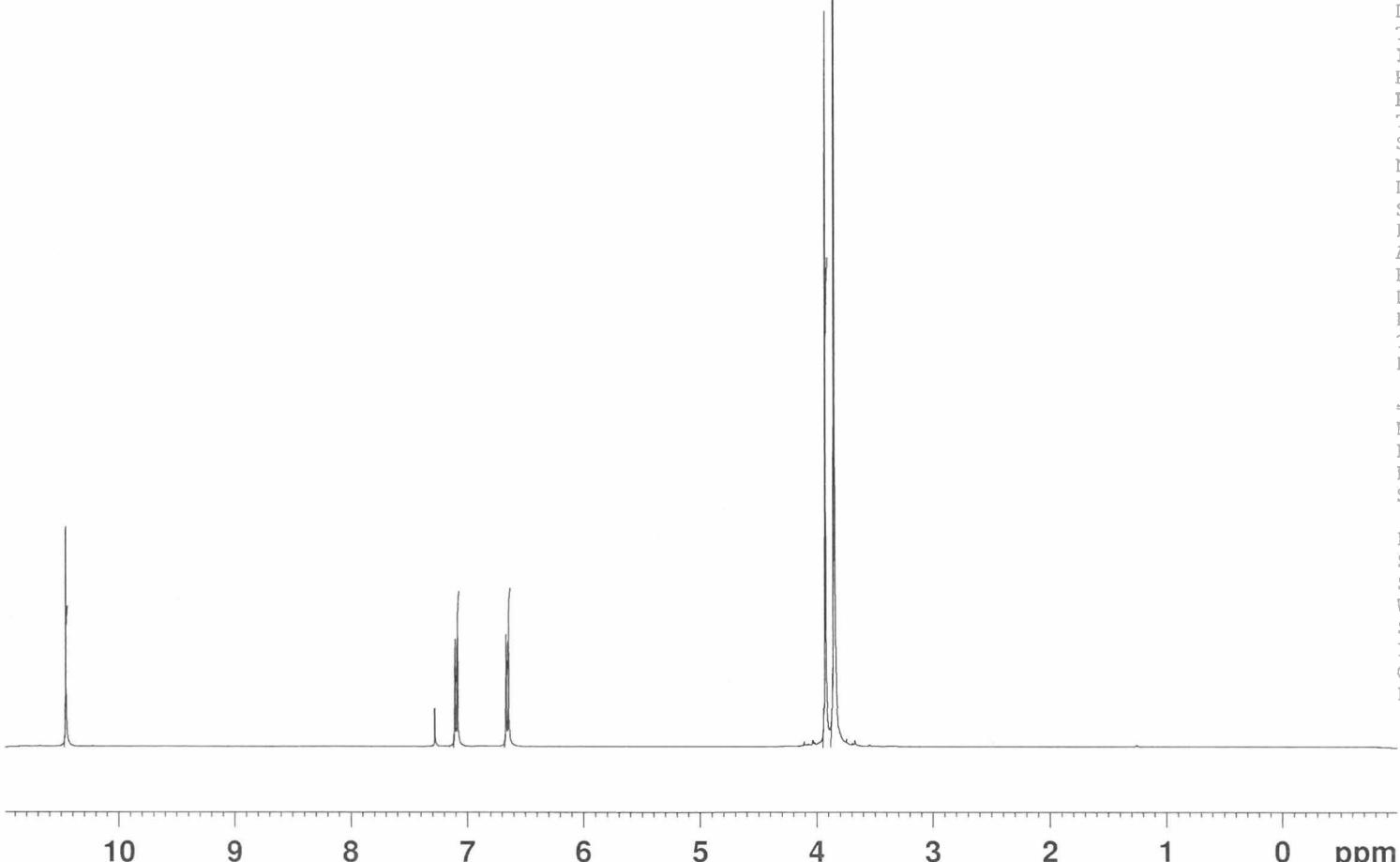


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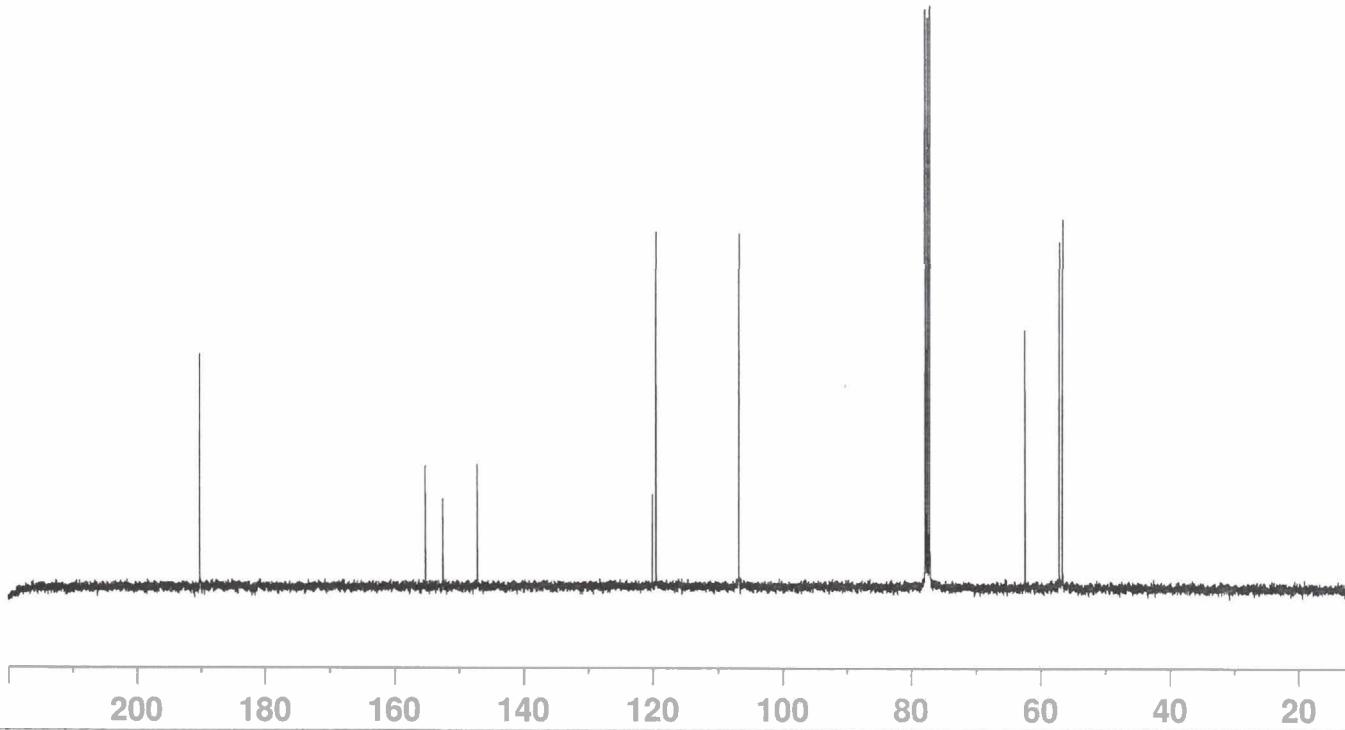
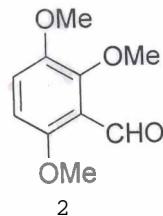
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0.90
0.92

2.81
5.87



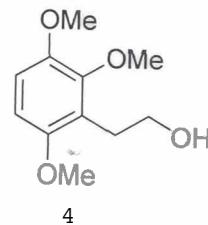
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 FIDRES 0.353213 Hz
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 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

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 PL1 2.00 dB
 SFO1 100.6232933 MHz

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 PL13 18.00 dB
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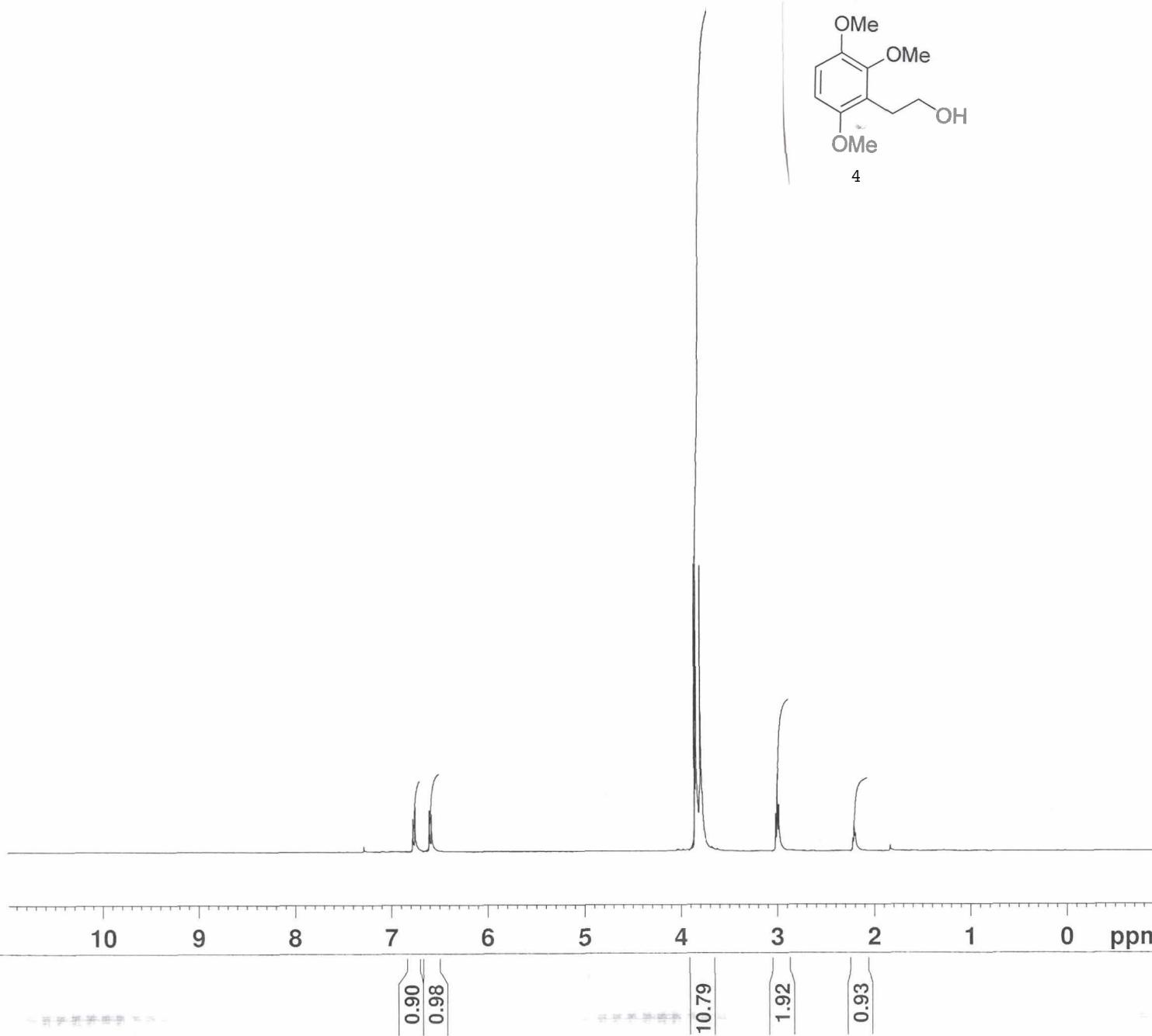


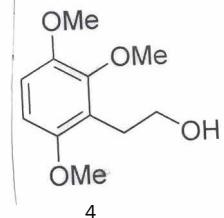
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SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 64
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
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F2 - Processing parameters
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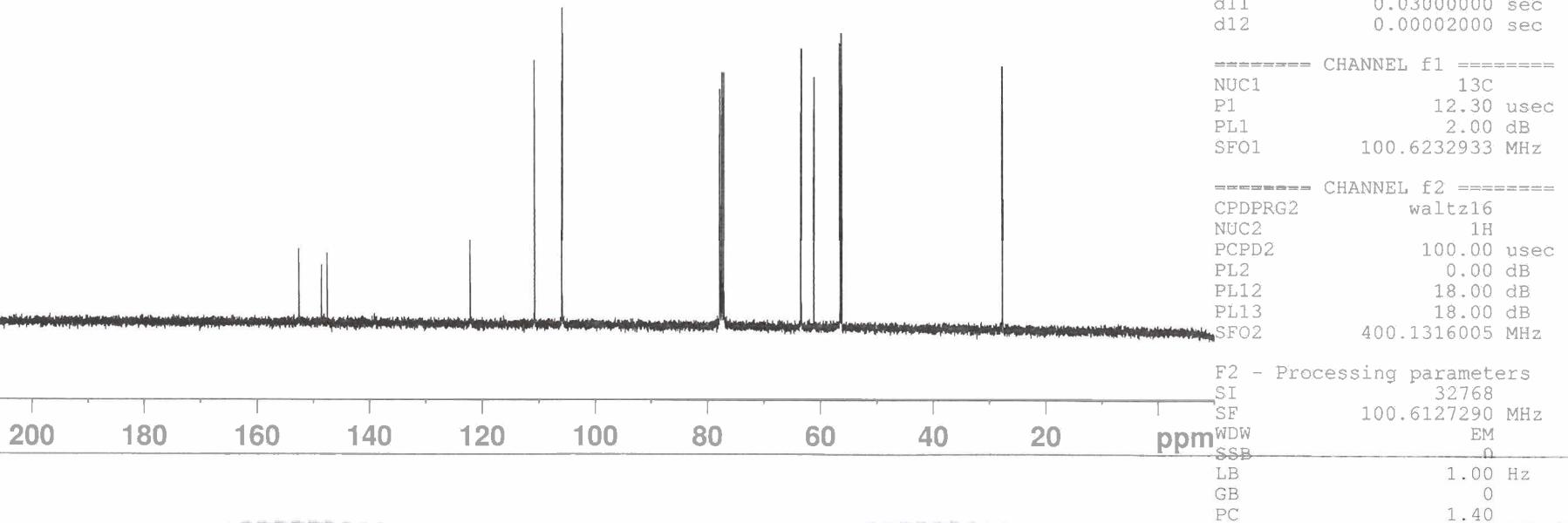


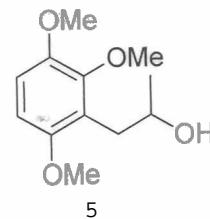
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 SOLVENT CDC13
 NS 403
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 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 512
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz





Current Data Parameters
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EXPNO 1
PROCNO 1

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SOLVENT CDCl3
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DS 2
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FIDRES 0.146157 Hz
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RG 64
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

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P1 7.70 usec
PL1 -6.00 dB
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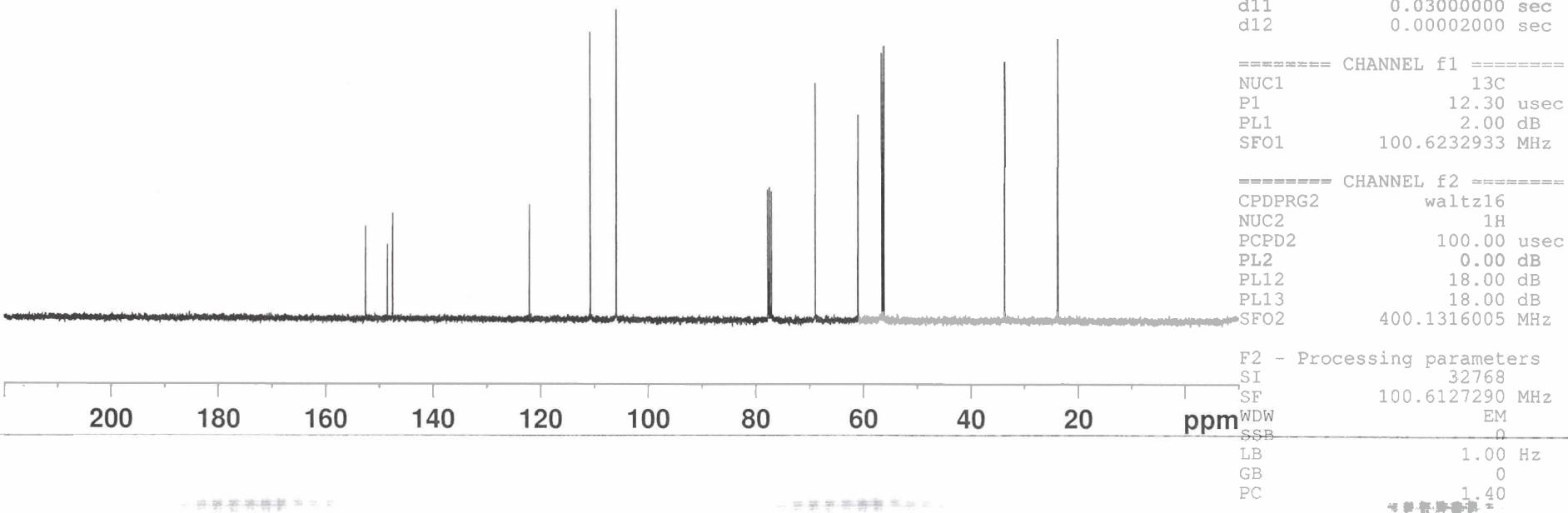
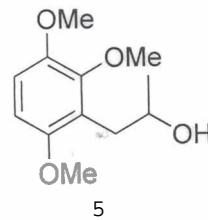
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0.99

1.06
9.14

2.04
1.11

3.04



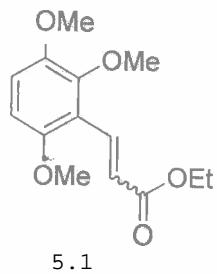
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 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
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 TE 300.0 K
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 d11 0.03000000 sec
 d12 0.00002000 sec

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 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
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 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
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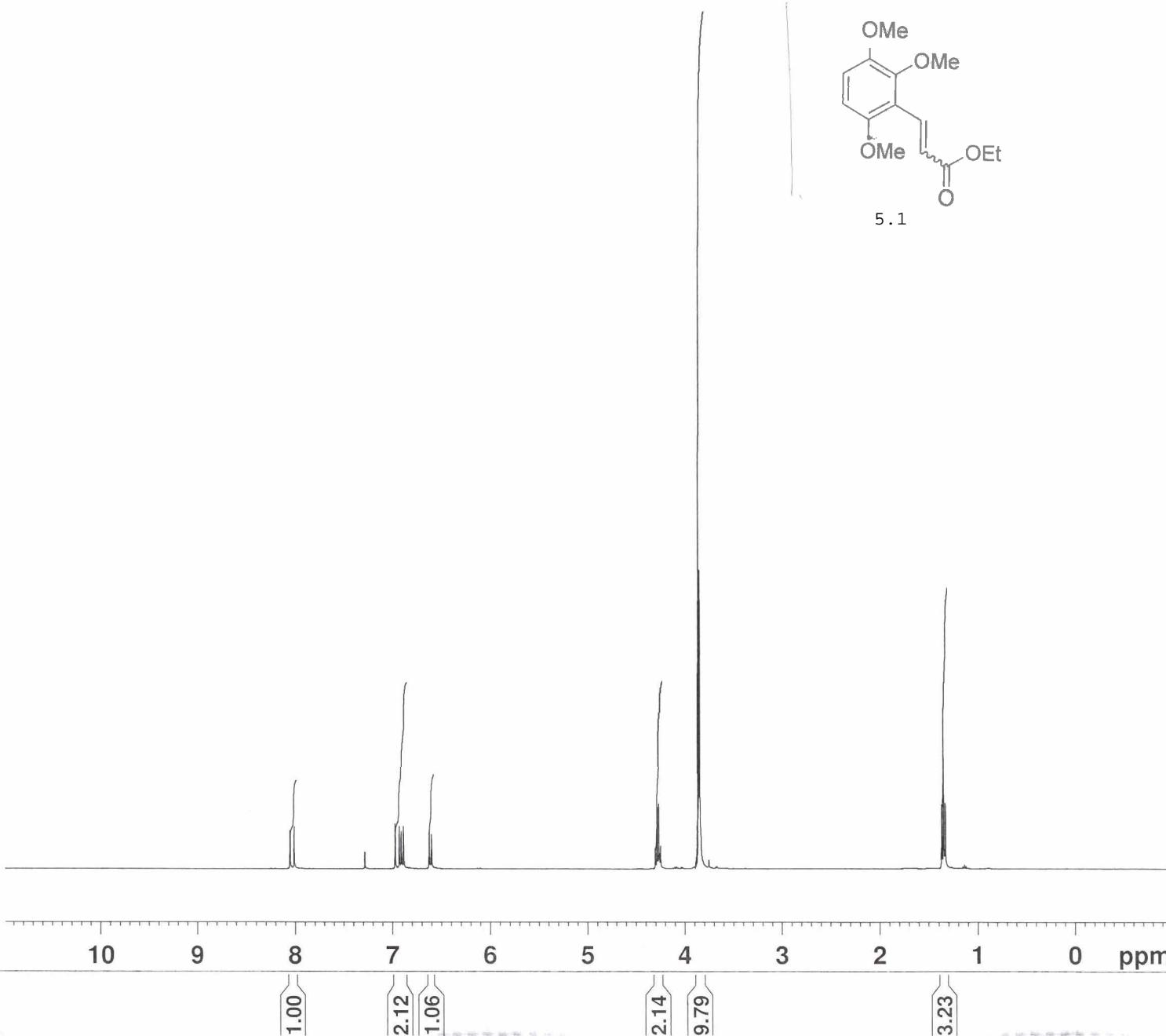


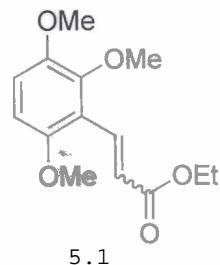
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 SOLVENT CDC13
 NS 16
 DS 2
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 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 101.6
 DW 104.400 usec
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 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
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 P1 7.70 usec
 PL1 -6.00 dB
 SFO1 400.1320007 MHz

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Current Data Parameters
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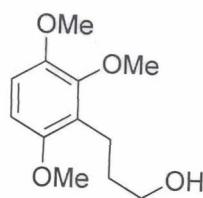
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 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
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 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
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F2 - Processing parameters
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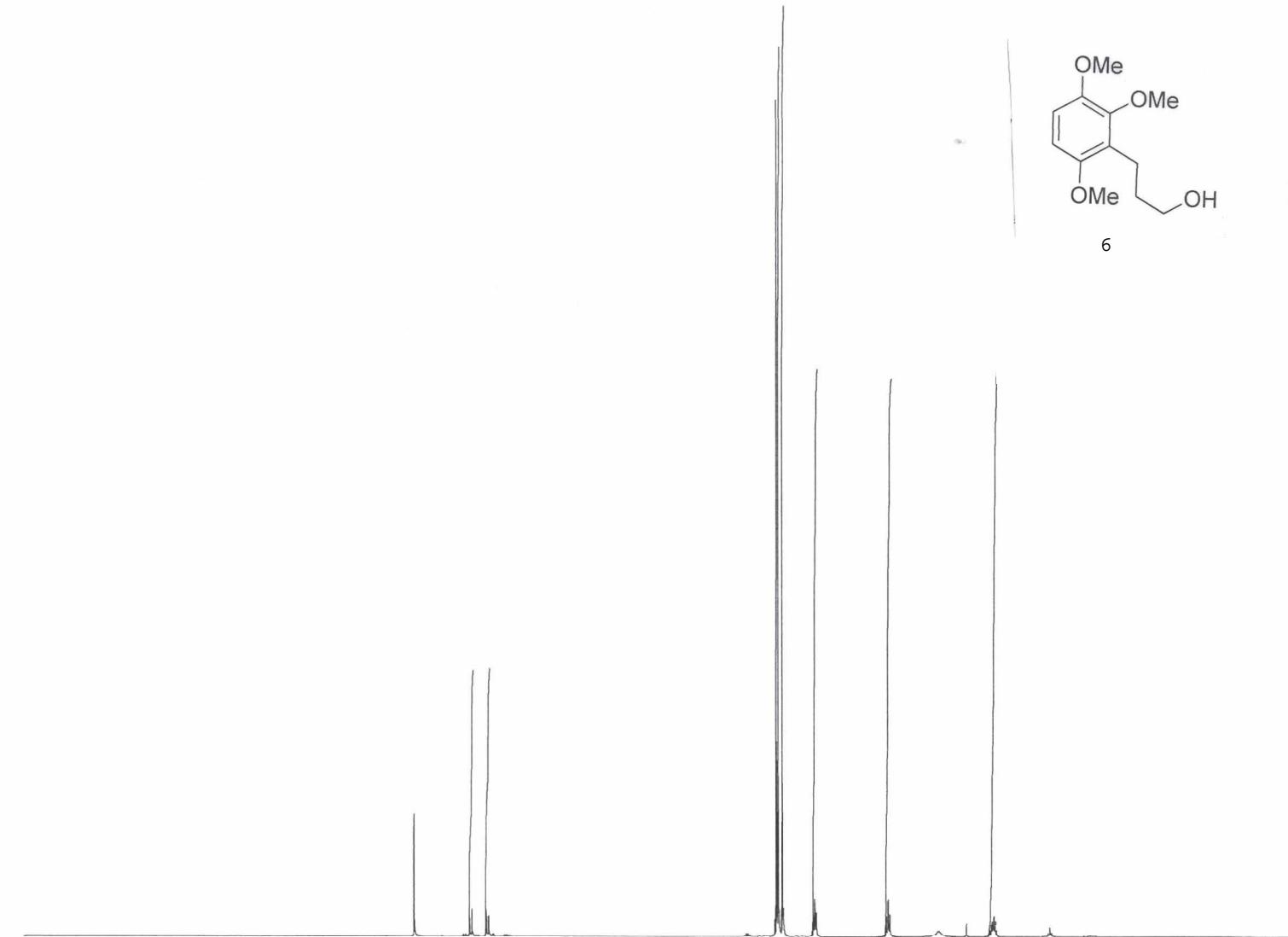
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 SOLVENT CDC13
 NS 64
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 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 114
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.0000000 sec

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 P1 7.70 usec
 PL1 -6.00 dB
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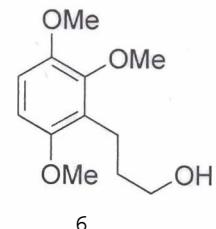
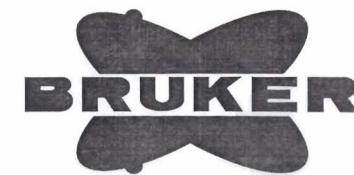


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1.08

3.36
3.58
3.74
2.28
2.25

2.30



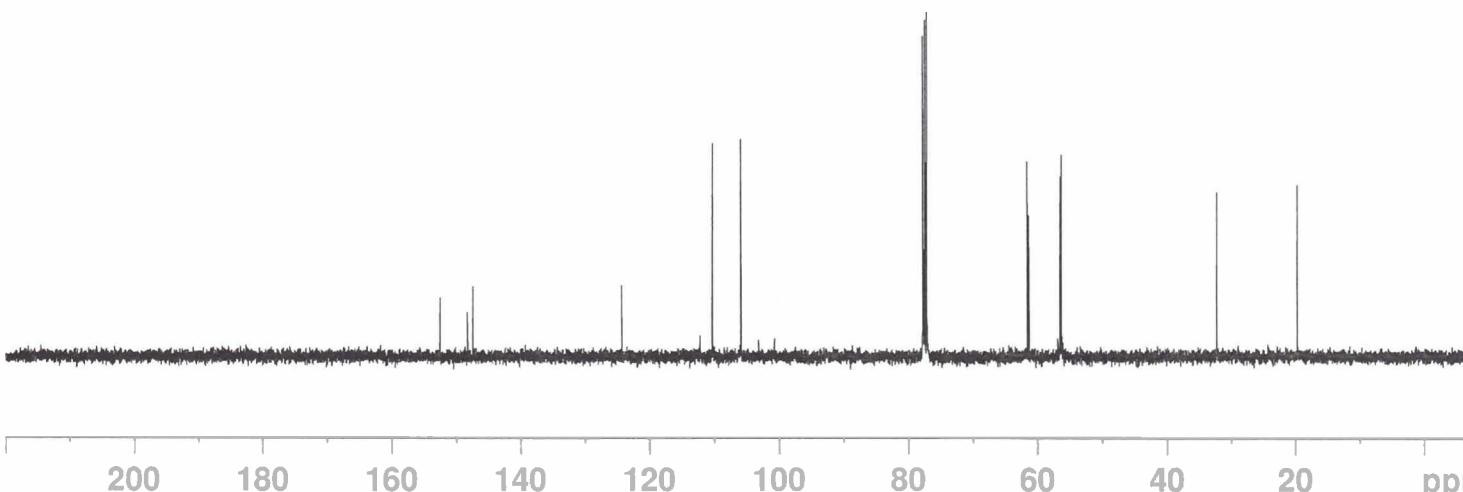
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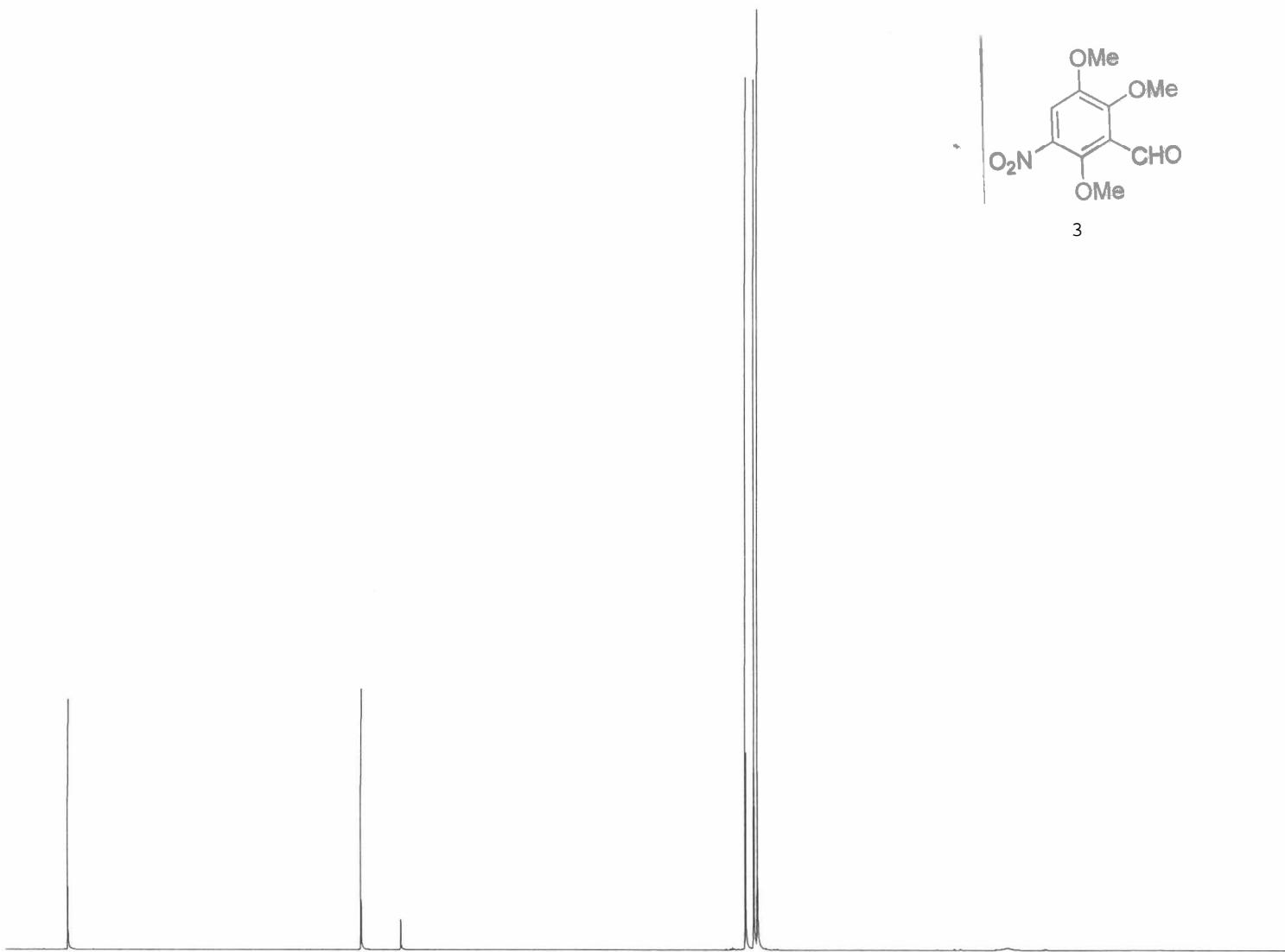
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AQ 1.4156276 sec
RG 4096
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DE 4.50 usec
TE 300.0 K
D1 0.05000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.30 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
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PL2 0.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
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Current Data Parameters
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 PROCNO 1

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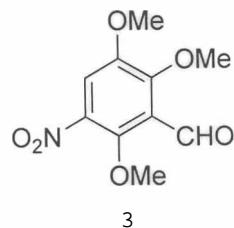
===== CHANNEL f1 ======
 NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

0.97

1.01

3.36
3.36
3.63
S18



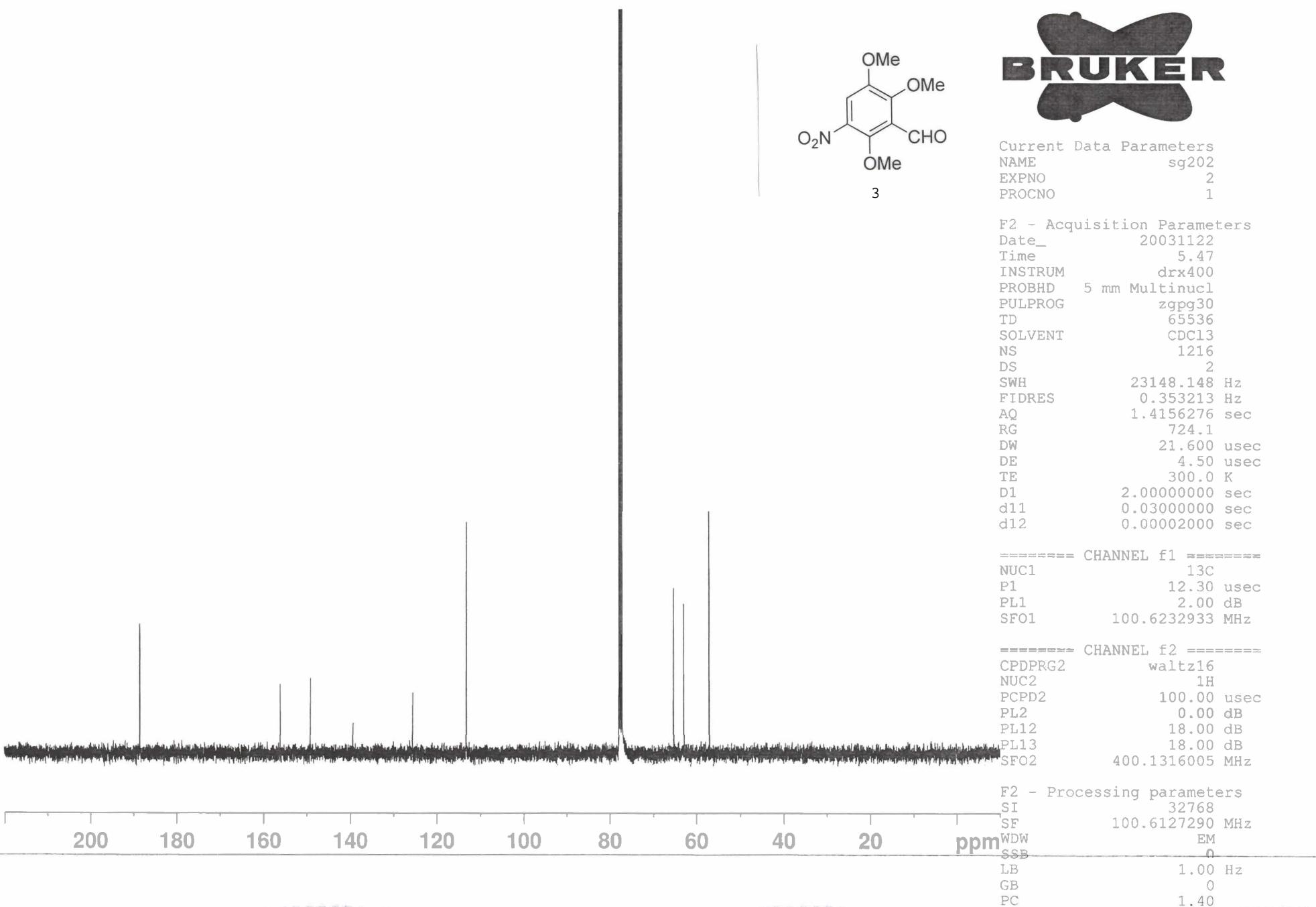
Current Data Parameters
NAME sg202
EXPNO 2
PROCNO 1

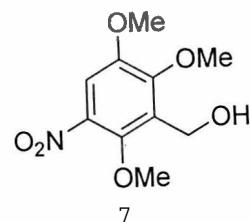
F2 - Acquisition Parameters
Date_ 20031122
Time 5.47
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1216
DS 2
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 724.1
DW 21.600 usec
DE 4.50 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.30 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



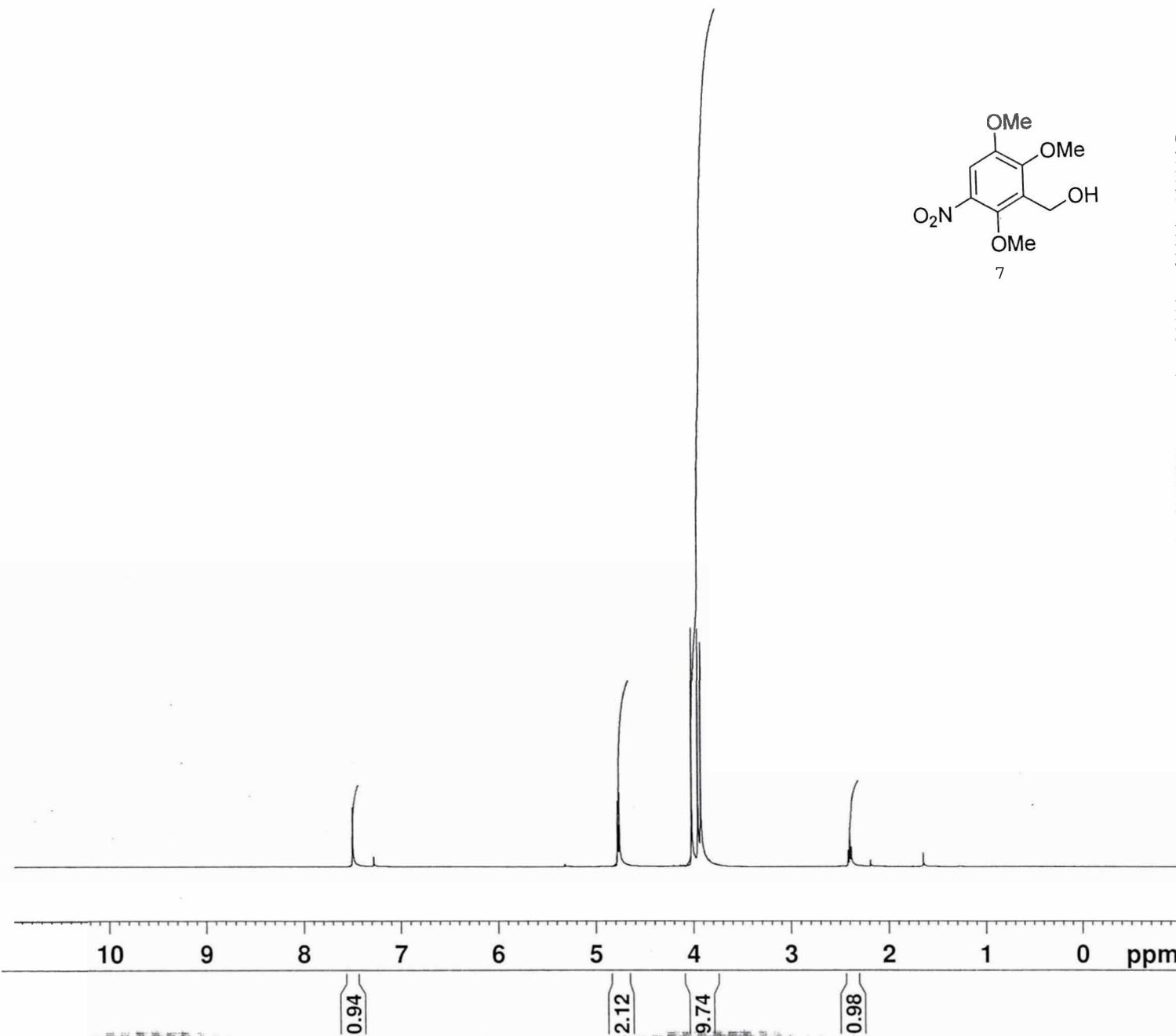


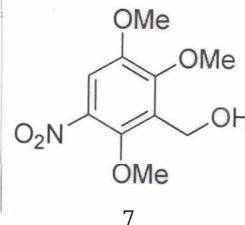
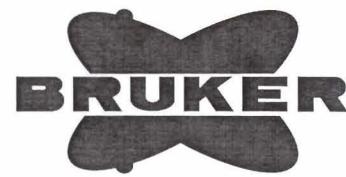
Current Data Parameters
 NAME gs123
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030308
 Time 23.43
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 143.7
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





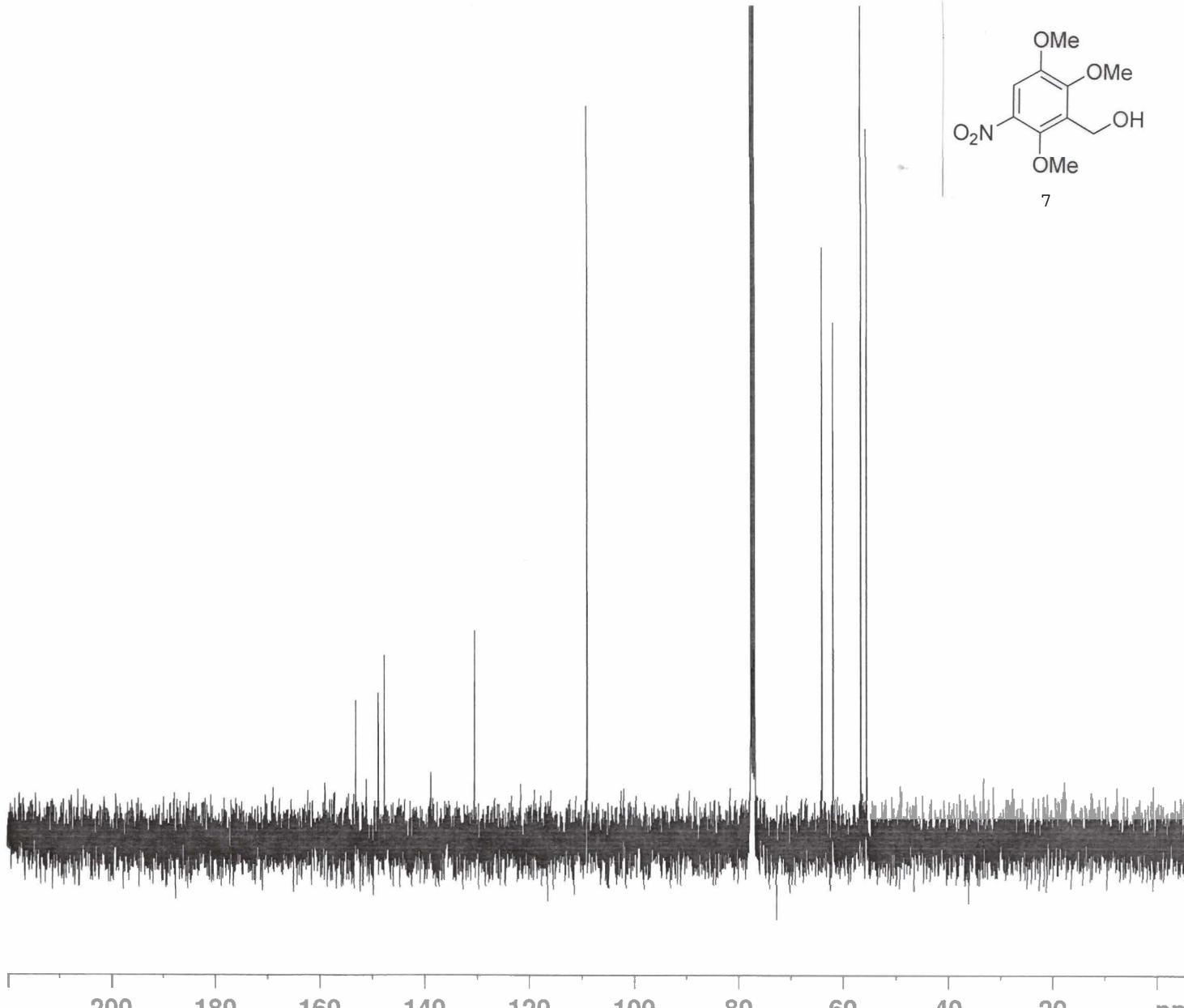
Current Data Parameters
NAME gs124
EXPNO 1
PROCNO 1

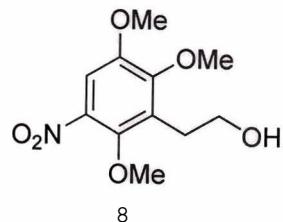
F2 - Acquisition Parameters
Date_ 20030308
Time 23.49
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zgppg30
TD 65536
SOLVENT CDC13
NS 452
DS 2
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 2580.3
DW 21.600 usec
DE 4.50 usec
TE 300.0 K
D1 0.05000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.30 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



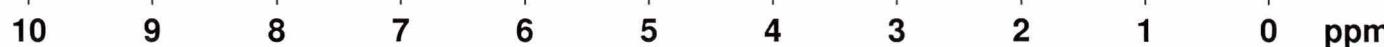


Current Data Parameters
 NAME gs125
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030310
 Time 19.08
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SFO1 400.1320007 MHz

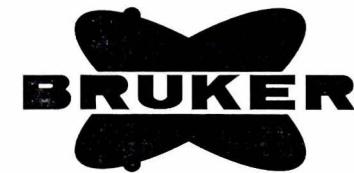
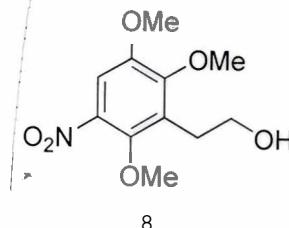
F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



6.24

17.67
37.27
19.71
12.94

6.17



Current Data Parameters
 NAME gs126
 EXPNO 1
 PROCNO 1

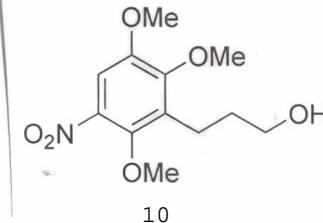
F2 - Acquisition Parameters
 Date_ 20030310
 Time 19.16
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 200
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 812.7
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 ======
 NUC1 ¹³C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 ======
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



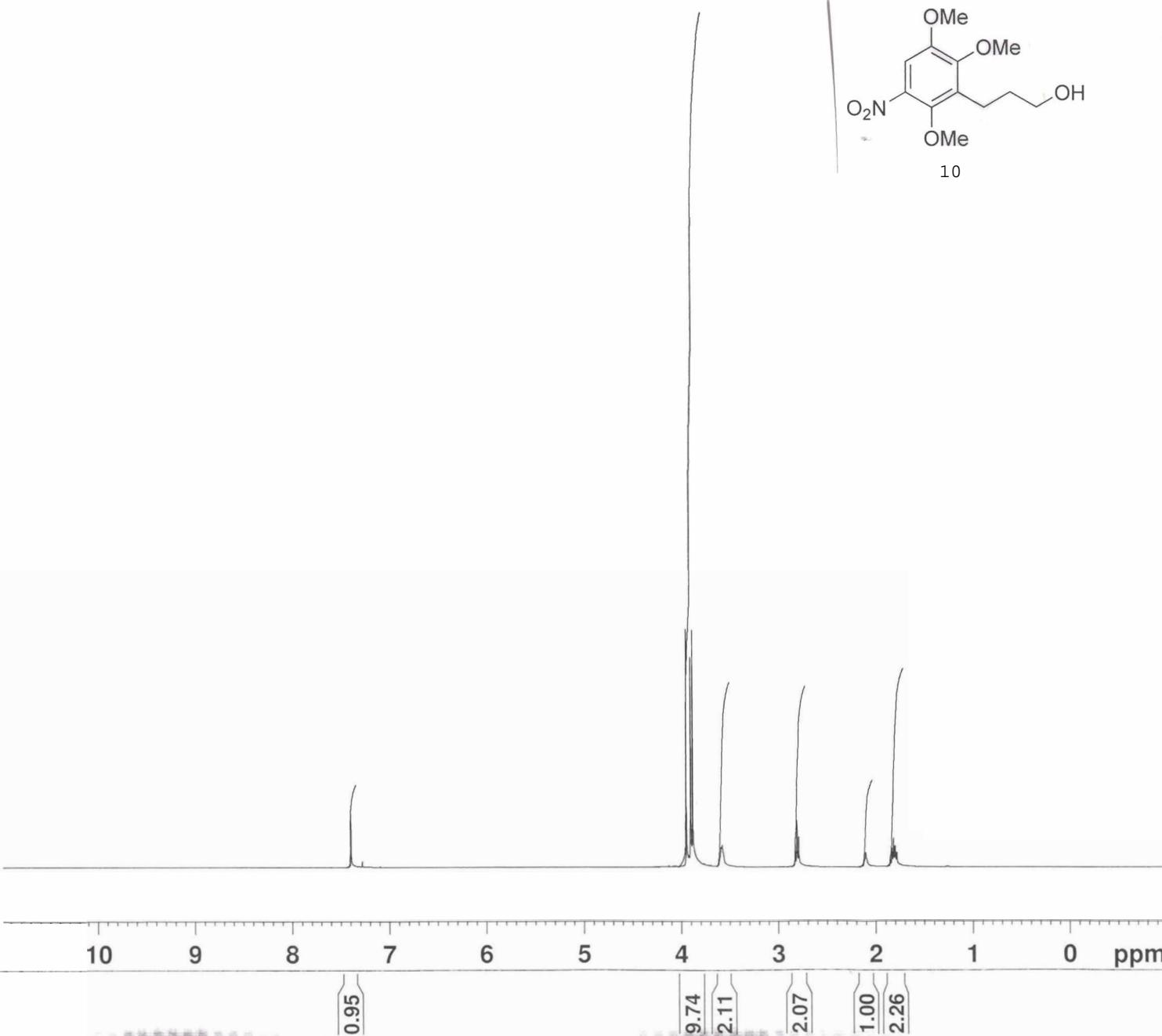


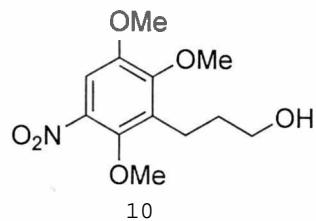
Current Data Parameters
 NAME gs127
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030312
 Time 2.18
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT **CDC13**
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.0000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME gs129
 EXPNO 1
 PROCNO 1

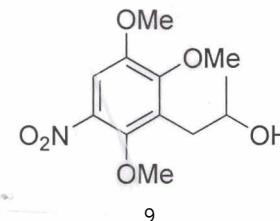
F2 - Acquisition Parameters
 Date_ 20030312
 Time 2.22
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 237
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 1625.5
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 WDW EM
 SSF 0
 LB 1.00 Hz
 GB 0
 PC 1.40



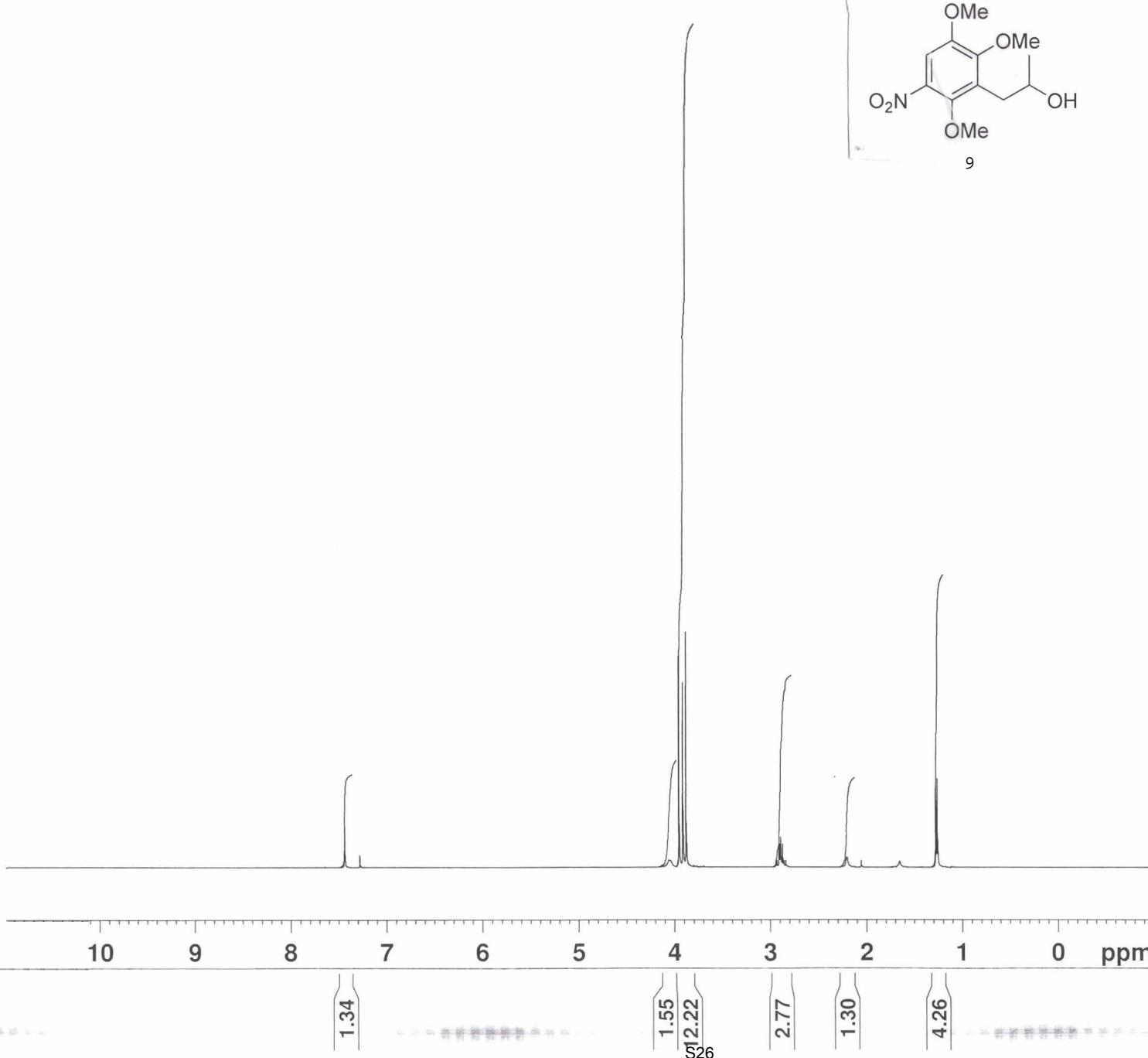


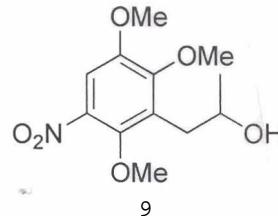
Current Data Parameters
NAME sg-002
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030607
Time 5.48
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 161.3
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
 NAME sg-003
 EXPNO 1
 PROCNO 1

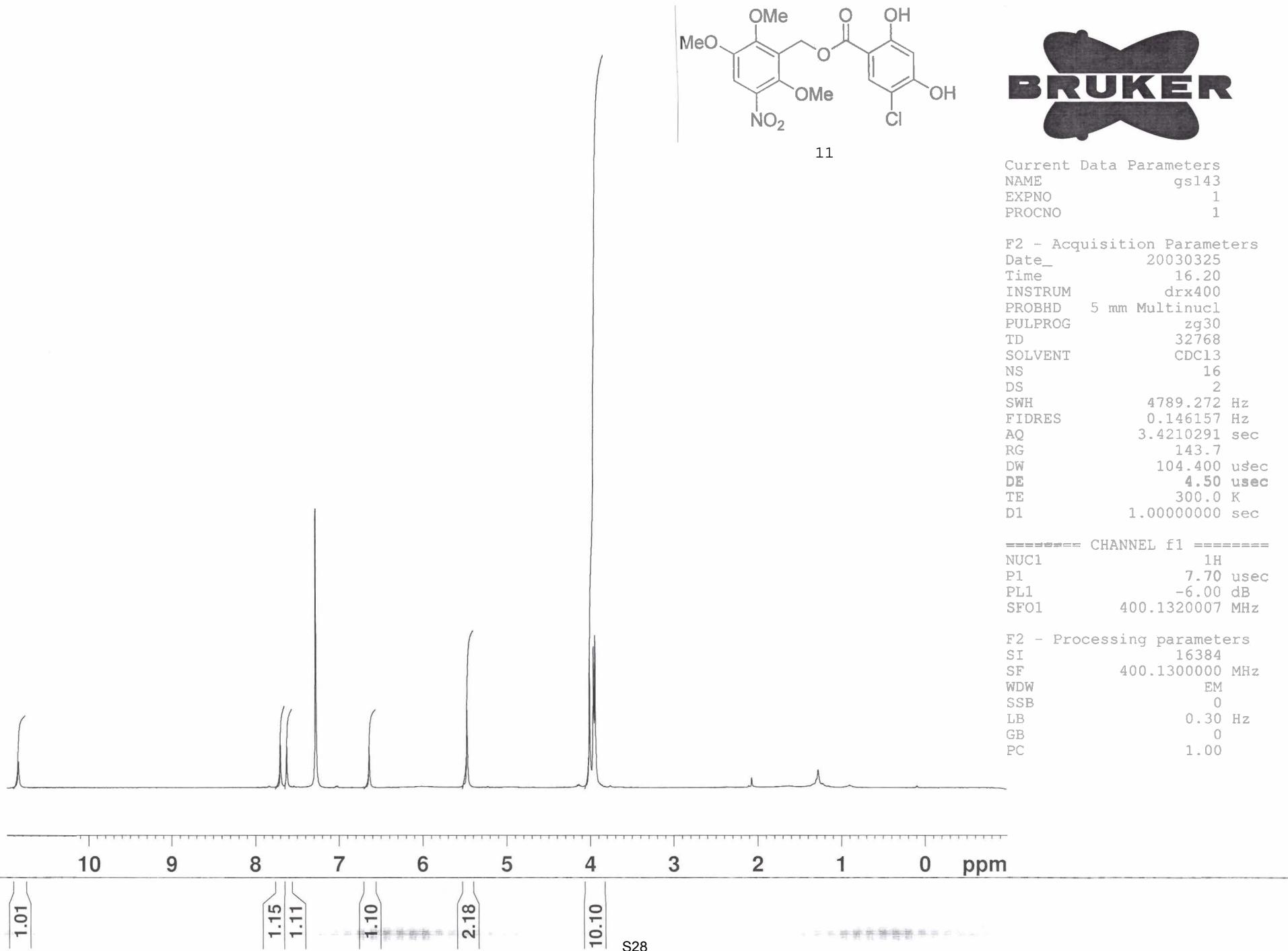
F2 - Acquisition Parameters
 Date_ 20030607
 Time 5.53
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 1290.2
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

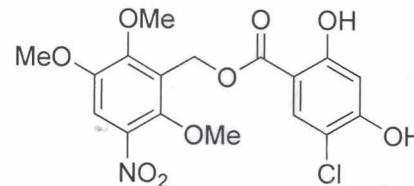
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40







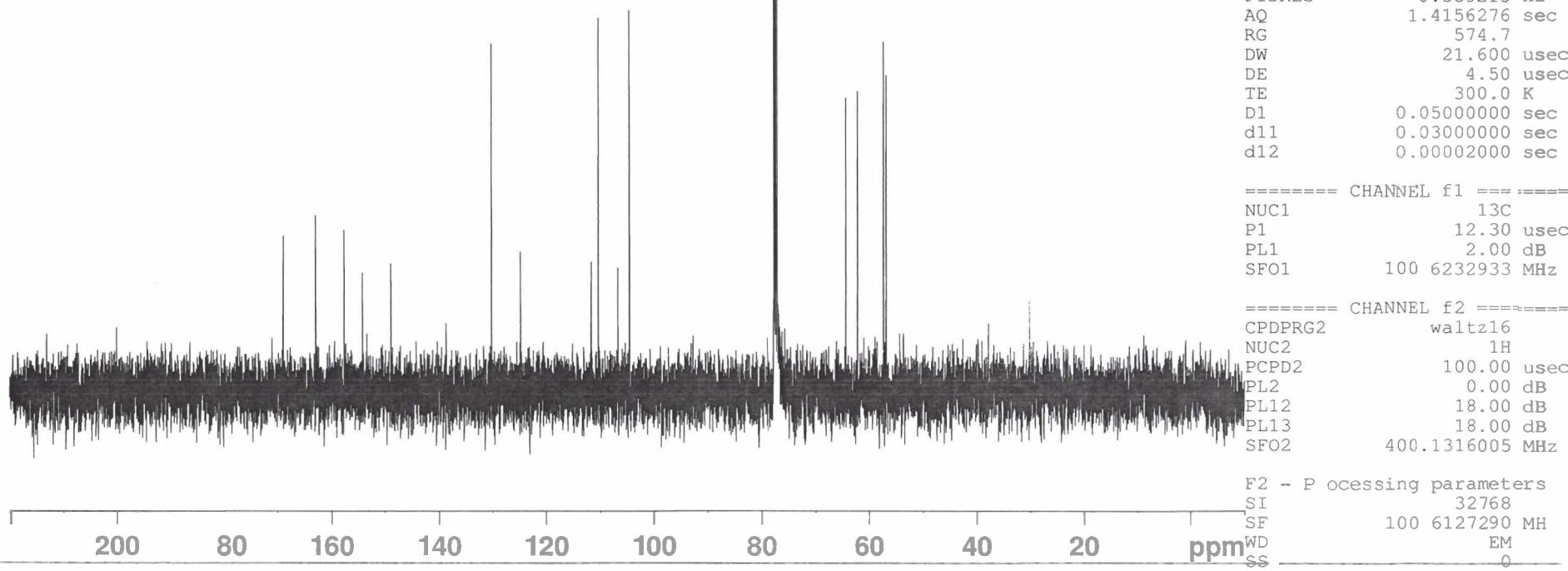
Current Data Parameters
 NAME gs159
 EXPNO 1
 PROCNO 1

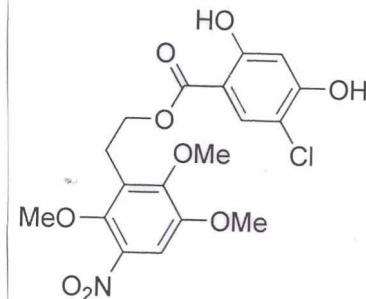
F2 - Acquisition Parameters
 Date_ 20030517
 Time 21.59
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zpg30
 TD 65536
 SOLVENT CDC13
 NS 781
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 574.7
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100 6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100 6127290 MHz
 WD EM
 SS 0
 LB 1.00 Hz
 GB 0
 PC 1.40



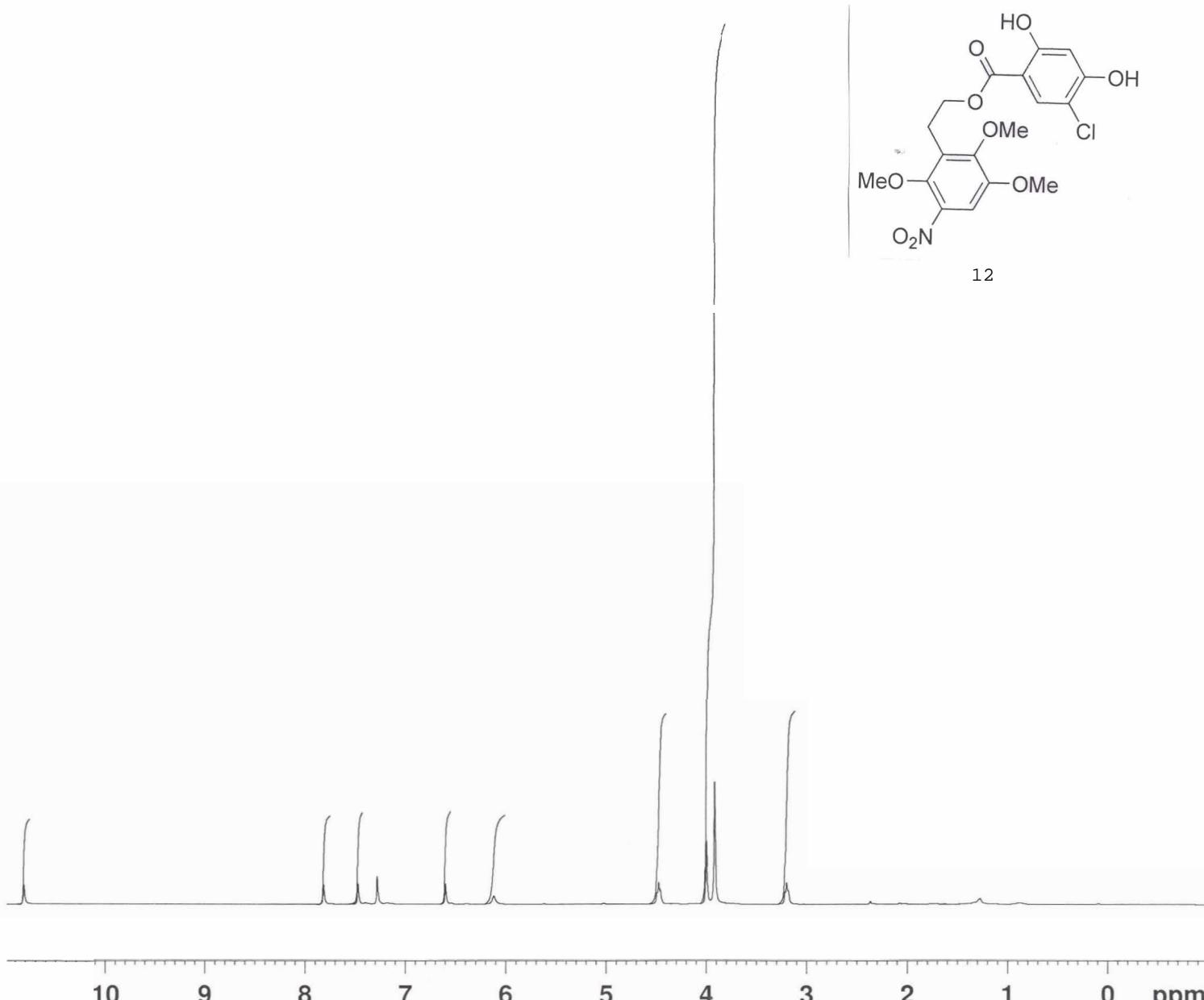


Current Data Parameters
NAME gs148
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030326
Time 19.44
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 90.5
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



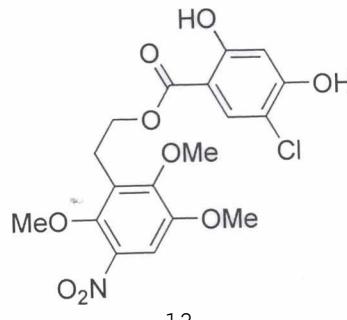
0.97

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

1.01 1.05 1.07 1.02

2.18 10.05 2.20

S30



Current Data Parameters
 NAME gs149
 EXPNO 1
 PROCNO 1

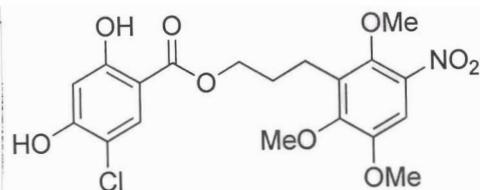
F2 - Acquisition Parameters
 Date_ 20030326
 Time 19.48
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 564
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 812.7
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 ======
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

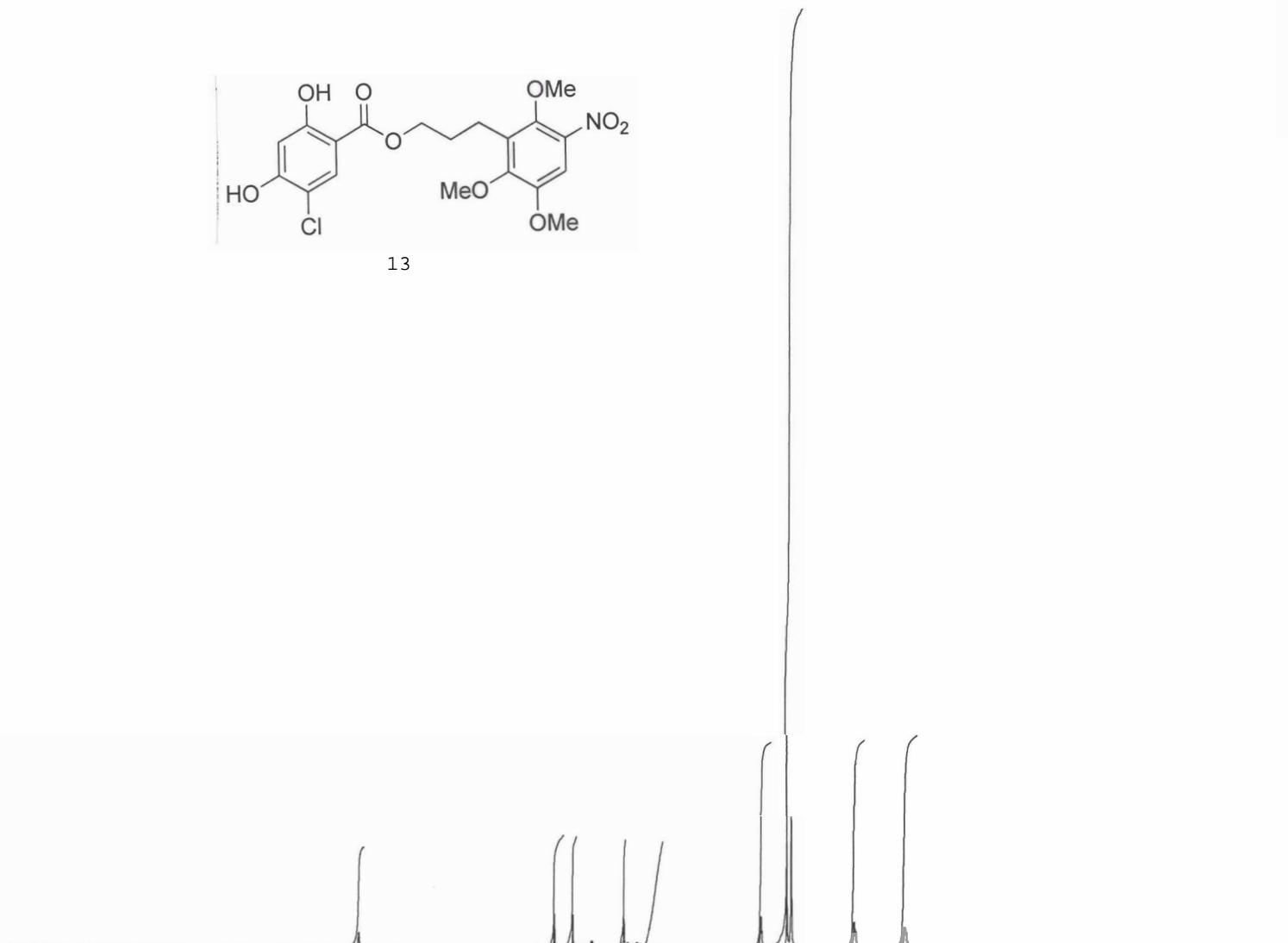
===== CHANNEL f2 ======
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





13



16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

4.76 5.37
5.30 5.15
5.07 9.78
9.86
10.07

S32

Current Data Parameters
NAME gang11
EXPNO 1
PROQNO 1

F2 - Acquisition Parameters
Date_ 20060513
Time 16.03
INSTRUM drx400
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 -5.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



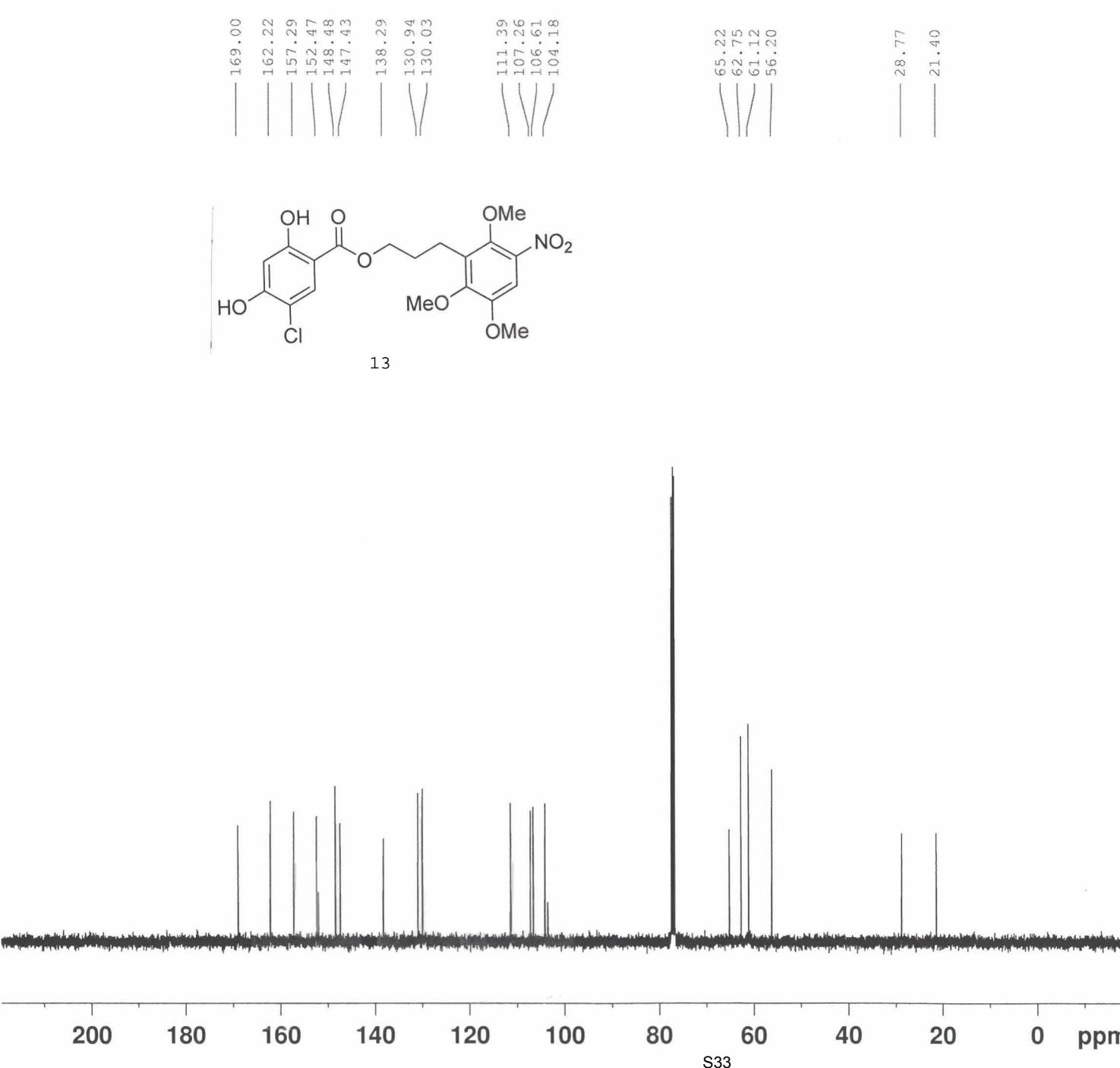
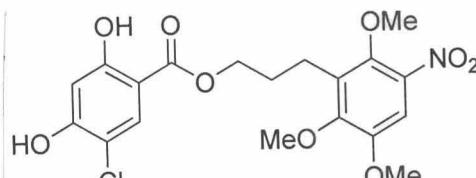
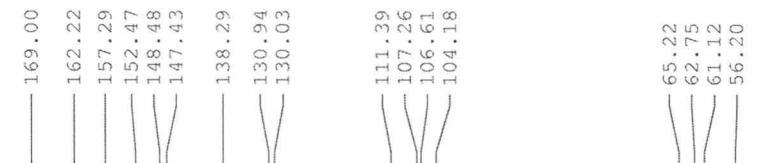
Current Data Parameters
 NAME gang11
 EXPNO 2
 PROCNO 1

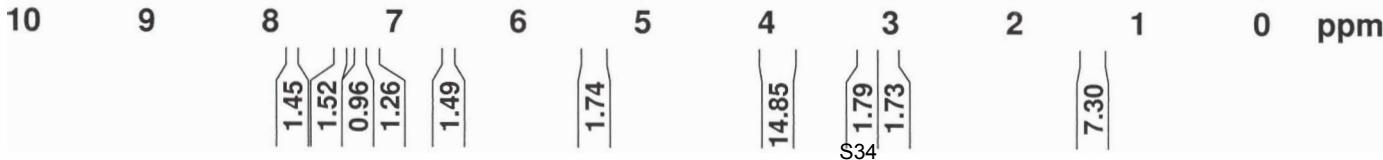
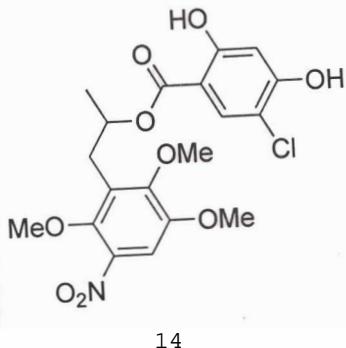
F2 - Acquisition Parameters
 Date_ 20060513
 Time 16.12
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 154
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.85 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPDRG 100.00 usec
 PL2 -5.00 dB
 PL12 14.58 dB
 PL13 120.00 dB
 SFO2 400.1316005 MHz

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



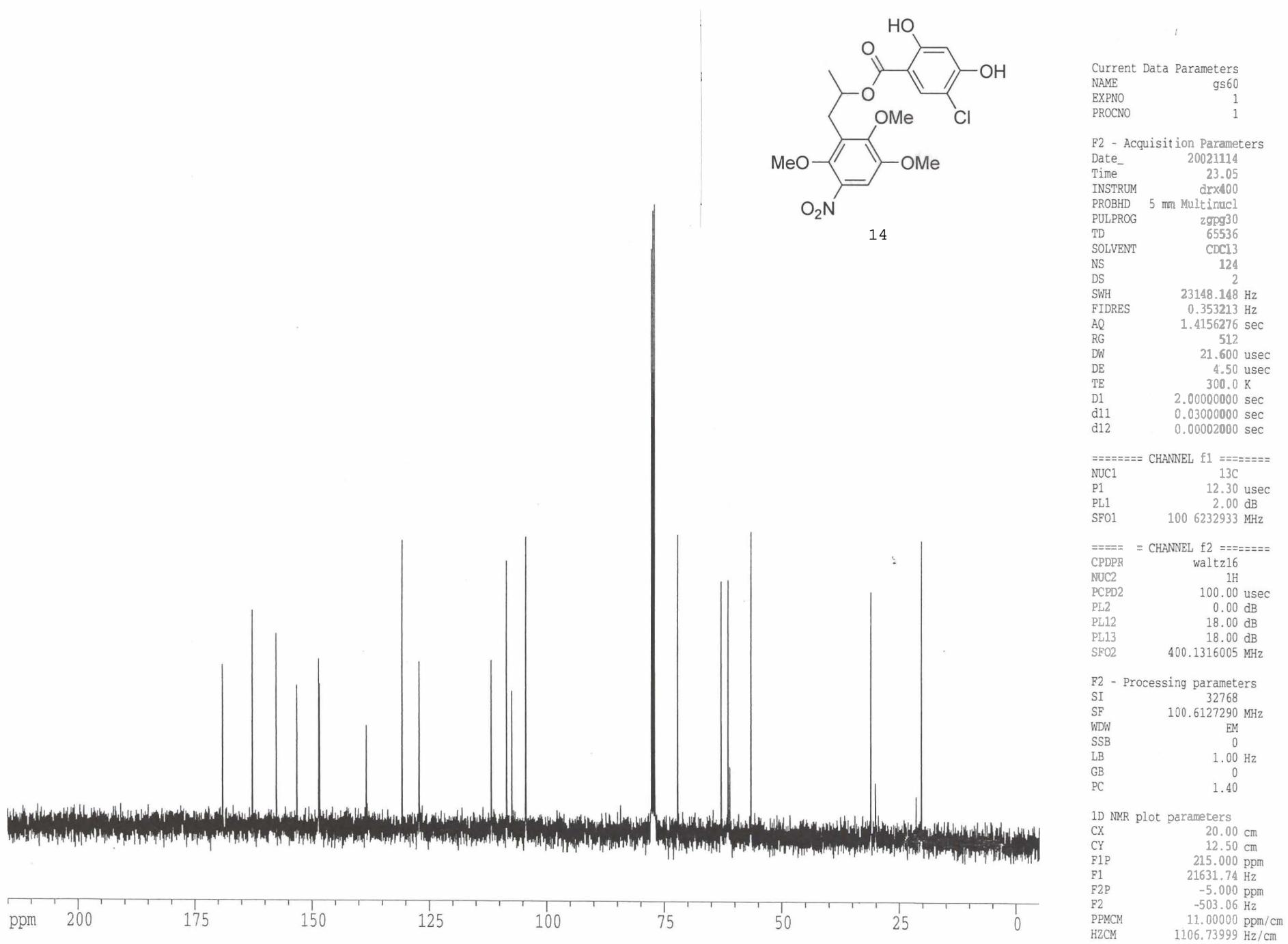


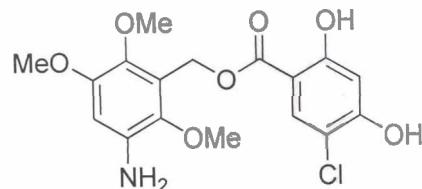
Current Data Parameters
NAME sg0015
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030614
Time 21.31
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 101.6
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



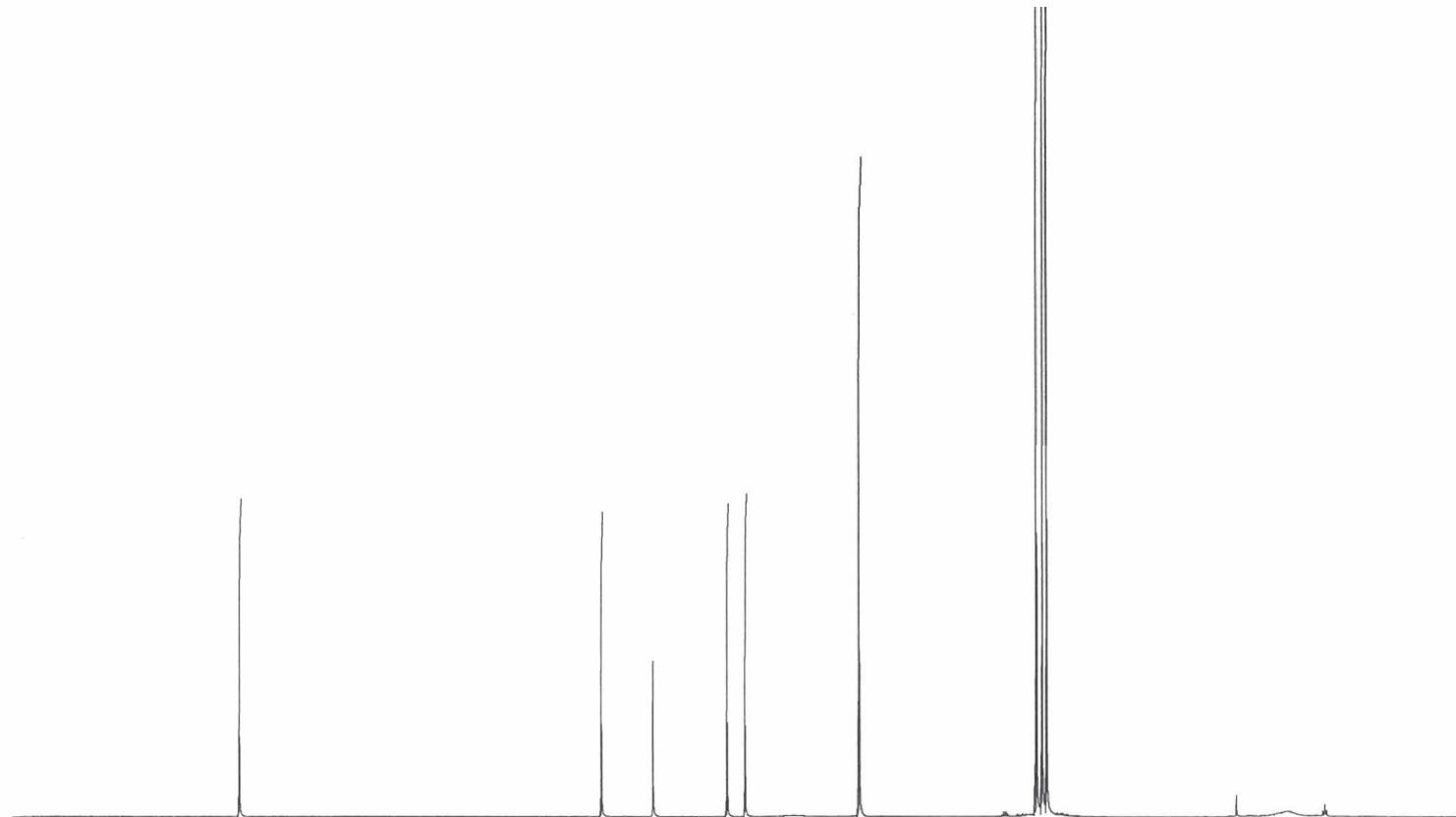


Current Data Parameters
 NAME sg205
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20031122
 Time 6.50
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 181
 DW 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SF01 400.1326008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



12 11 10 9 8 7 6 5 4 3 2 1 ppm

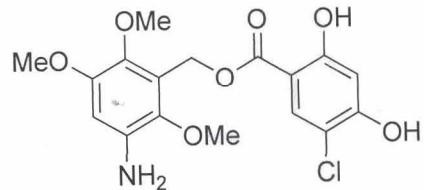
1.04

1.00

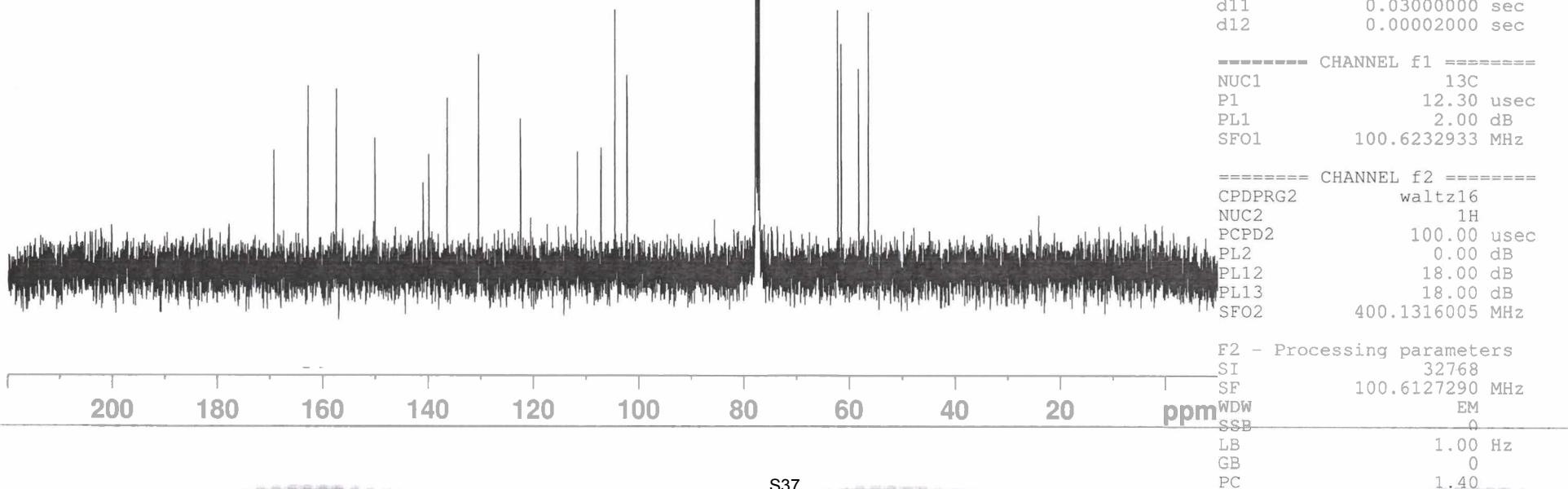
1.03
1.06

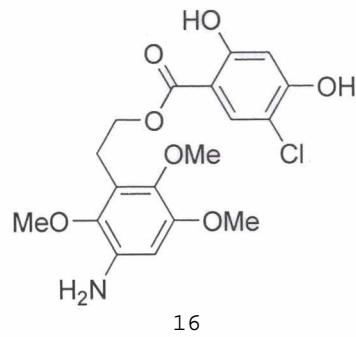
2.16

3.39
3.50
3.42



15



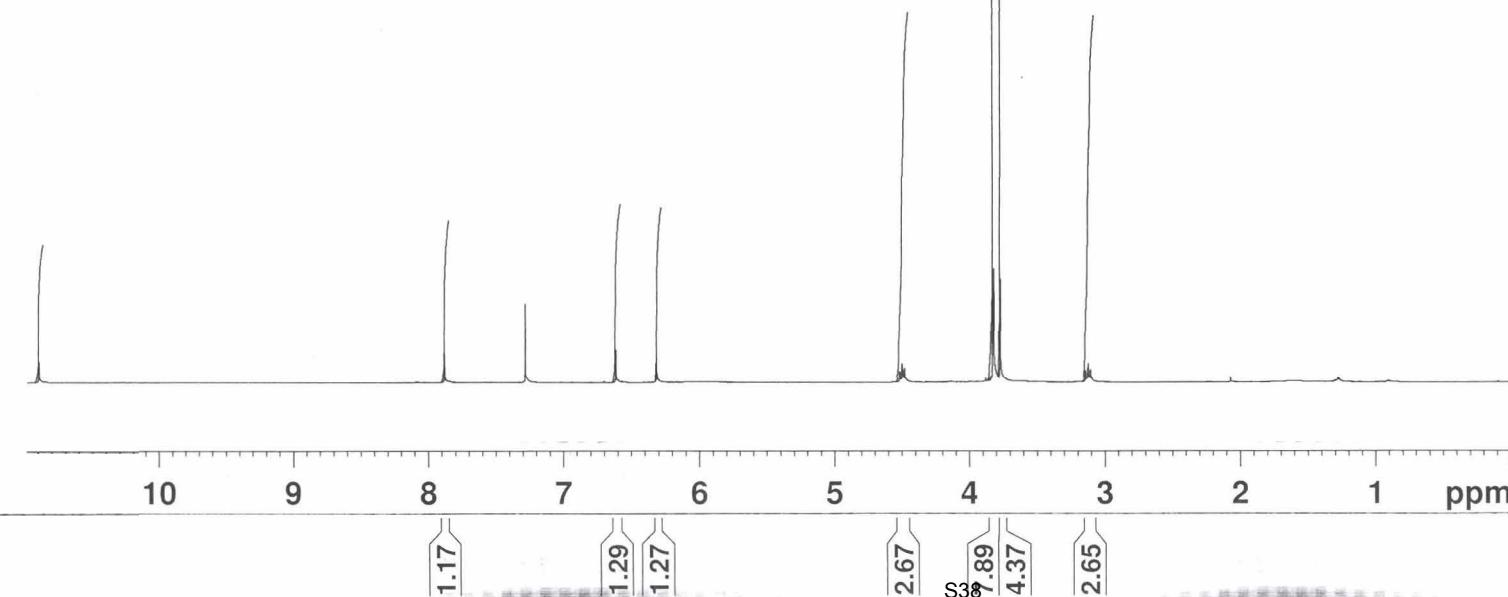


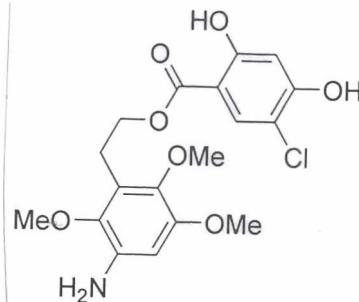
Current Data Parameters
 NAME sg241
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20031211
 Time 5.27
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 228.1
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

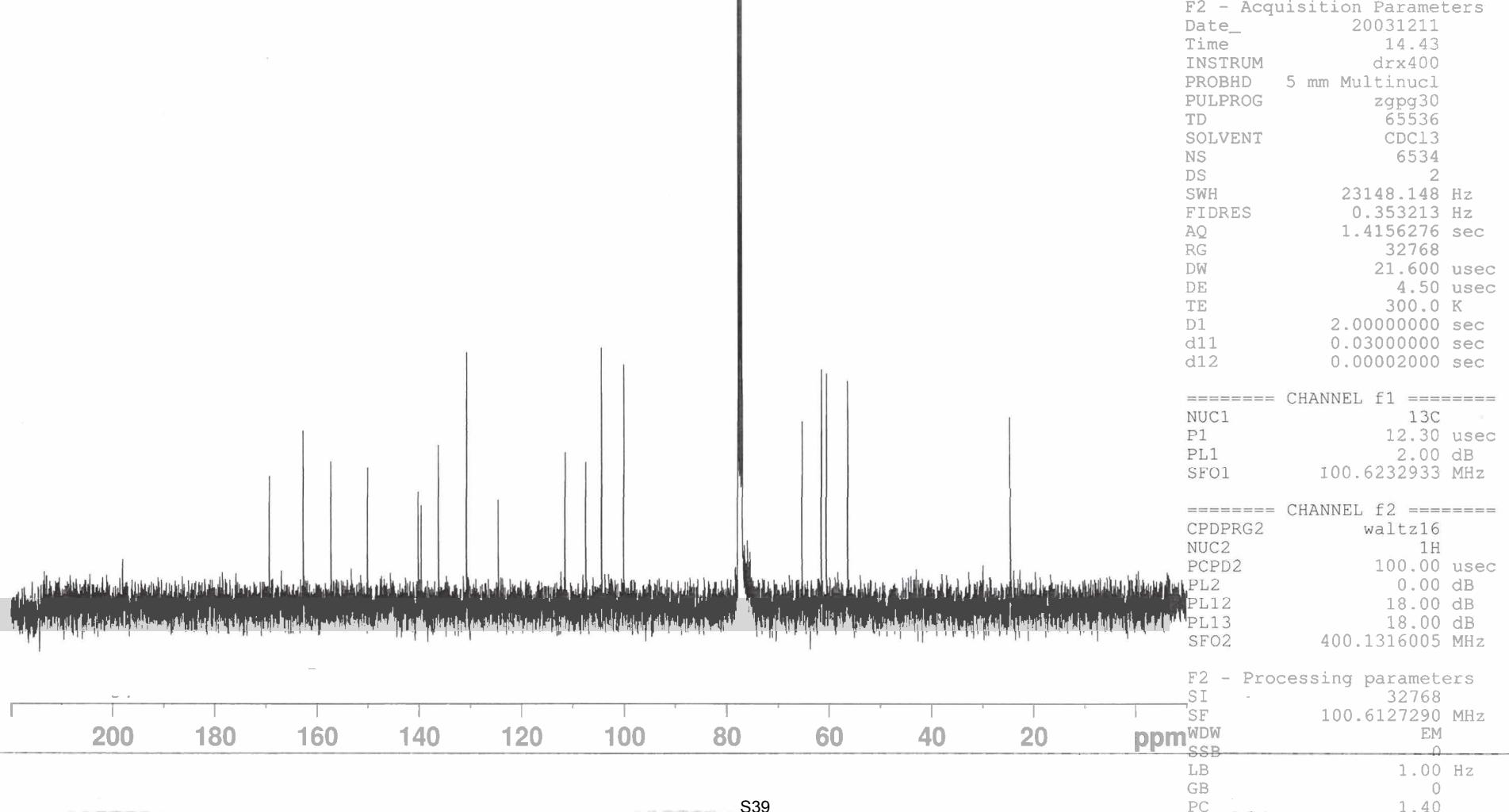
===== CHANNEL f1 =====
 NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SFO1 400.1320007 MHz

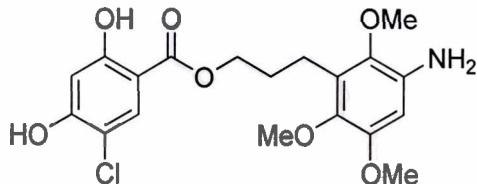
F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



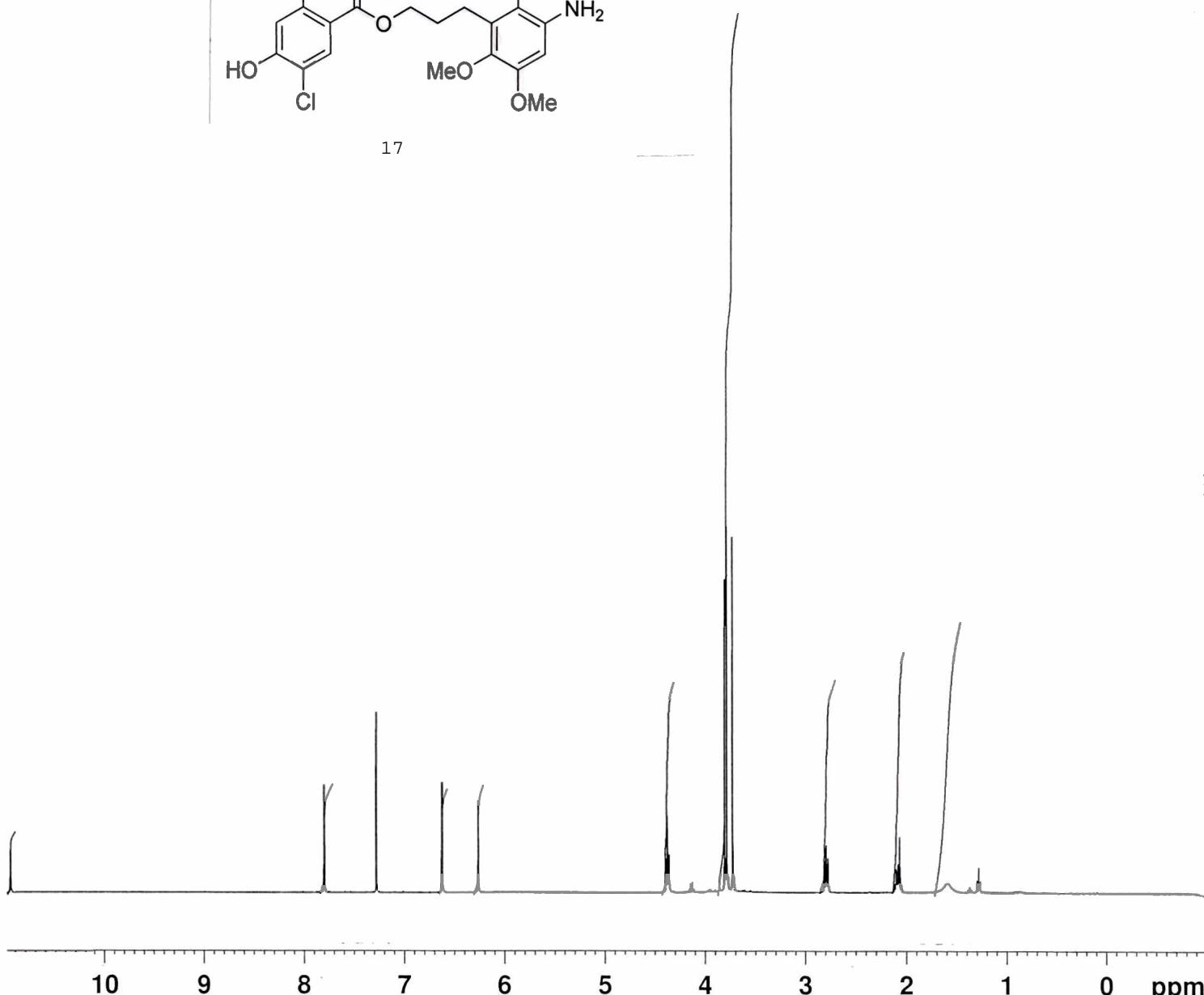


16





17



Current Data Parameters

NAME gs177
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030531
Time 5.00
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 256
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

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

NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters

SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

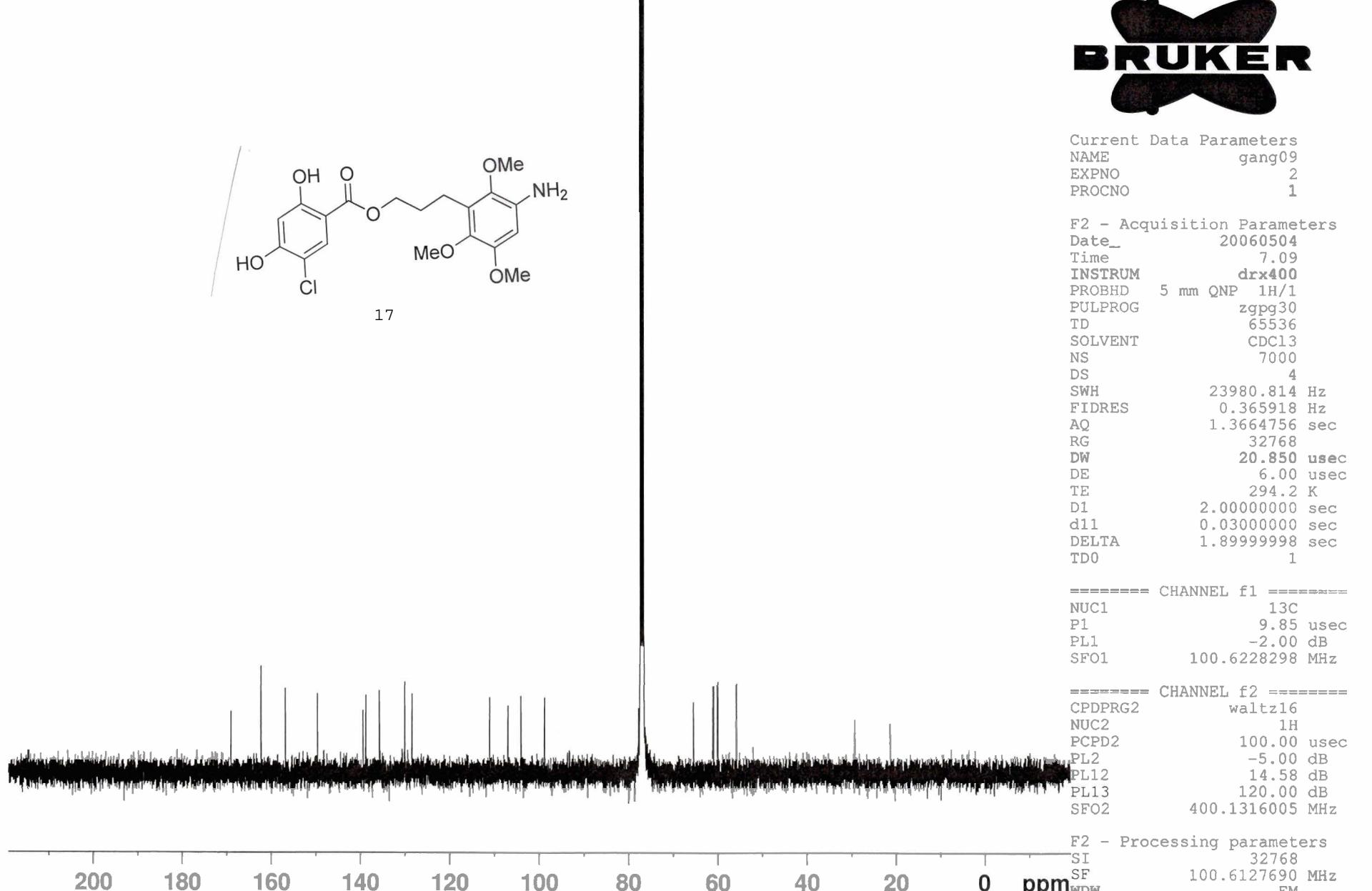
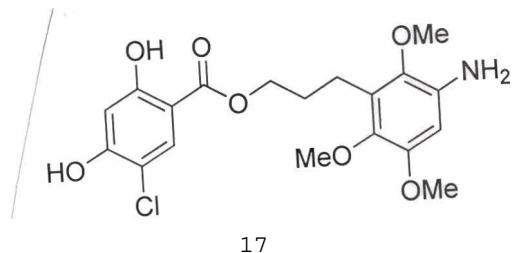
Current Data Parameters
 NAME gang09
 EXPNO 2
 PROCNO 1

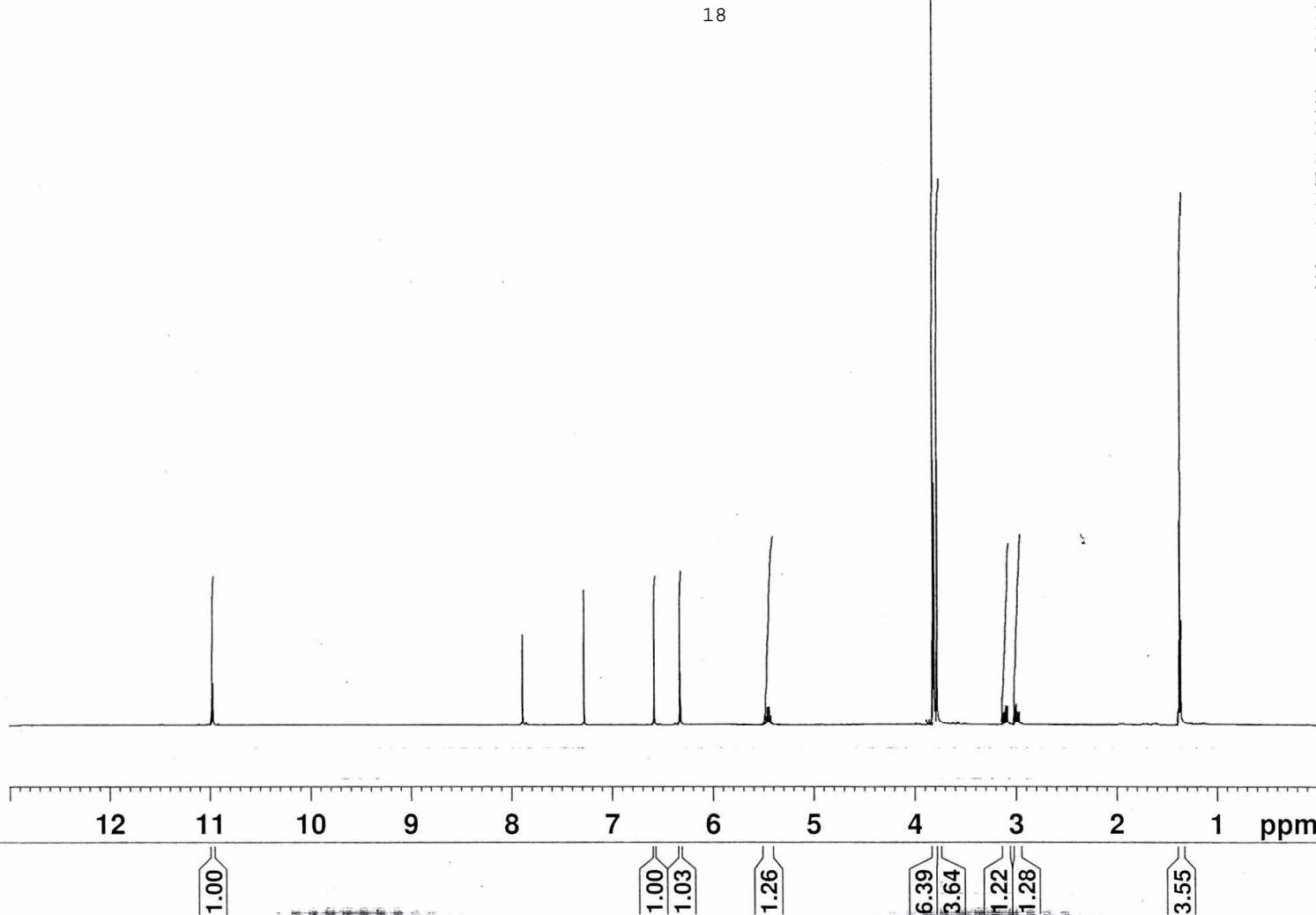
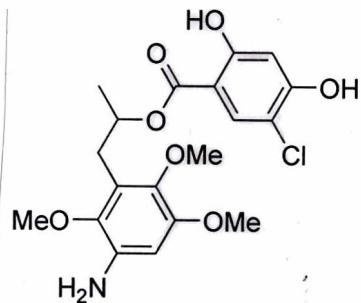
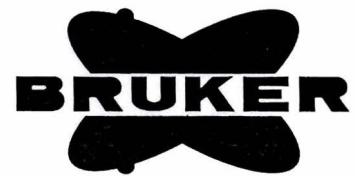
F2 - Acquisition Parameters
 Date_ 20060504
 Time 7.09
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/1
 PULPROG zpgpg30
 TD 65536
 SOLVENT CDCl3
 NS 7000
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.85 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -5.00 dB
 PL12 14.58 dB
 PL13 120.00 dB
 SFO2 400.1316005 MHz

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



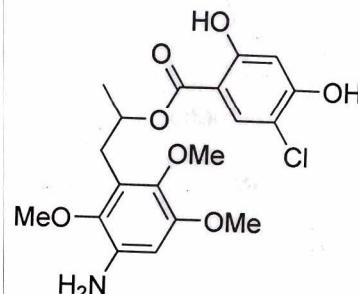


Current Data Parameters
NAME sg206
EXPNO 2
PROCNO 1

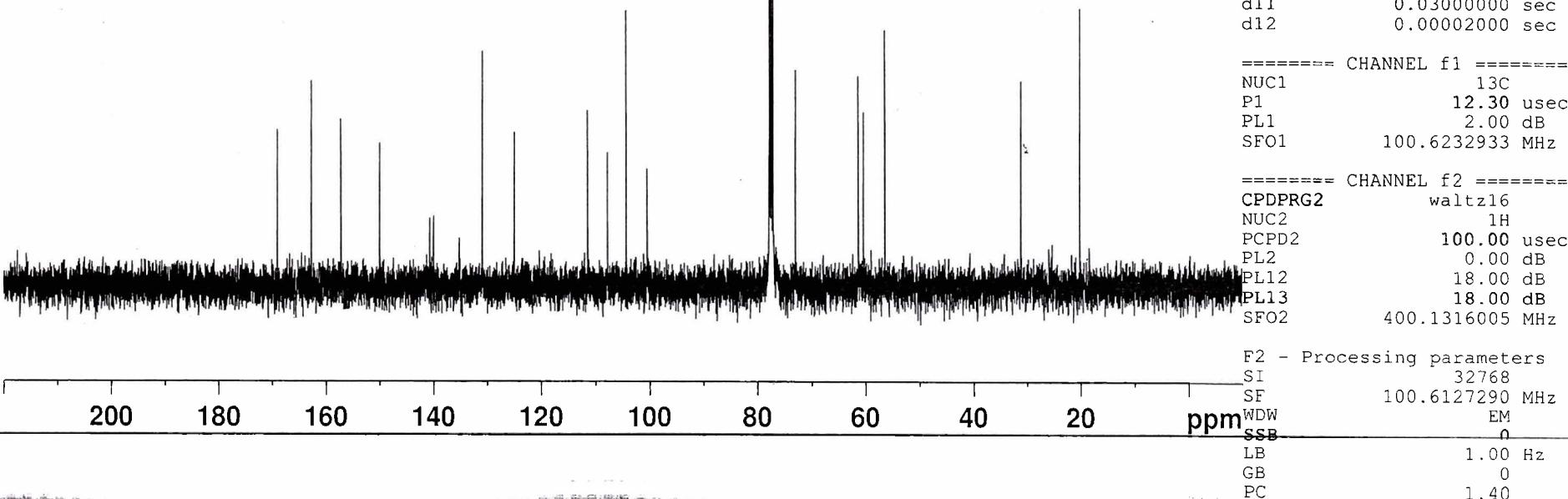
F2 - Acquisition Parameters
Date_ 20031124
Time 6.41
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS Z
SWH 5208.333 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 161.3
DW 96.000 usec
DE 4.50 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1326008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



18



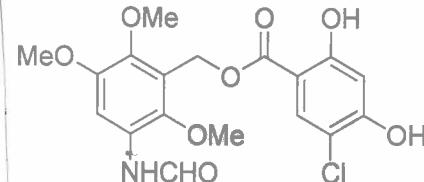
Current Data Parameters
 NAME sg207
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20031124
 Time 6.45
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCL3
 NS 857
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 2580.3
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 ======
 NUC1 ¹³C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 ======
 CPDPRG2 waltz16
 NUC2 ^{1H}
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

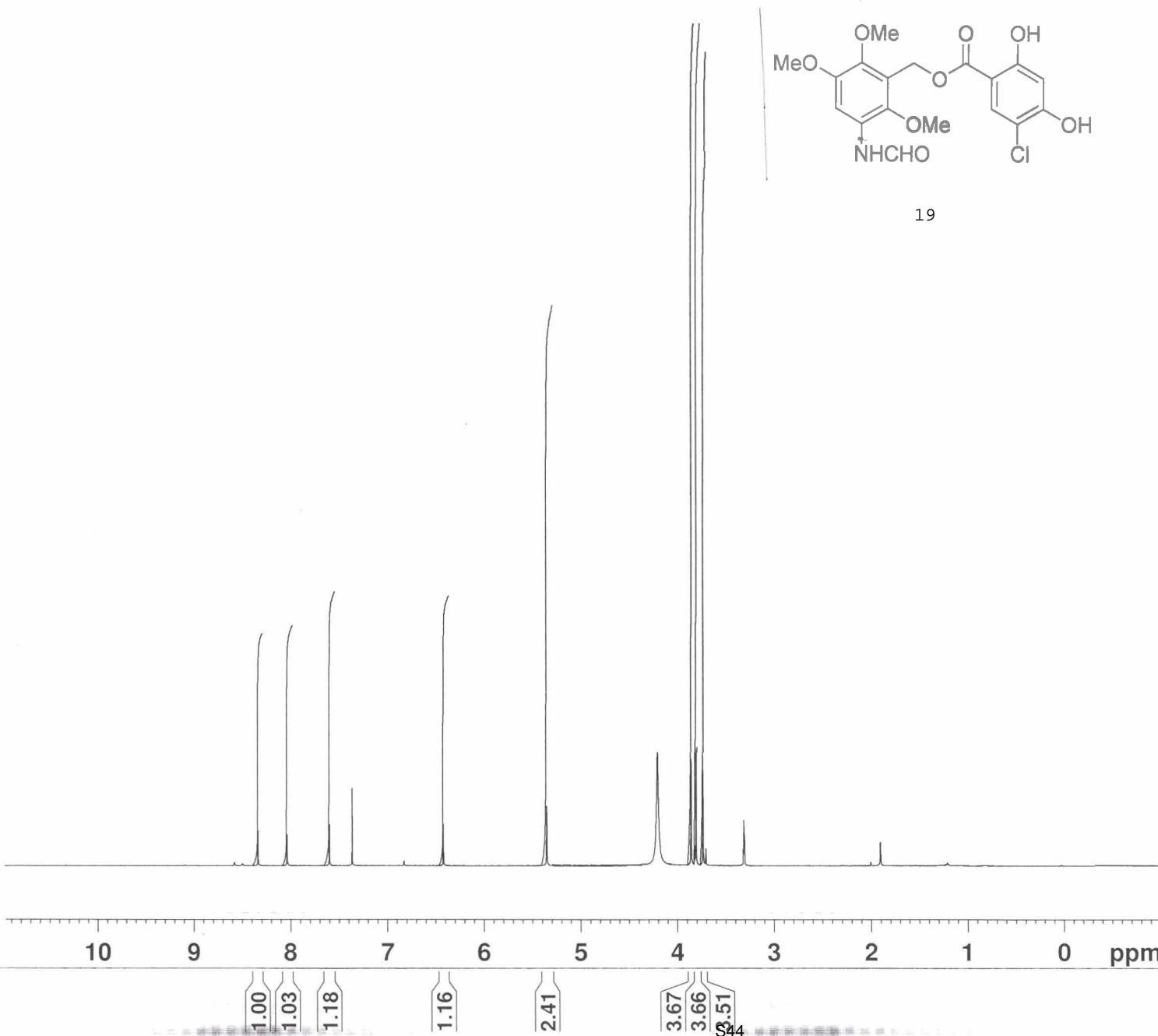


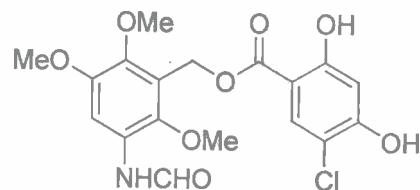
Current Data Parameters
 NAME methoxy
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060321
 Time 5.03
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT MeOH
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 406.4
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

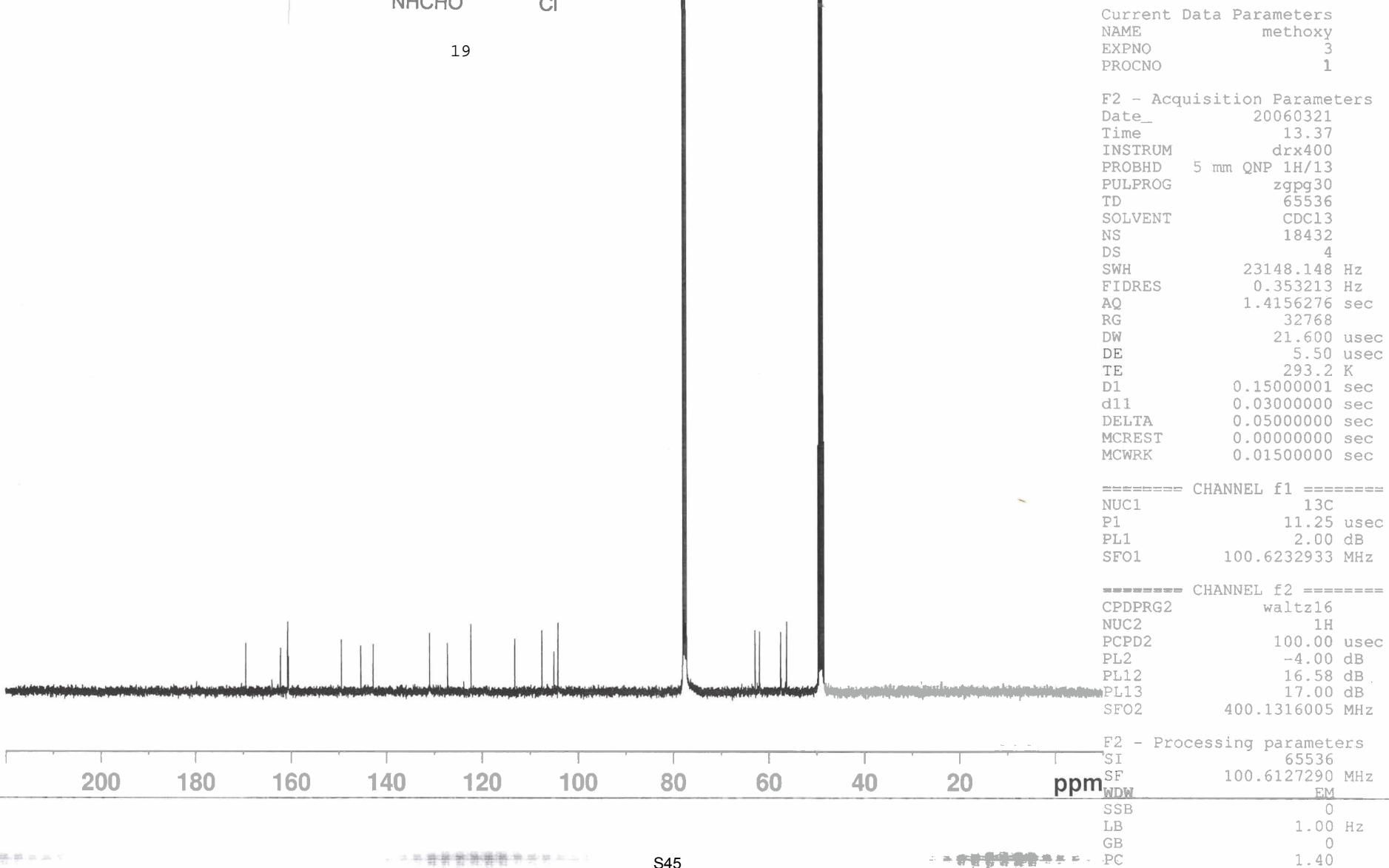
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

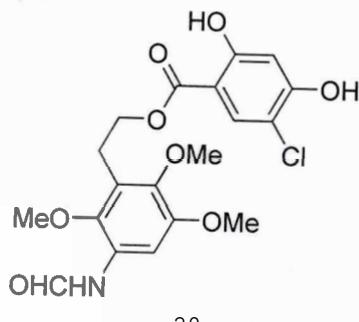
F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



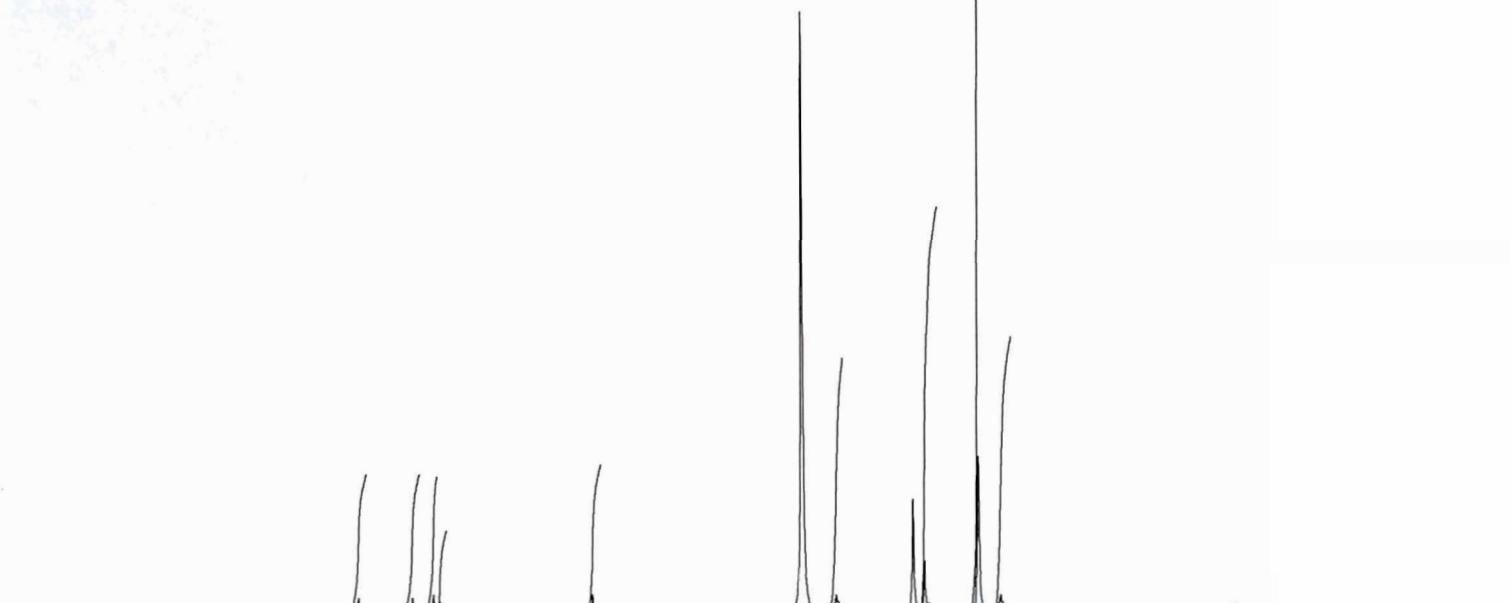


19





20



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

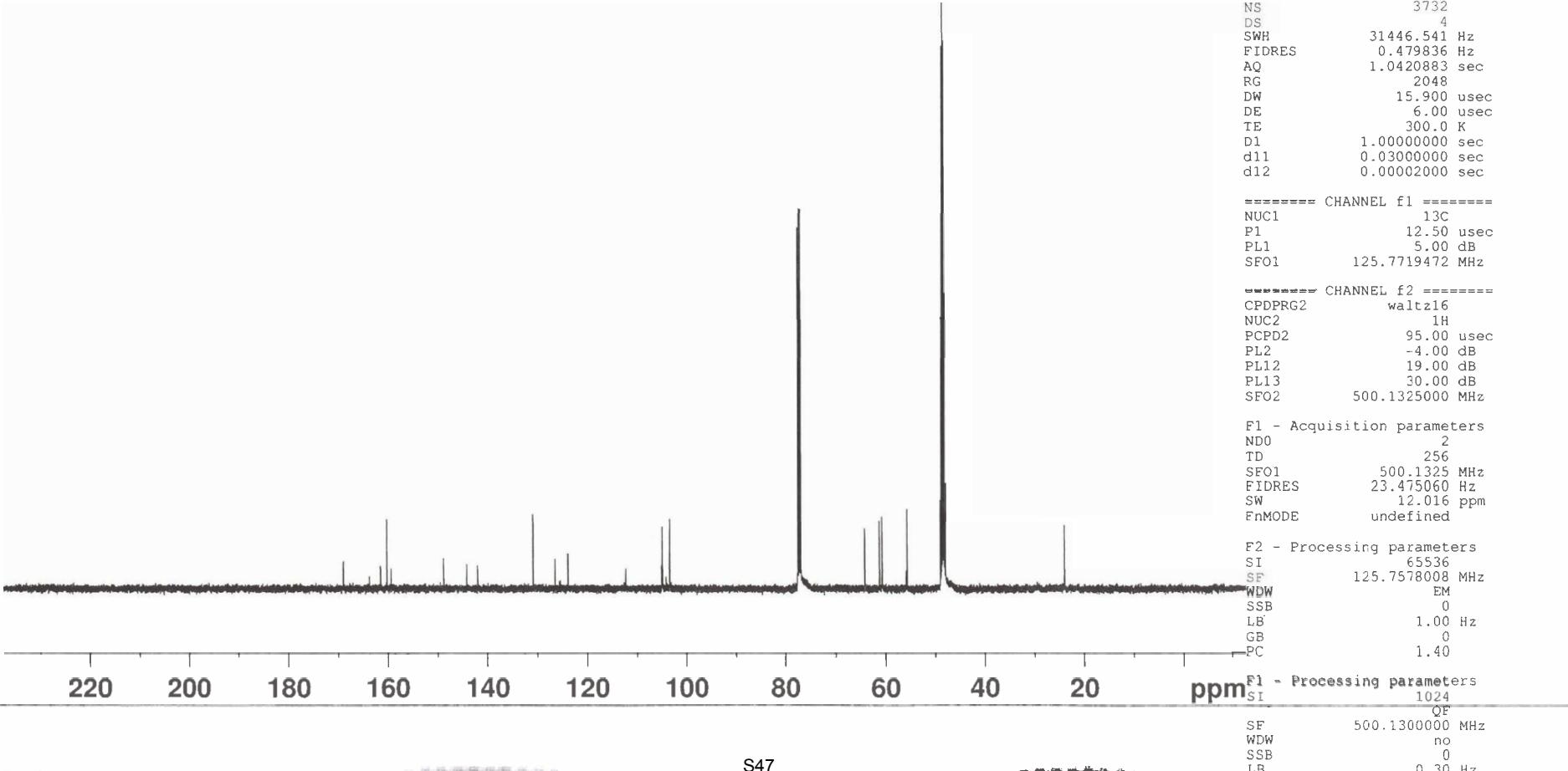
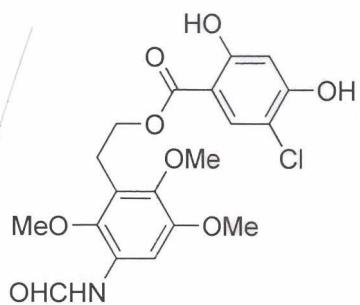
1.00
1.01
0.99
0.61
1.08
1.83
2.90
2.67
1.98
1.96

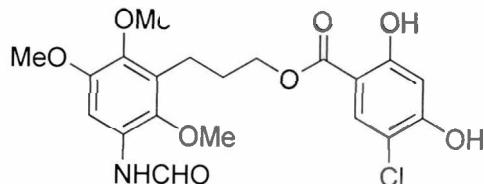
Current Data Parameters
NAME sg0037
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030629
Time 4.26
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT MeOH
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 181
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

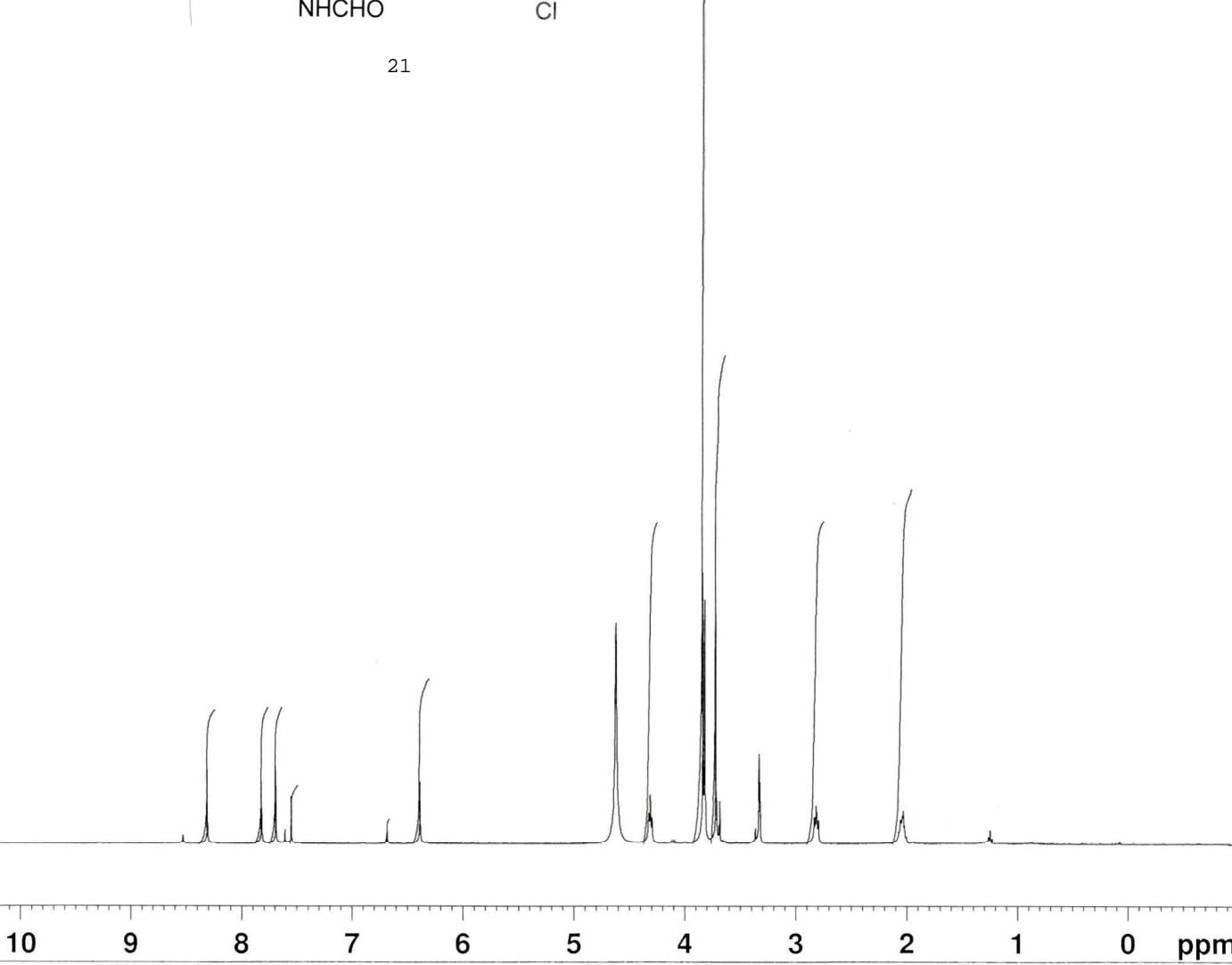
===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





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Current Data Parameters
NAME sg0045
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030702
Time 15.59
INSTRUM drx400
PROBHD 5 mm Multincl
PULPROG zg30
TD 32768
SOLVENT MeOH
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 181
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

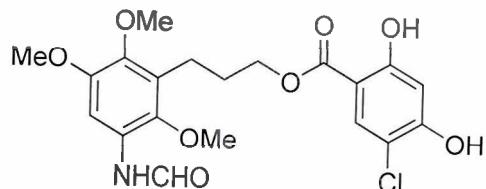
===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

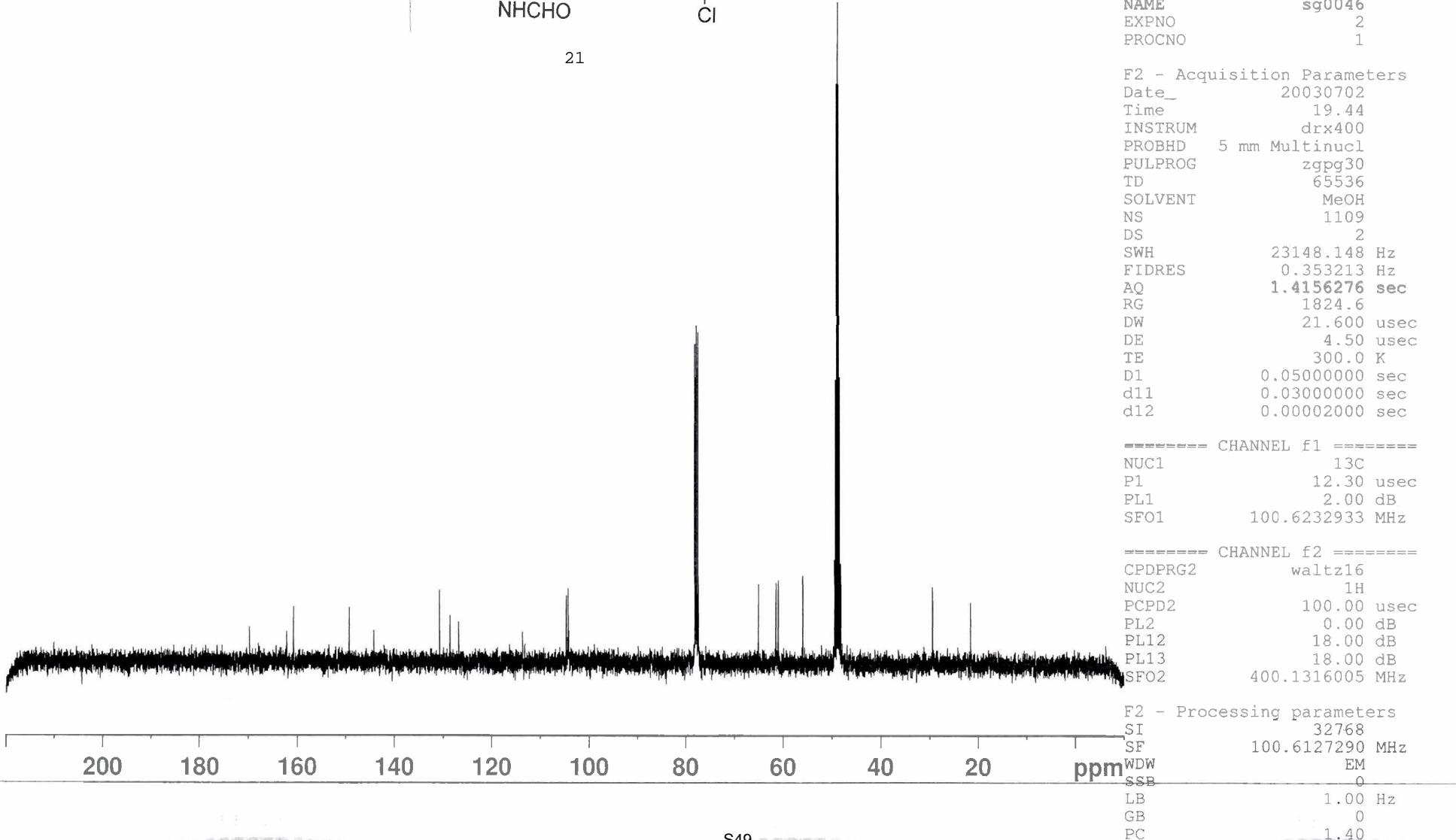
10 9 8 7 6 5 4 3 2 1 0 ppm

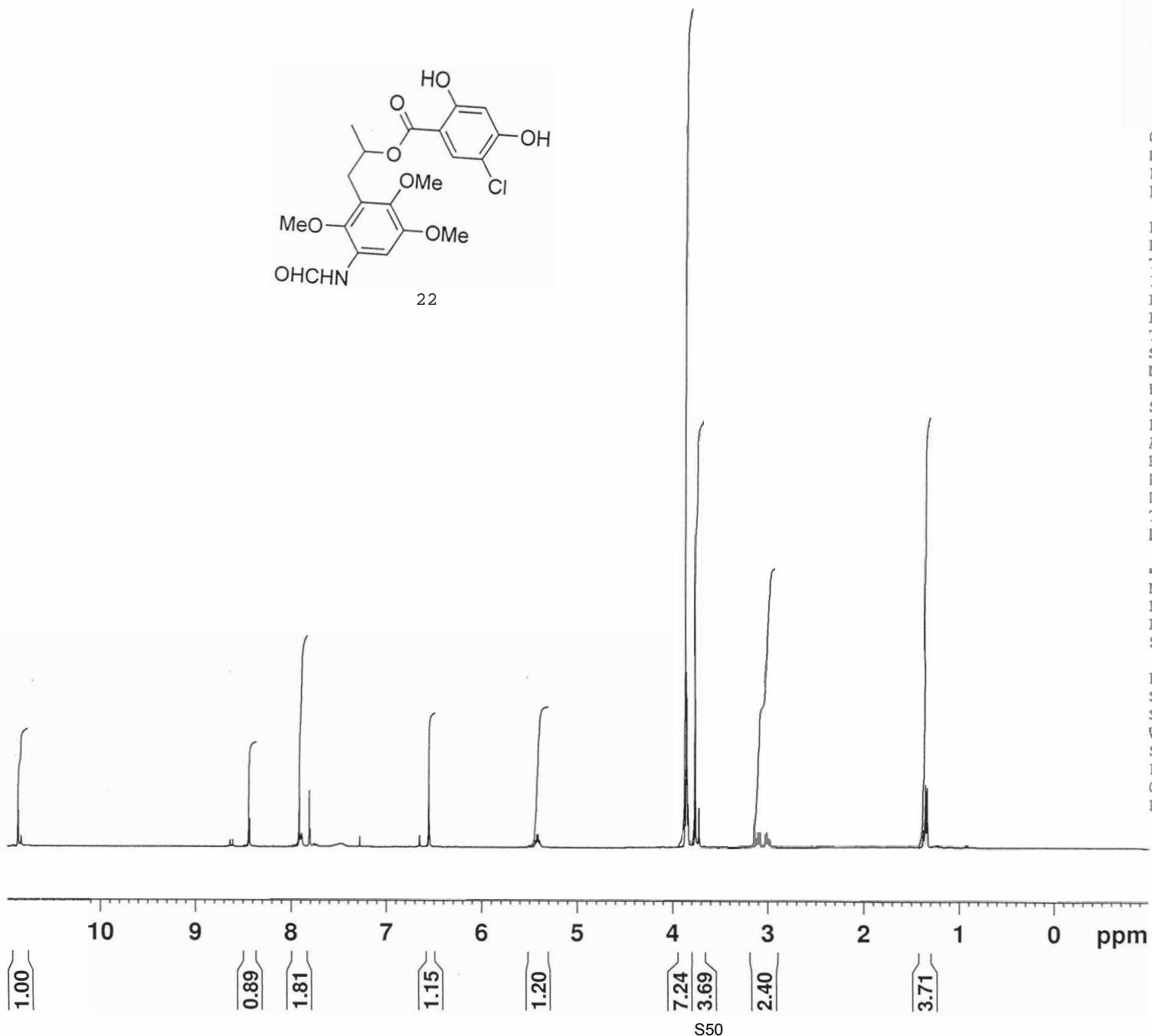
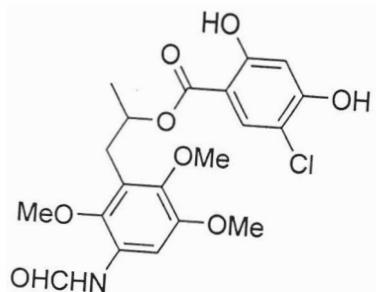
1.03
1.05
1.05
0.46
0.20
1.27

2.48
7.47
3.76
2.48
2.73



21





Current Data Parameters

NAME	sg-112
EXPNO	2
PROCNO	1

F2 - Acquisition Parameter

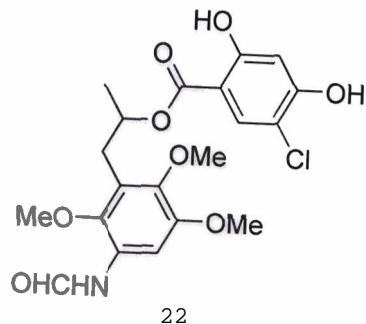
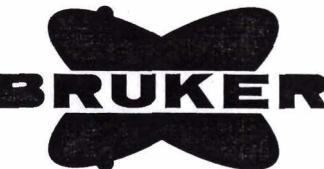
Date_	20030822
Time	6.28
INSTRUM	drx400
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	32
DS	2
SWH	4789.272 Hz
FIDRES	0.146157 Hz
AQ	3.4210291 se
RG	64
DW	104.400 us
DE	4.50 us
TE	300.0 K
D1	1.00000000 se

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

NUC1	1H
P1	7.70 us
PL1	-6.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	16384
SF	400.13000000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



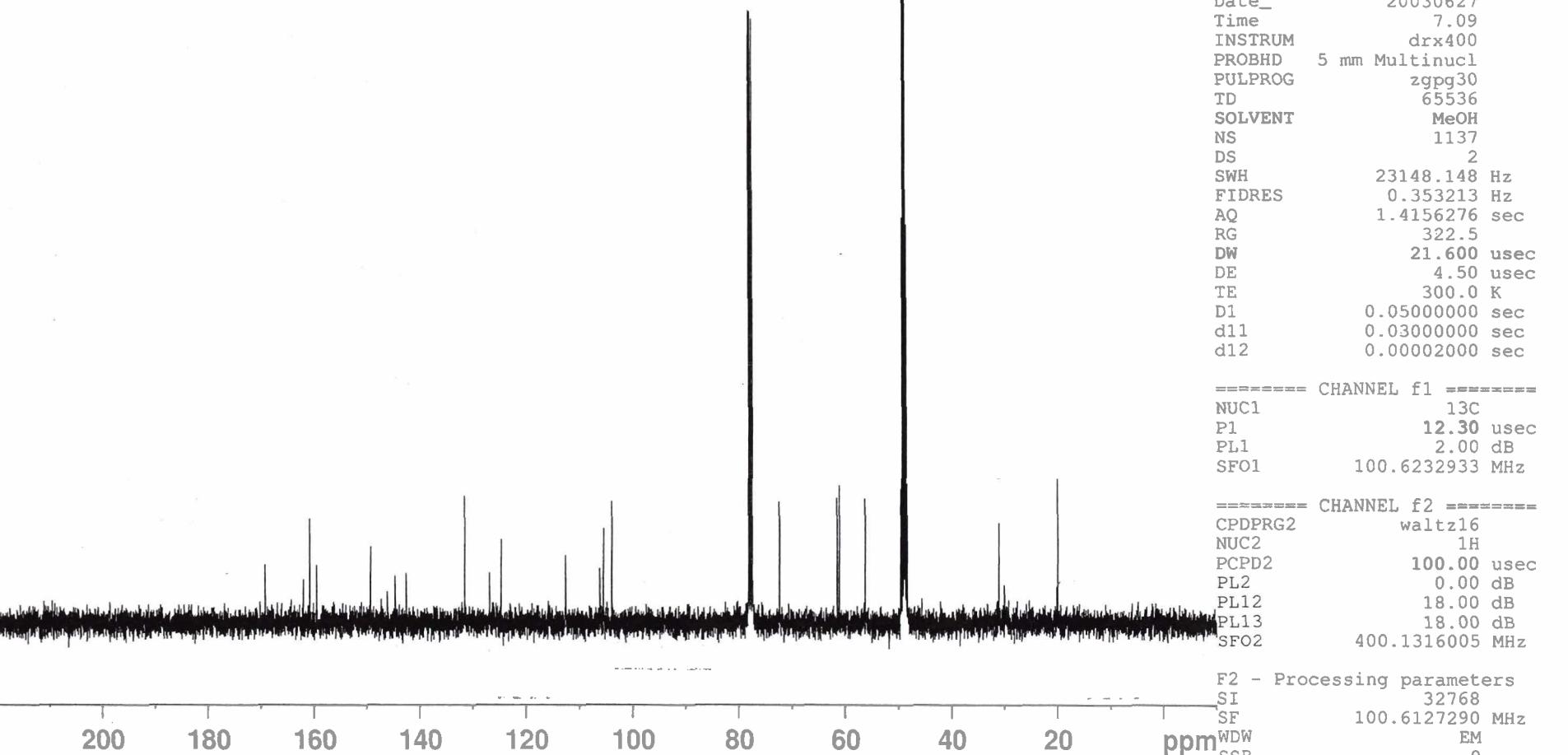
Current Data Parameters
NAME sg0035
EXPNO 2
PROCNO 1

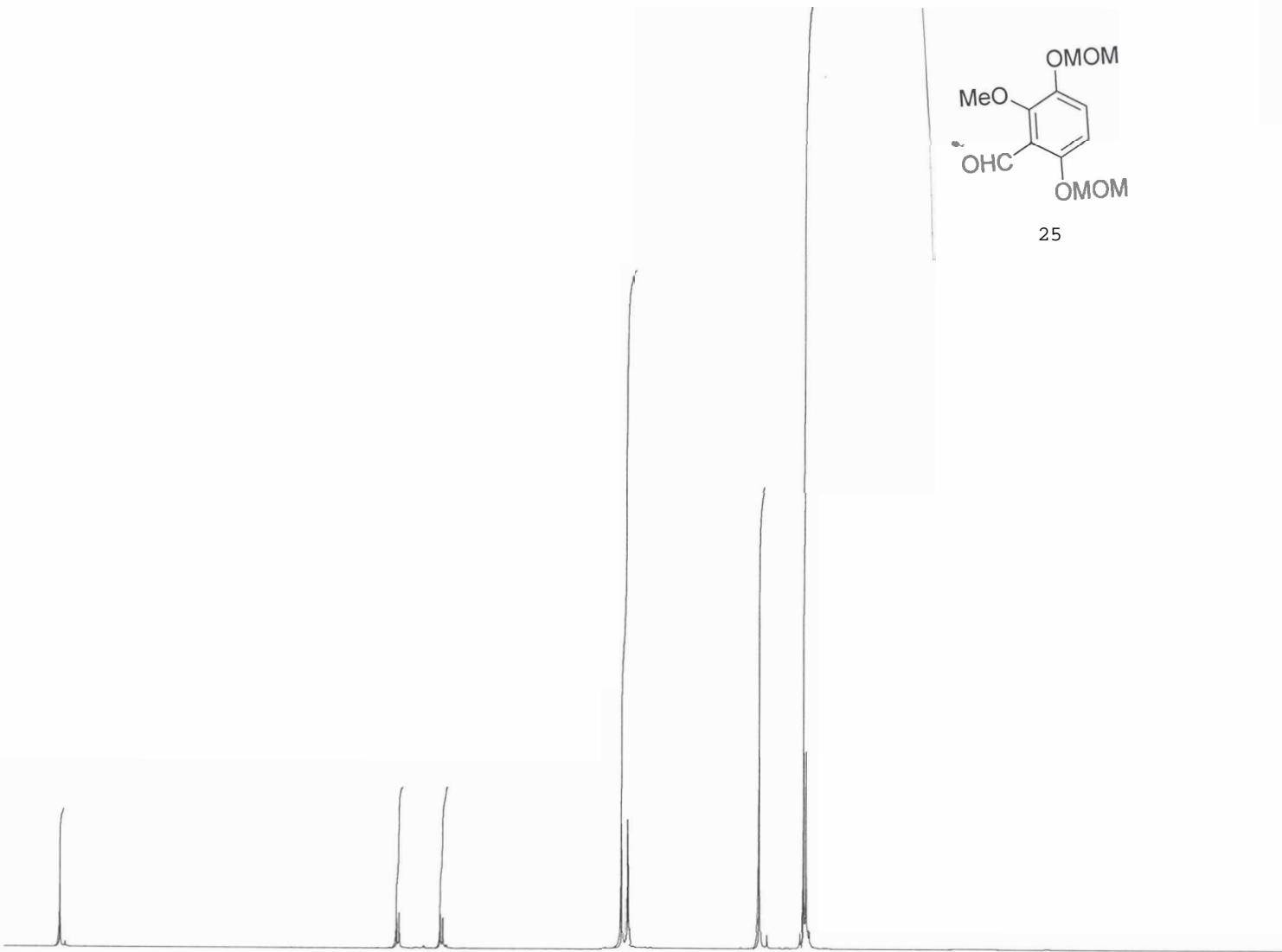
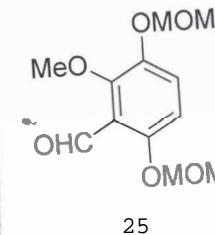
F2 - Acquisition Parameters
Date_ 20030627
Time 7.09
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT MeOH
NS 1137
DS 2
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 322.5
DW 21.600 usec
DE 4.50 usec
TE 300.0 K
D1 0.05000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.30 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME sg-128
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030922
Time 4.31
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 90.5
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SF01 400.1320007 MHz

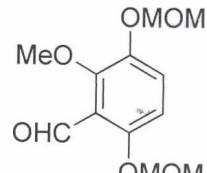
F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1 00

1.00

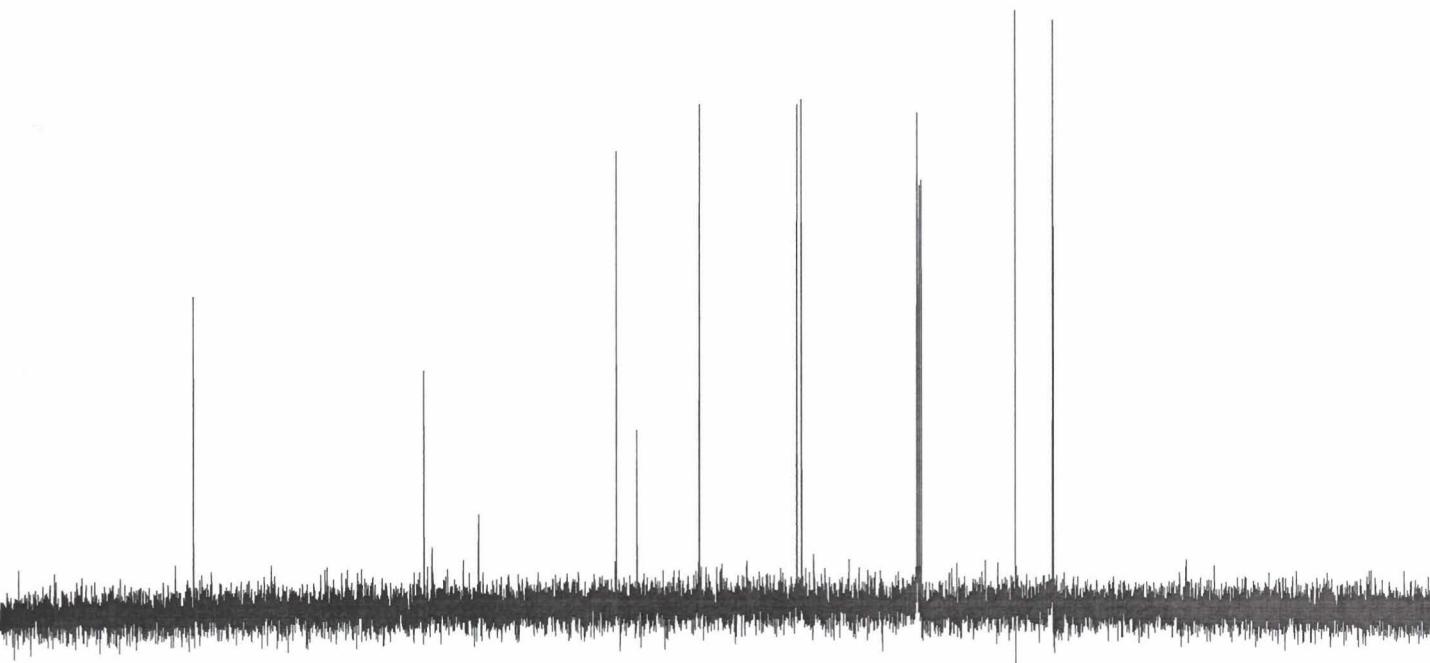
1.17
1.17

4.92

3.35
6.84



25



200

180

160

140

120

100

80

60

40

20

ppm

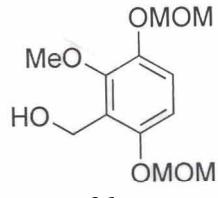
Current Data Parameters
 NAME sg-129
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030922
 Time 4.35
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 58
 DS 2
 SW 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 1290.2
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100 6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 16384
 SF 100.6127288 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME | sg-130
 EXPNO | 1
 PROCNO | 1

F2 - Acquisition Parameters
 Date_ 20031008
 Time 22.36
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SFO1 400.1320007 MHz

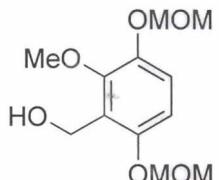
F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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

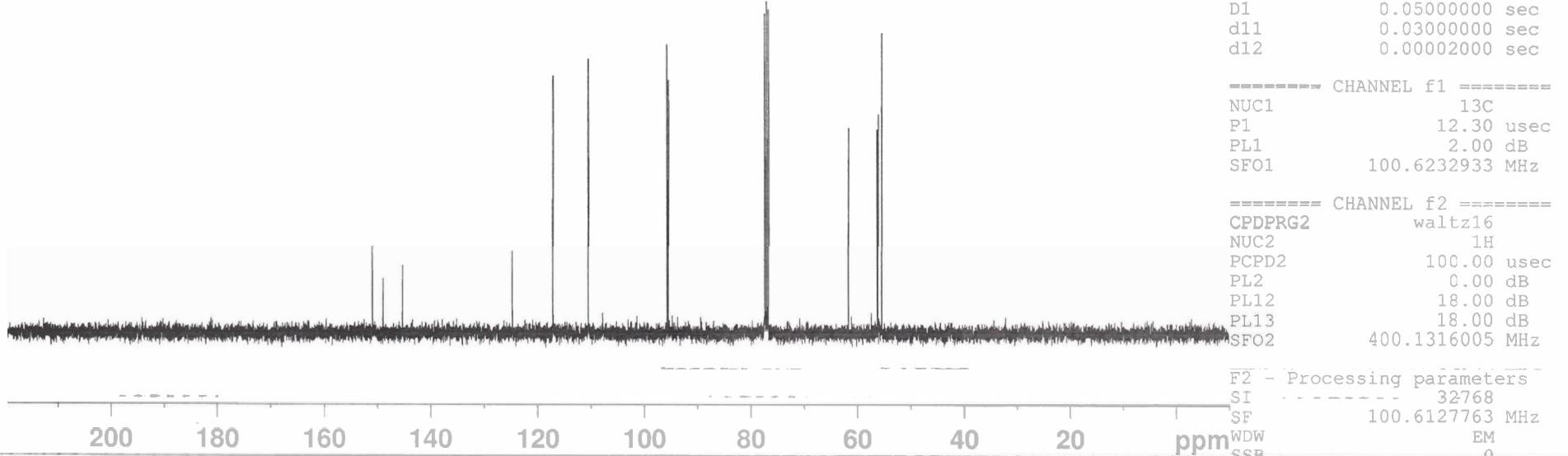
1.53
1.54

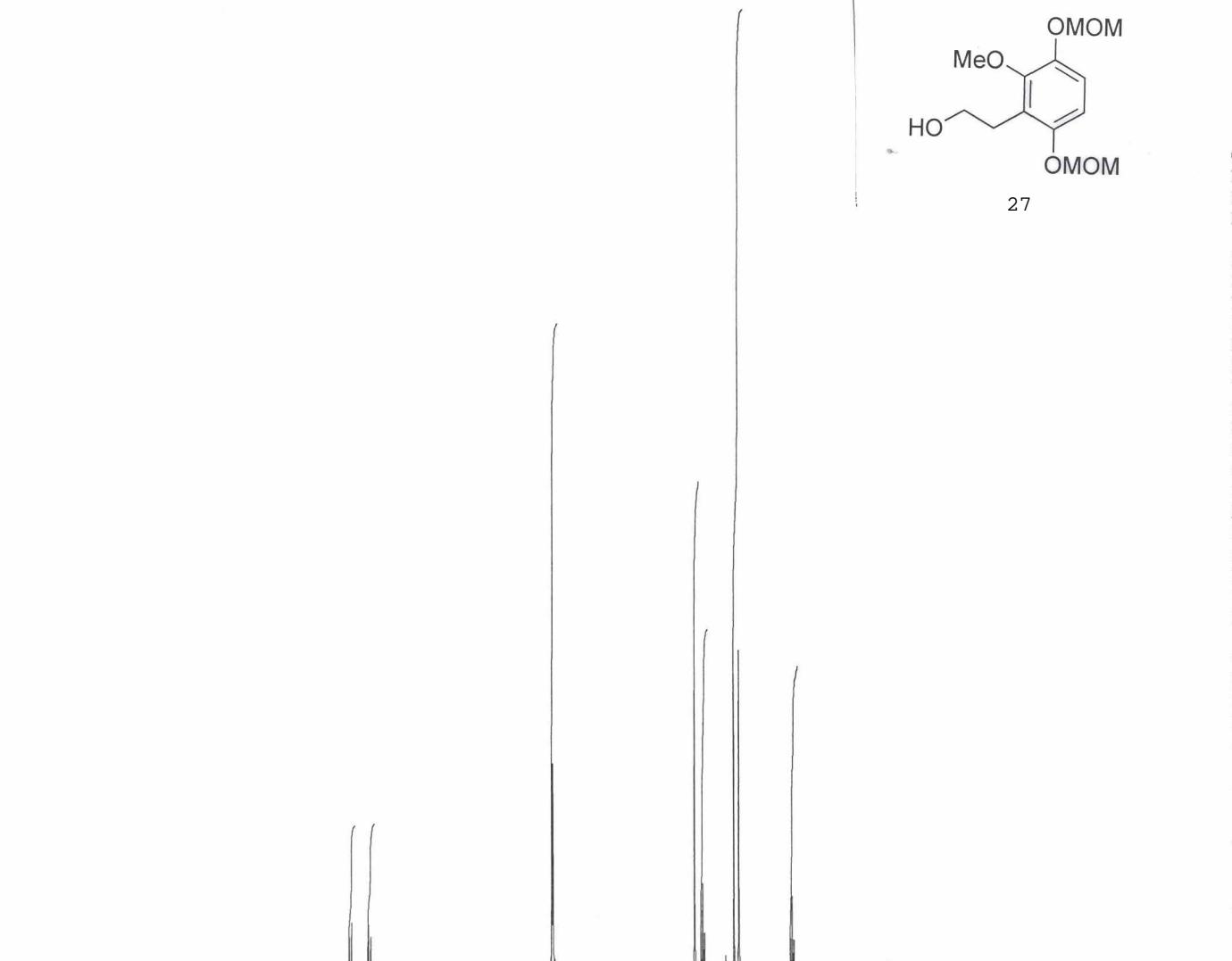
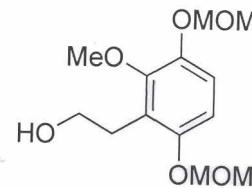
2.74
2.90
2.68

4.18
4.05
4.15



26





27

Current Data Parameters
NAME sg-132
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030923
Time 5.47
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 64
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

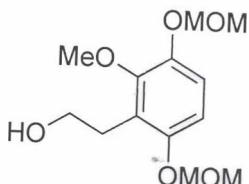
F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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

1.00
1.01

4.21

3.20
2.26
2.22
S56
2.02

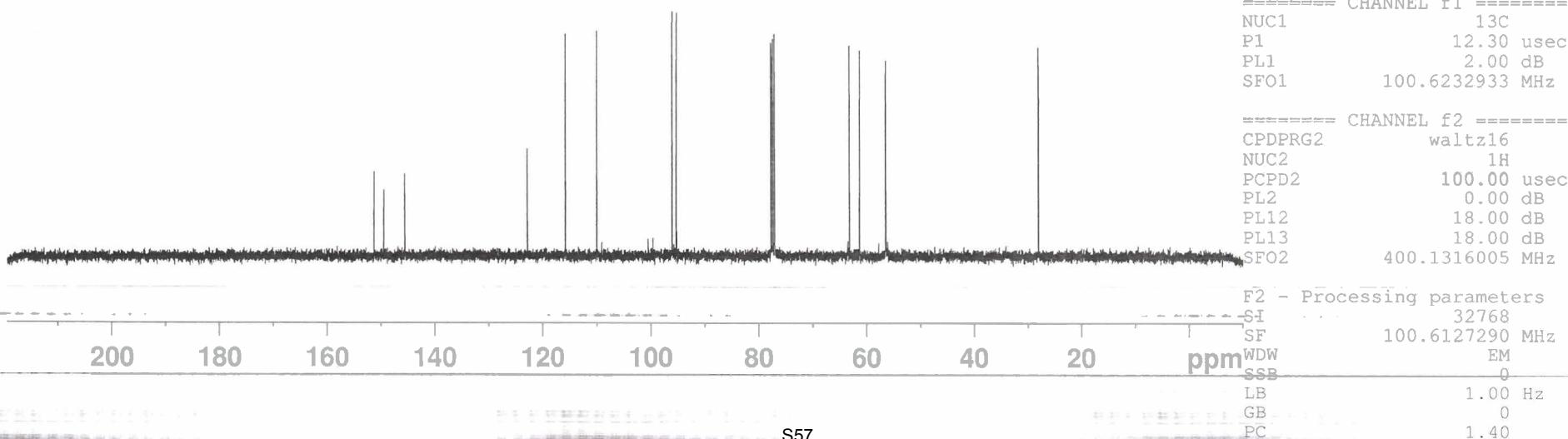


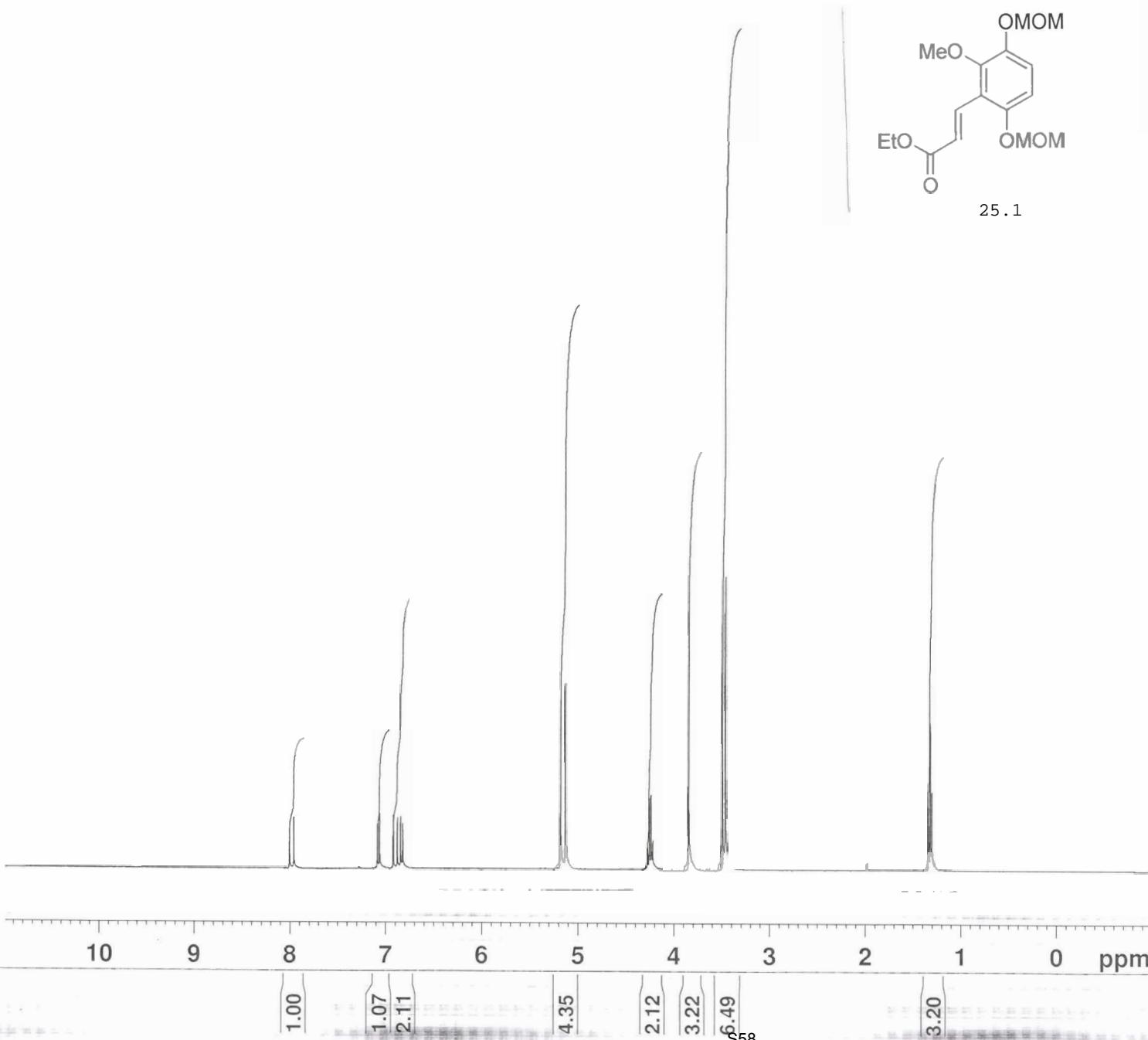
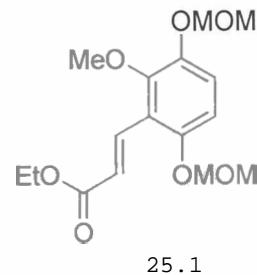
Current Data Parameters
 NAME sg-133
 EXPNO 2
 PROCNO 1

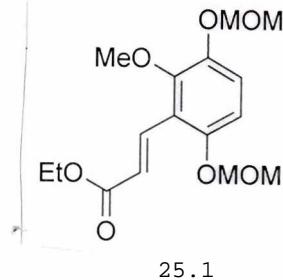
F2 - Acquisition Parameters
 Date_ 20030923
 Time 5.52
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 111
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 1448.2
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 ======
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 ======
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz







Current Data Parameters
 NAME sg434
 EXPNO 2
 PROCNO 1

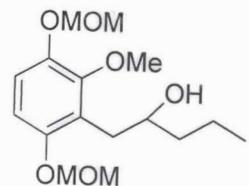
F2 - Acquisition Parameters
 Date_ 20050406
 Time 2.56
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 83
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0

200 180 160 140 120 100 80 60 40 20 ppm

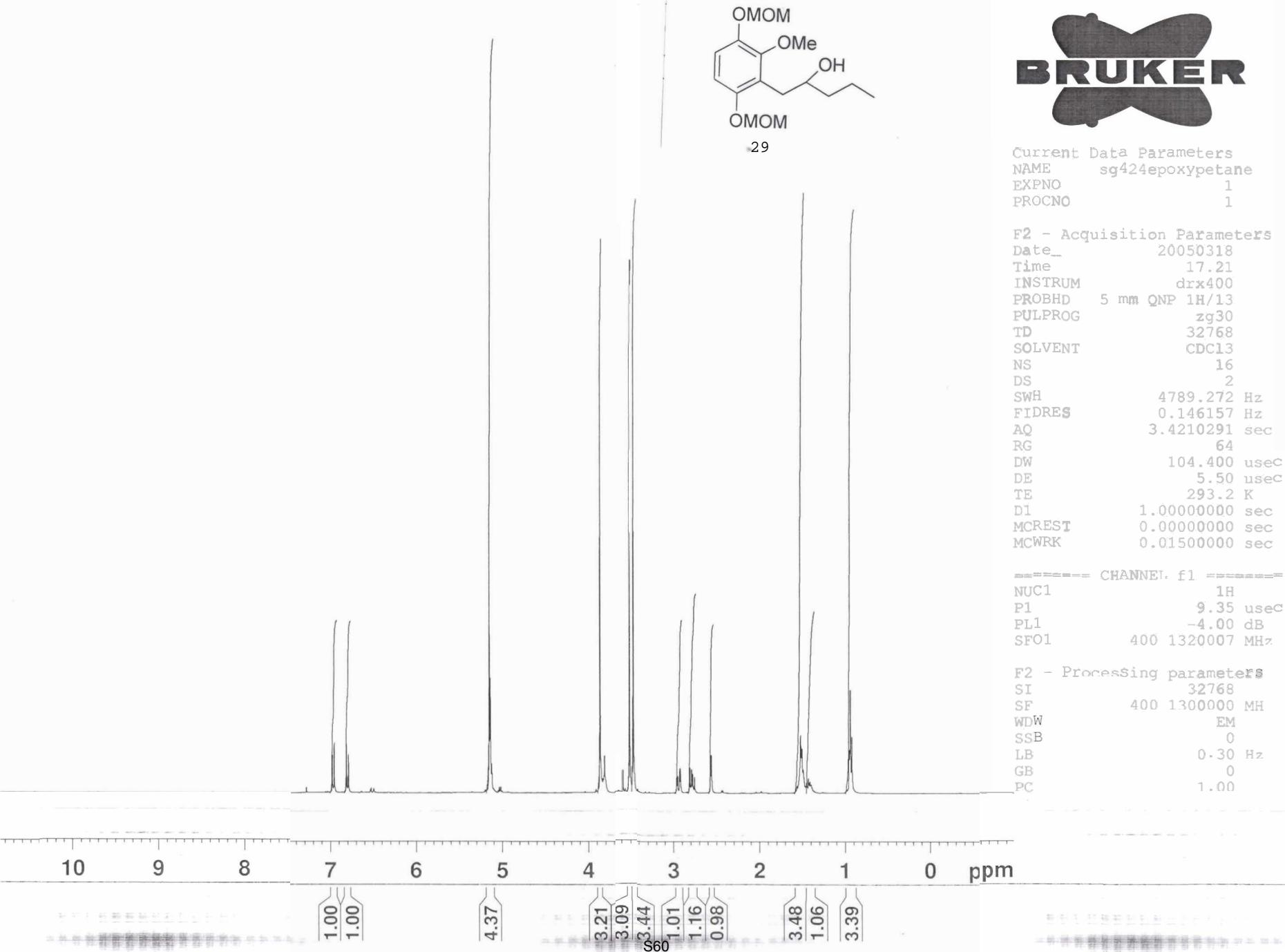


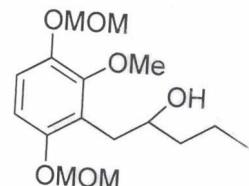
Current Data Parameters
 NAME sg424epoxypetane
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20050318
 Time 17.21
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL: f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400 1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400 1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





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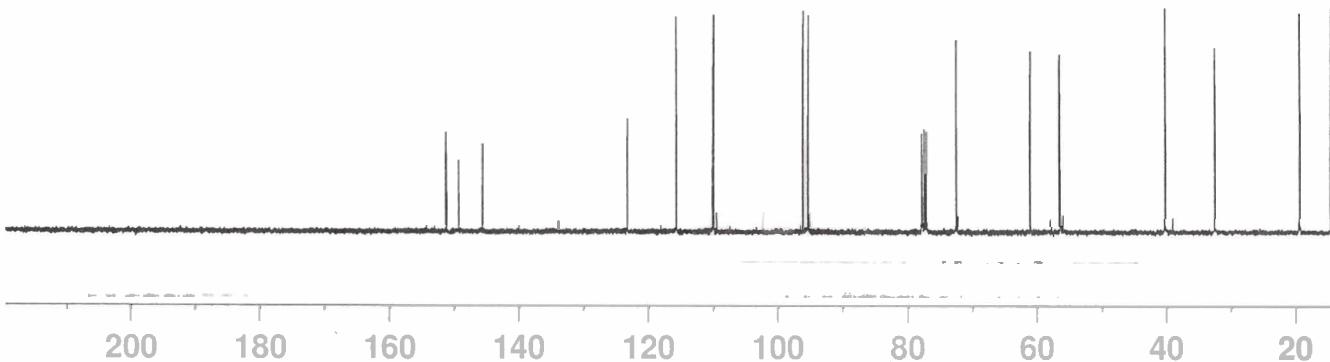
Current Data Parameters
 NAME sg424epoxypetane
 EXPNO 2
 PROCNO 1

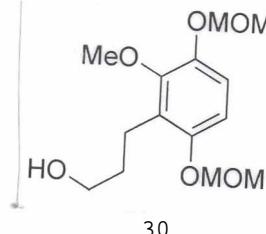
F2 - Acquisition Parameters
 Date_ 20050318
 Time 17.26
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 205
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPDP2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0





Current Data Parameters
NAME sg431
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050330
Time 19.38
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 45.3
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

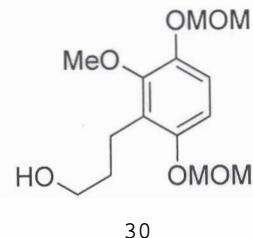
===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 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

0.50 0.51 2.09 1.56 4.19 1.00 0.50 0.98

S62



30



Current Data Parameters
 NAME sg431
 EXPNO 2
 PROCNO 1

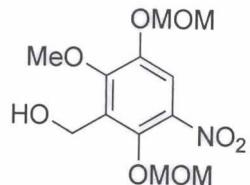
F2 - Acquisition Parameters
 Date_ 20050330
 Time 19.42
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 48
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 ======
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

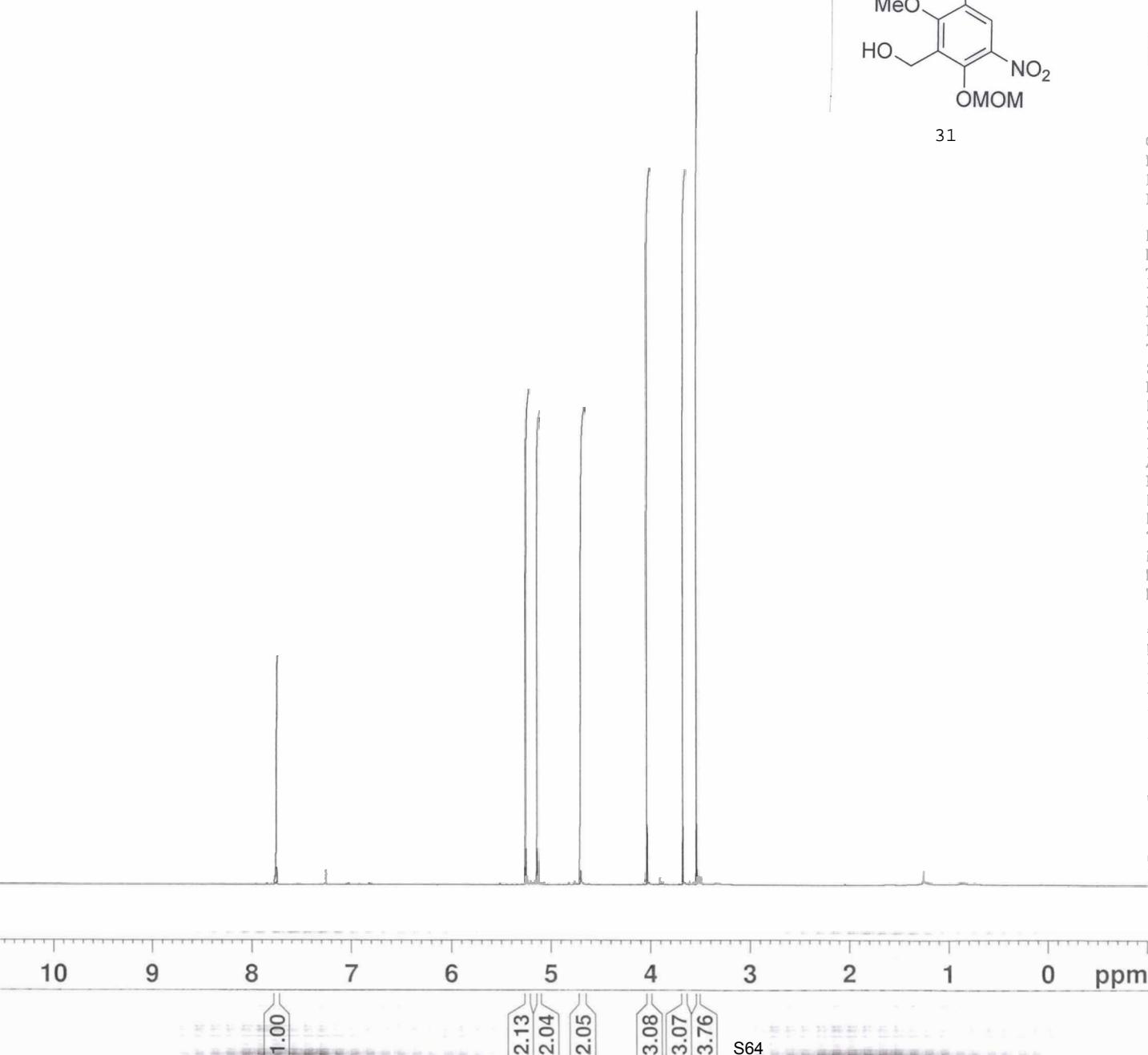
===== CHANNEL f2 ======
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.612/290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0.00

200 180 160 140 120 100 80 60 40 20 ppm



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Current Data Parameters
NAME 1cmomnitration
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060324
Time 5.02
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 256
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

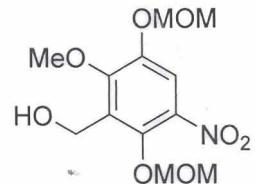
10 9 8 7 6 5 4 3 2 1 0 ppm

1.00

2.13
2.04
2.05

3.08
3.07
3.76

S64

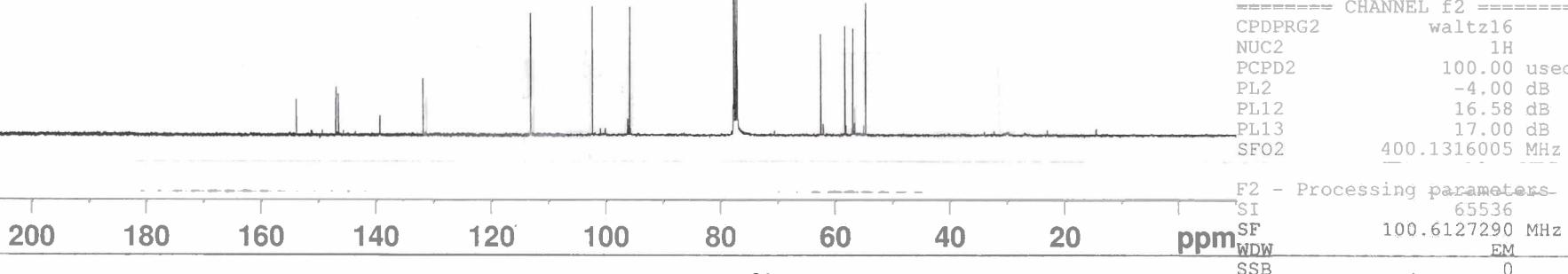


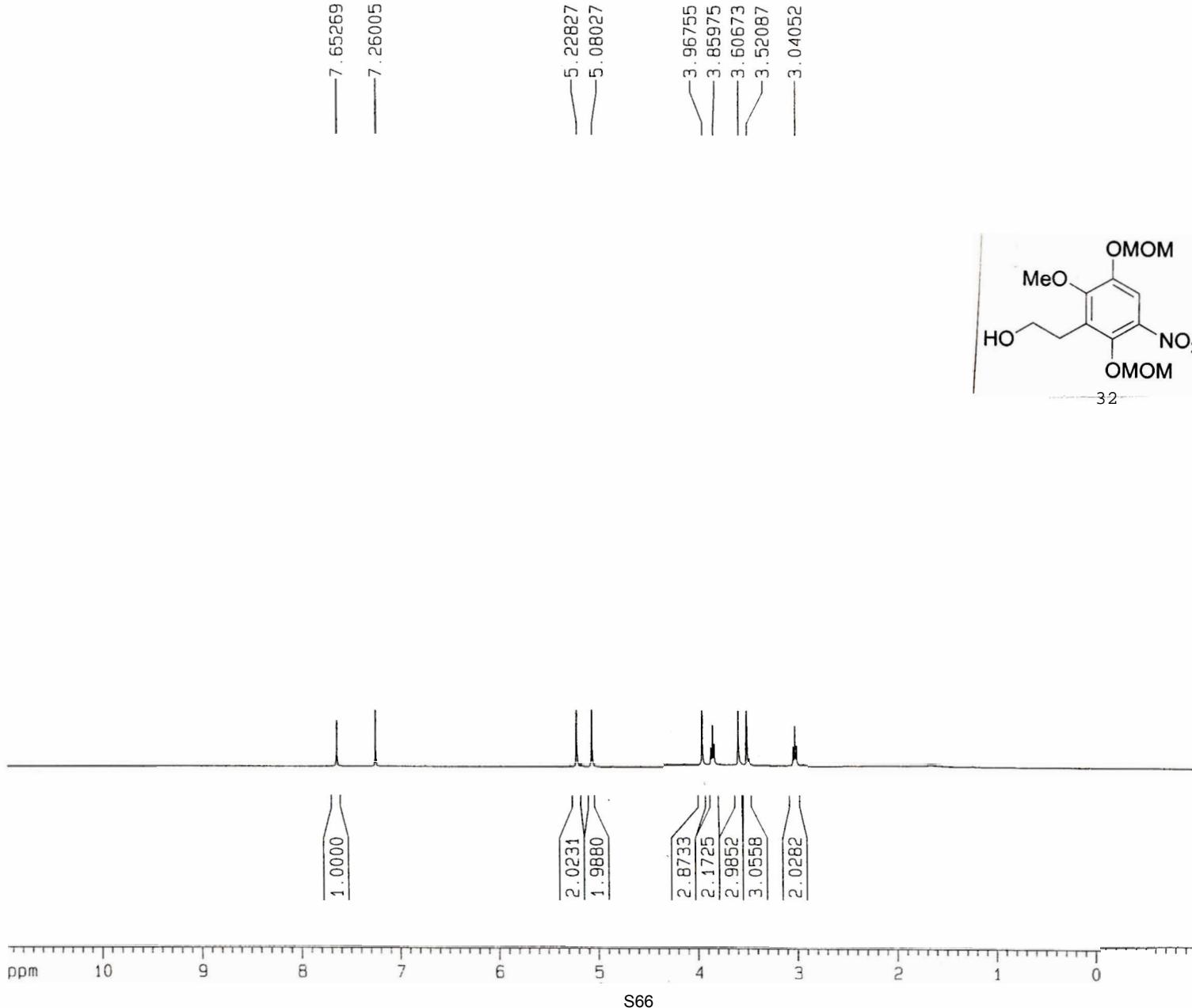
Current Data Parameters
 NAME lcmonitration
 EXPNO 2
 PROCNO 1

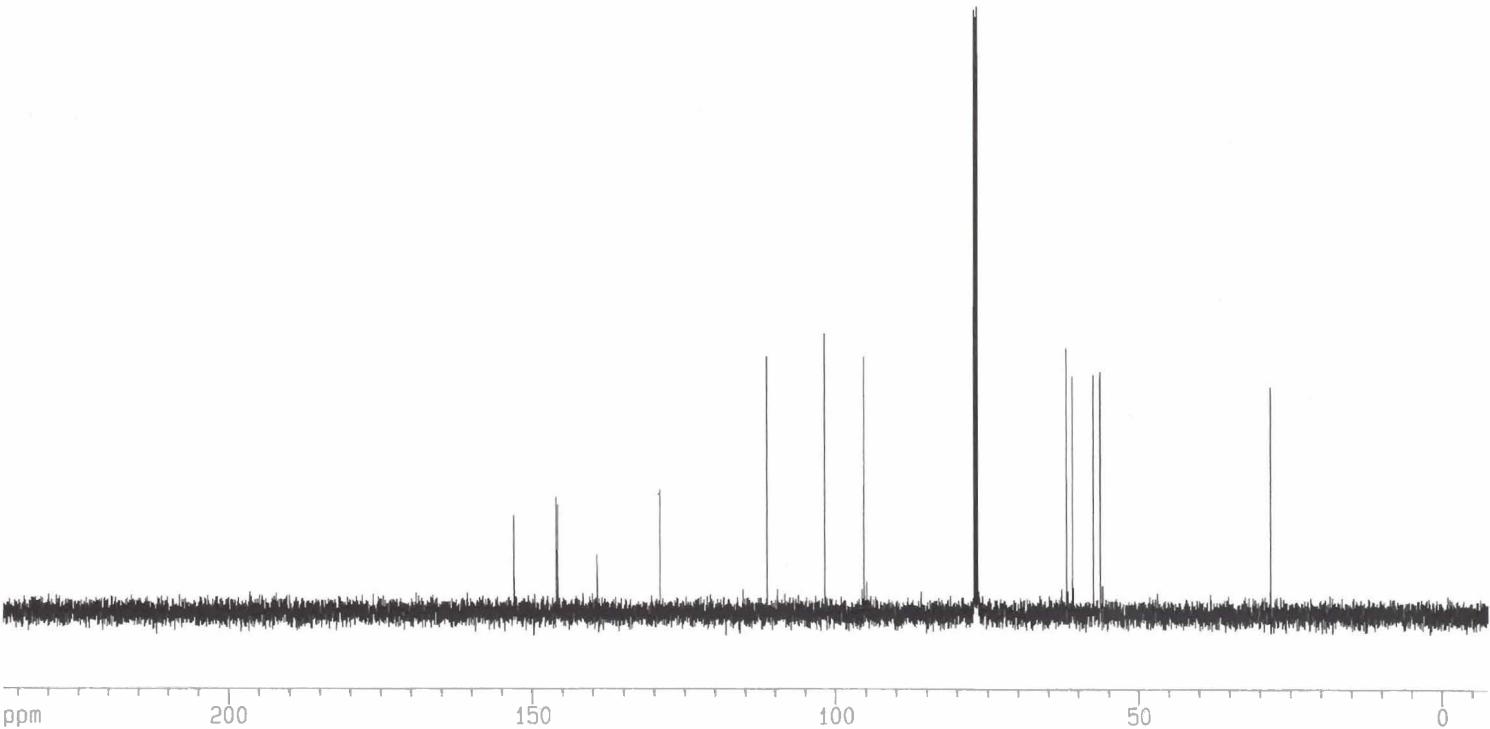
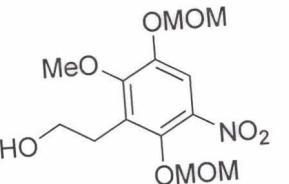
F2 - Acquisition Parameters
 Date_ 20060324
 Time 13.20
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16384
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 3649.1
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 ======
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 ======
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz







Current Data Parameters
 NAME 113
 EXPNO 2
 PROCN 1

F2 - Acquisition Parameters
 Date_ 20031226
 Time 21.01
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 68
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420883 sec
 RG 2048
 DW 15.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 d11 0.0300000 sec
 d12 0.00002000 sec

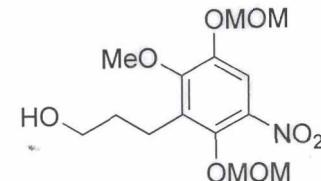
===== CHANNEL f1 =====
 NUC1 13C
 P1 6.50 usec
 PL1 5.00 dB
 SF01 125.7719472 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 95.00 usec
 PL2 -4.00 dB
 PL12 19.00 dB
 PL13 30.00 dB
 SF02 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578008 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 0F
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.30 Hz
 GB 0

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 242.517 ppm
 F1 30498.43 Hz
 F2P -7.539 ppm
 F2 -948.11 Hz
 F2PCM 12.50282 ppm/cm
 HZCM 1572.32703 Hz/cm

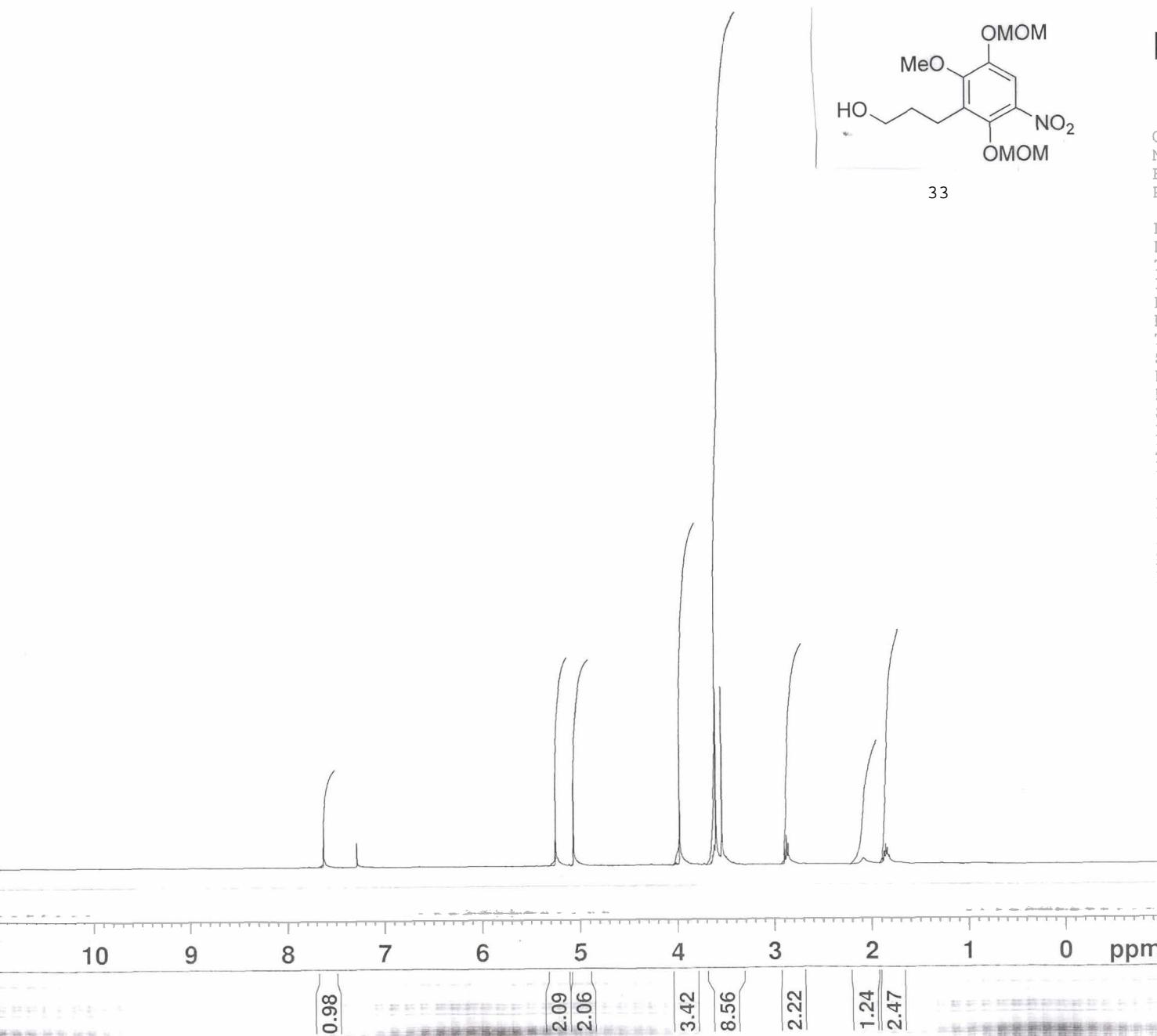


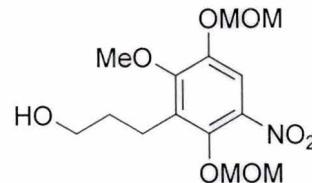
Current Data Parameters
 NAME sg432
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050331
 Time 17.30
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 181
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

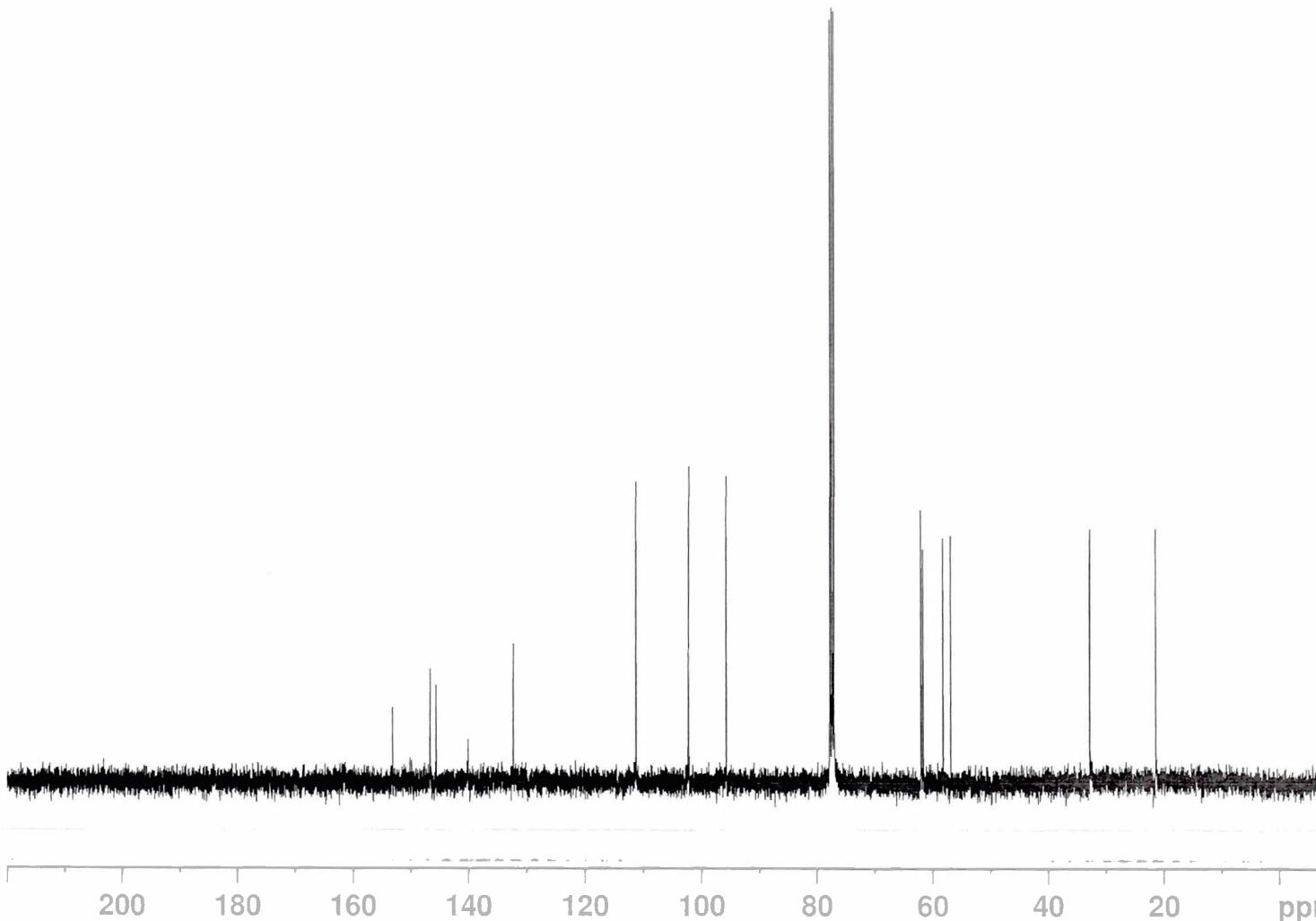
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





33



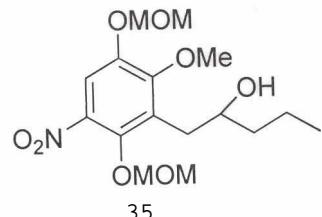
Current Data Parameters
NAME sg432
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050331
Time 17.46
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 794
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

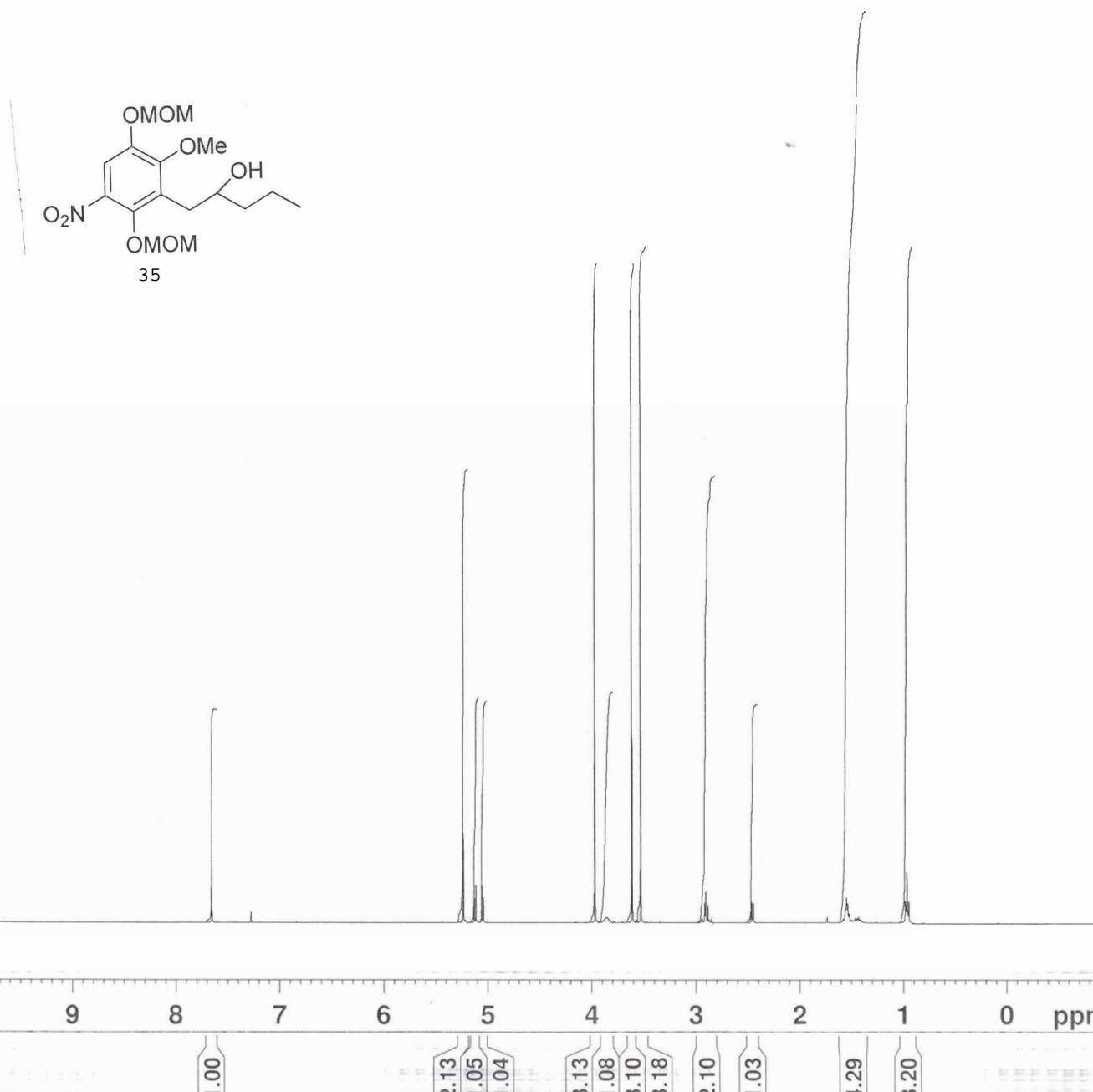
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0



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

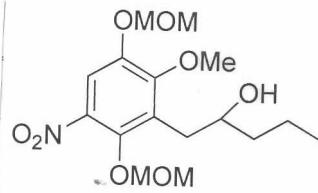


Current Data Parameters
NAME sg437
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20050408
Time 16.48
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 101.6
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME sg437
 EXPNO 2
 PROCNO 1

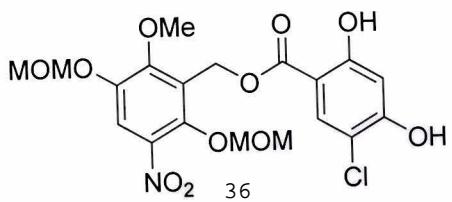
F2 - Acquisition Parameters
 Date 20050408
 Time 16.57
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 338
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

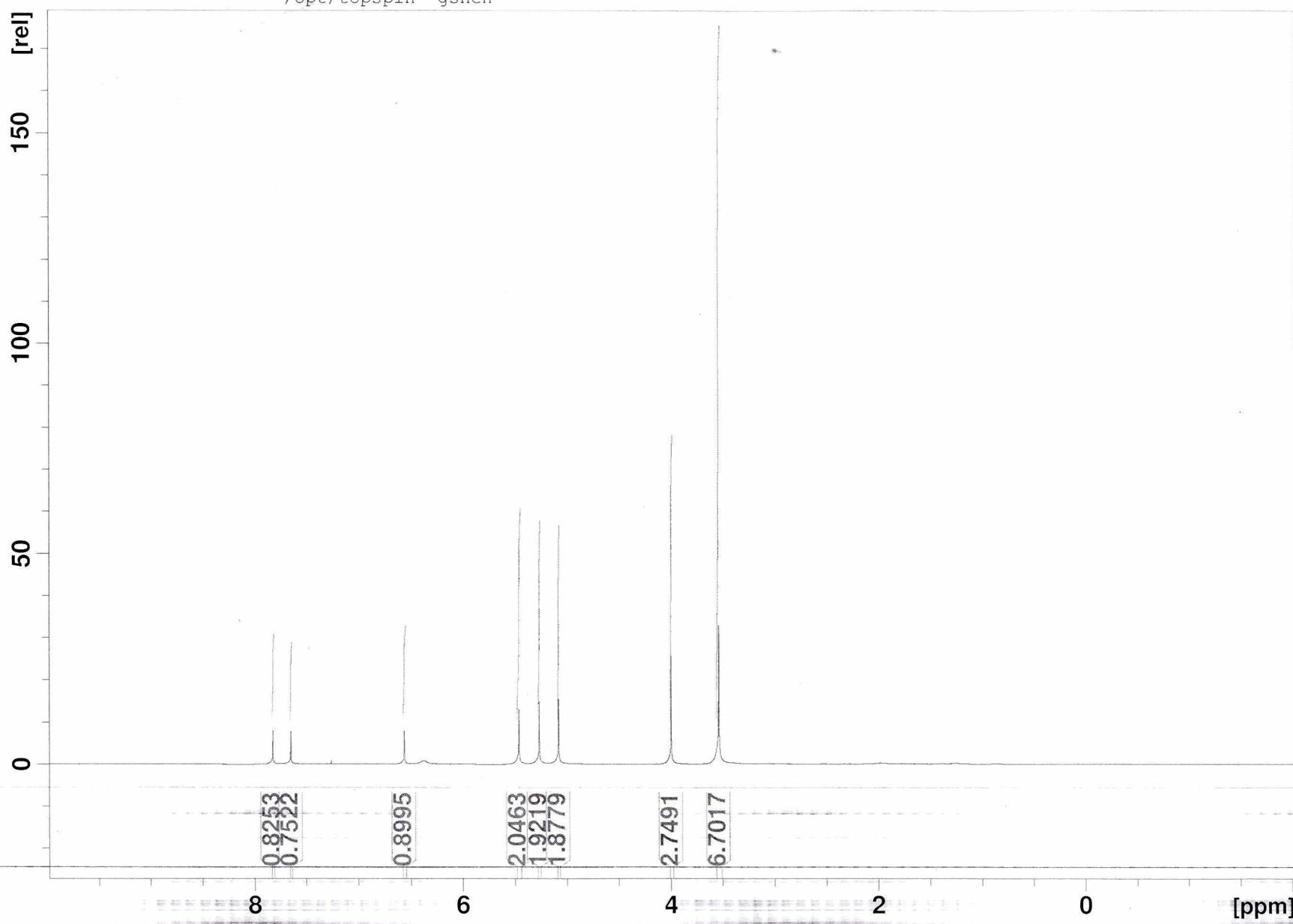
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

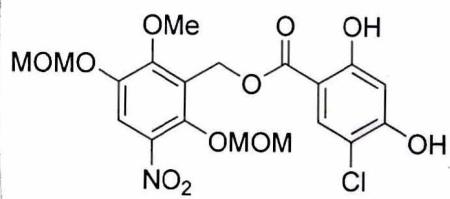
F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW
 SSB 0
 LB 1.00 Hz
 GB 0



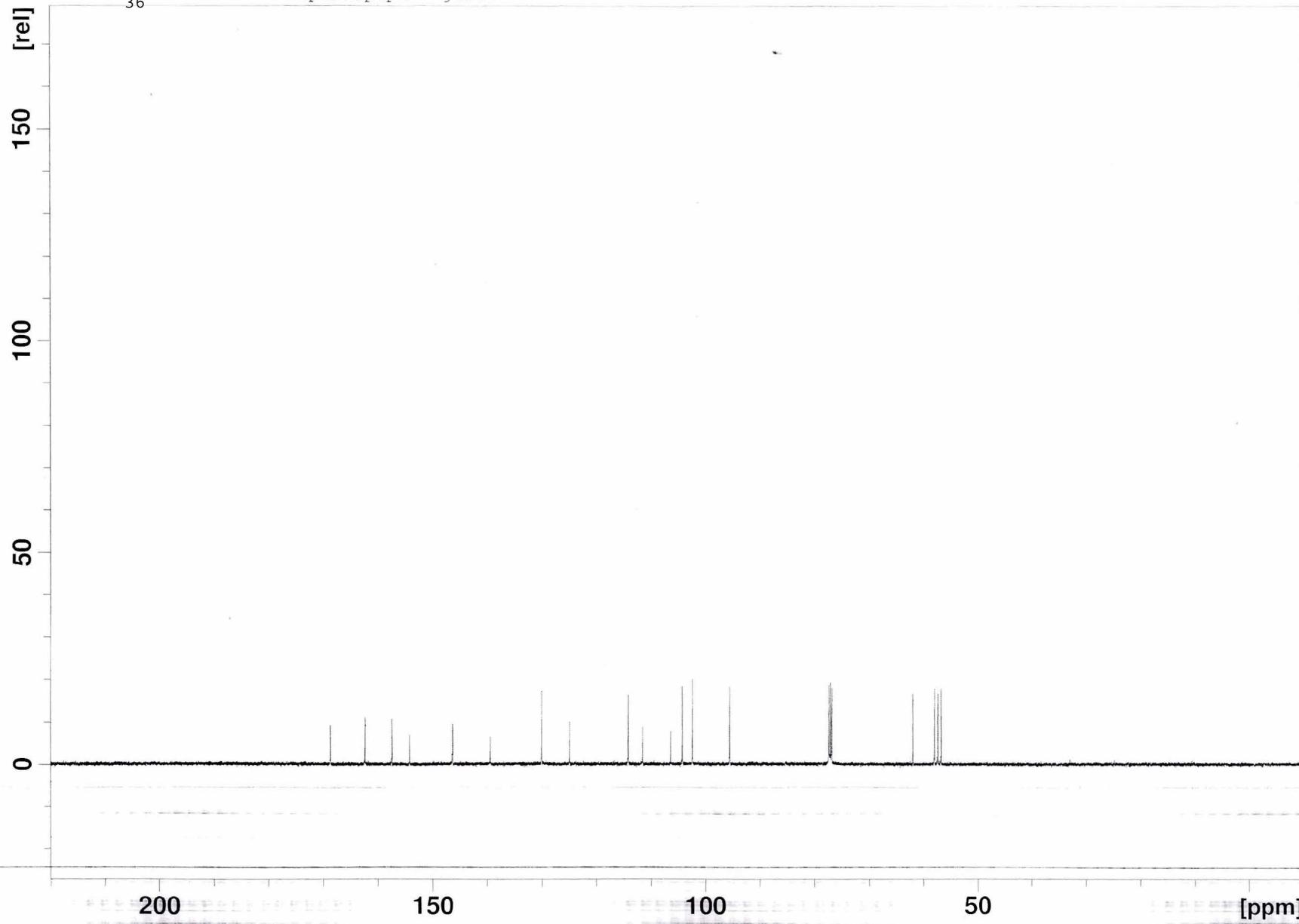


/opt/topspin gshen





/opt/topspin gshen



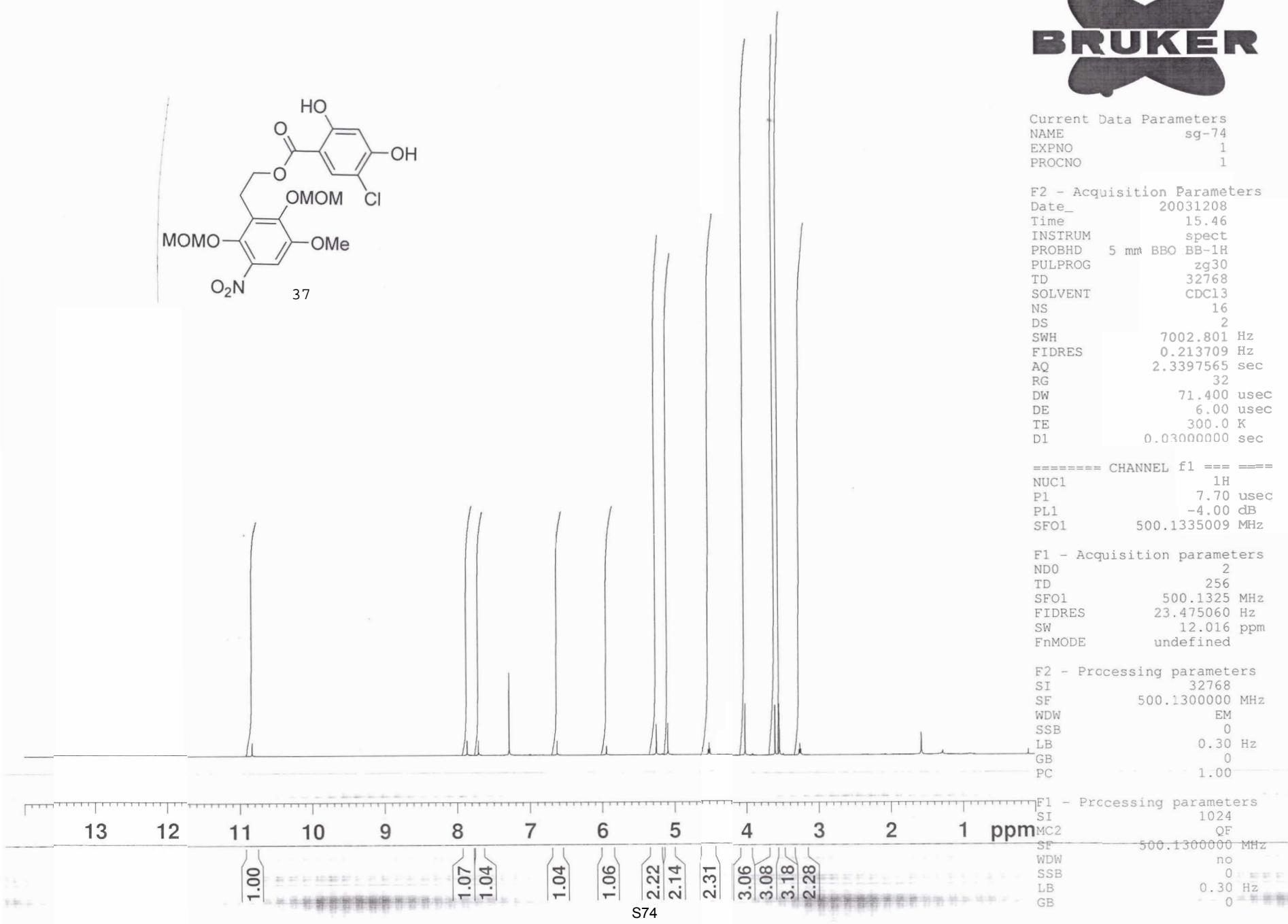
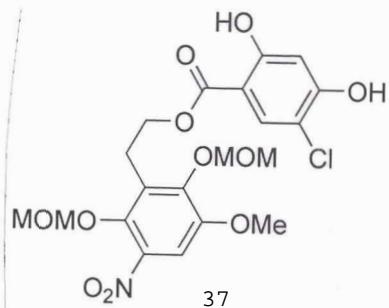
200

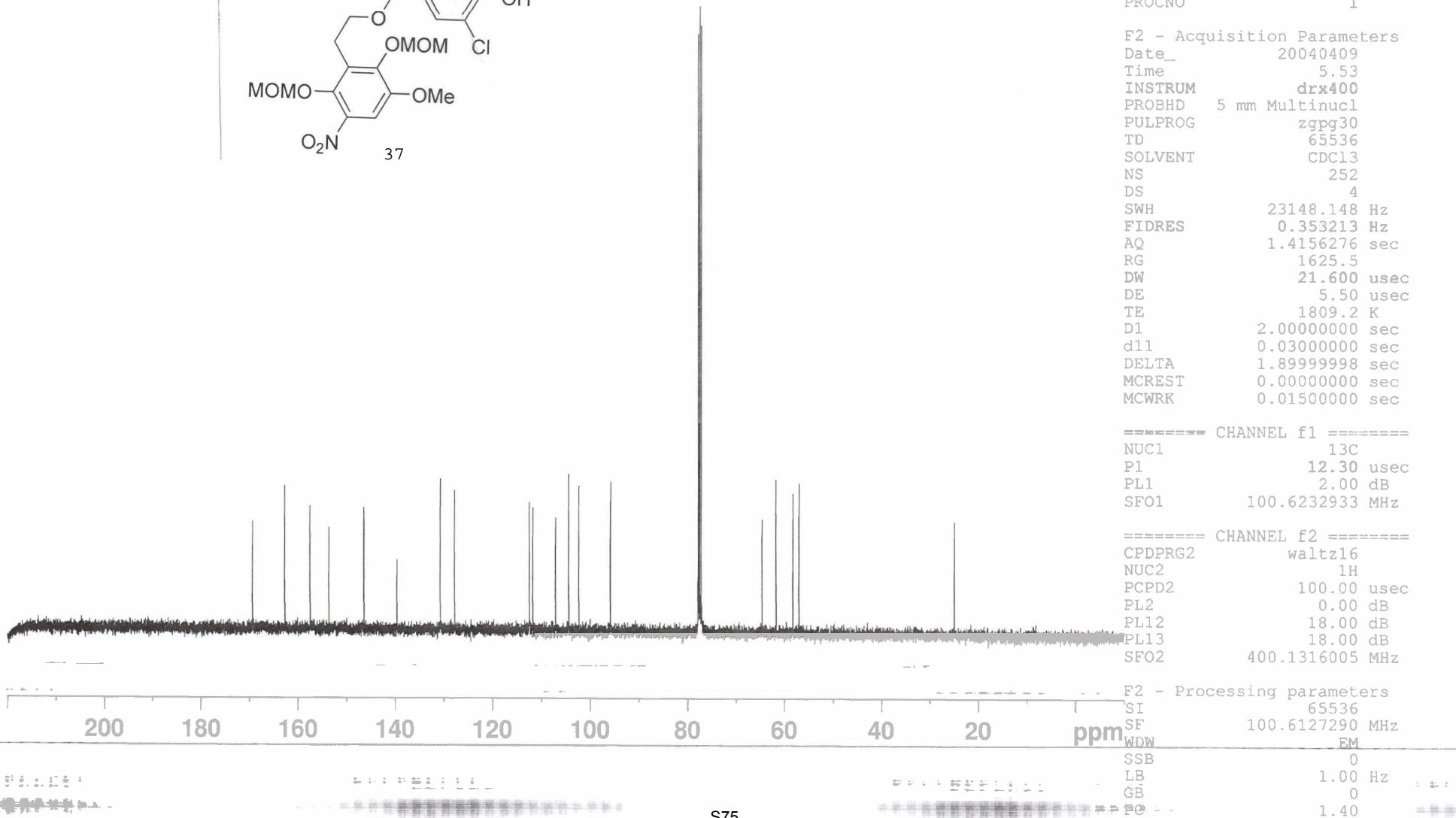
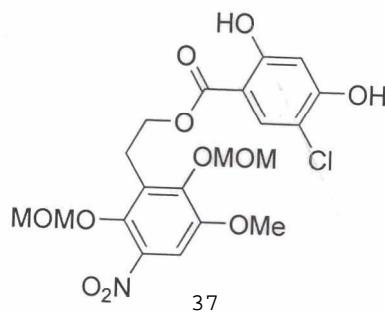
150

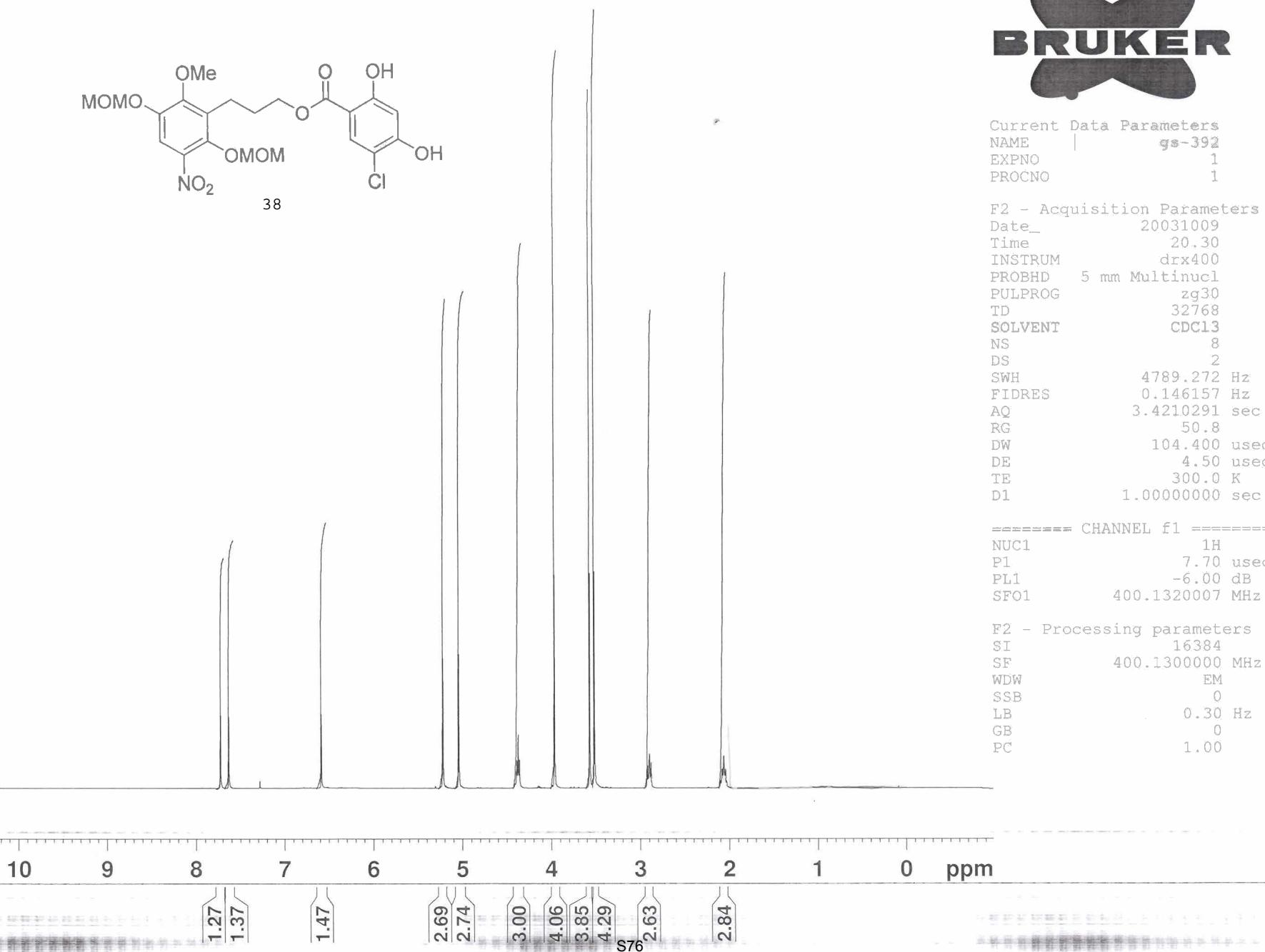
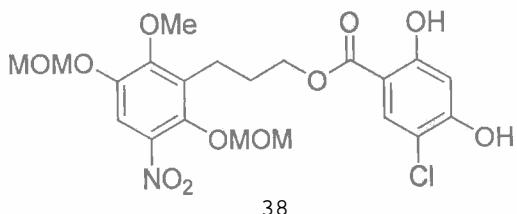
100

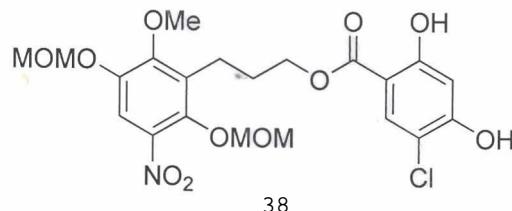
50

[ppm]









Current Data Parameters
 NAME | sg-95
 EXPNO | 1
 PROCNO | 1

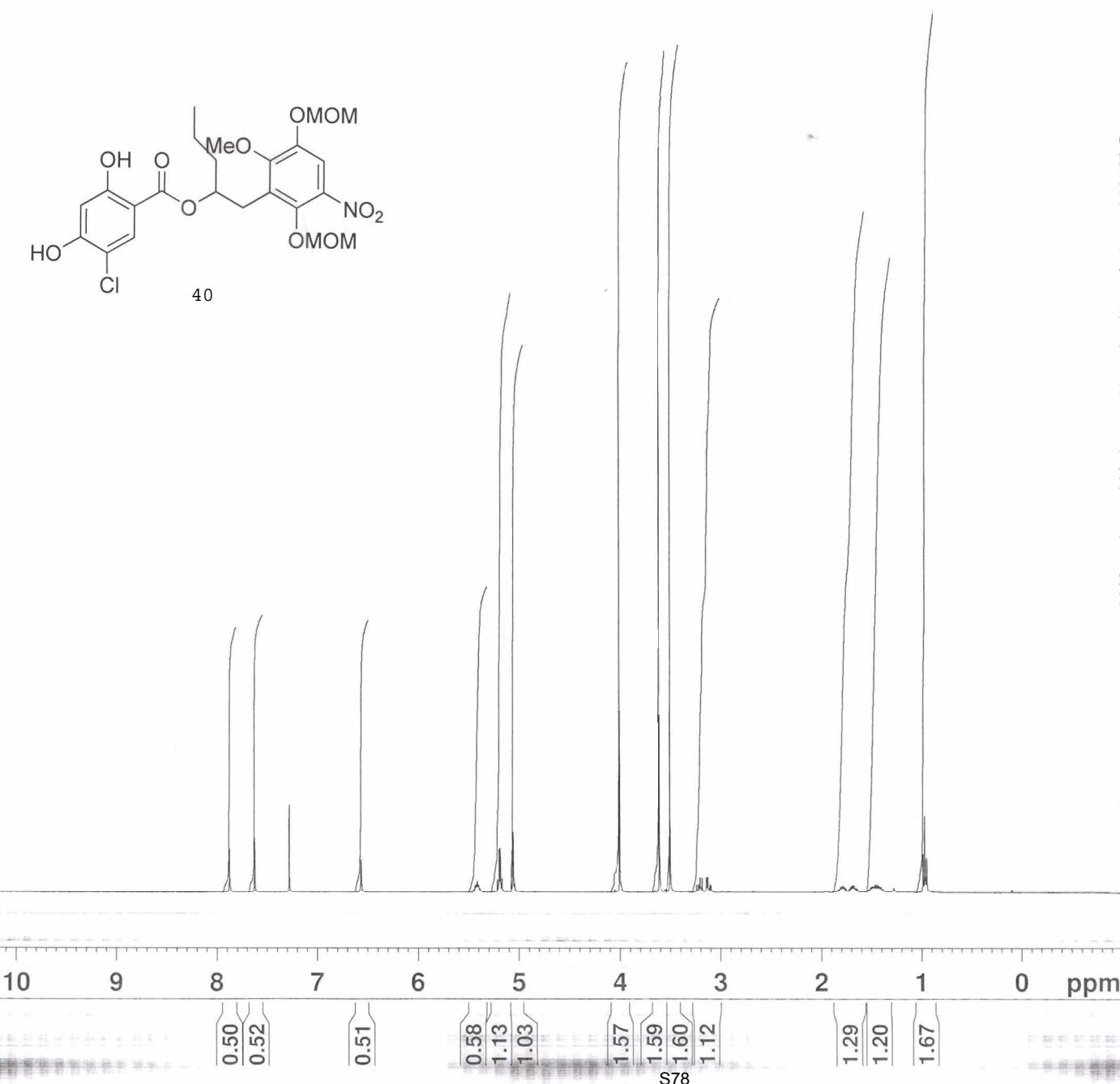
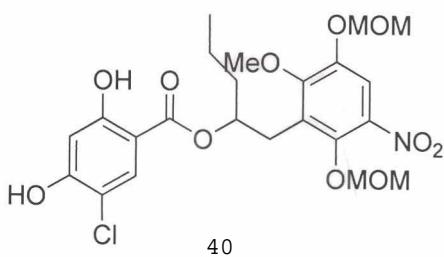
F2 - Acquisition Parameters
 Date_ 20031009
 Time 20.34
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgppg30
 TD 65536
 SOLVENT CDCl3
 NS 367
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 645.1
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPDRG2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0



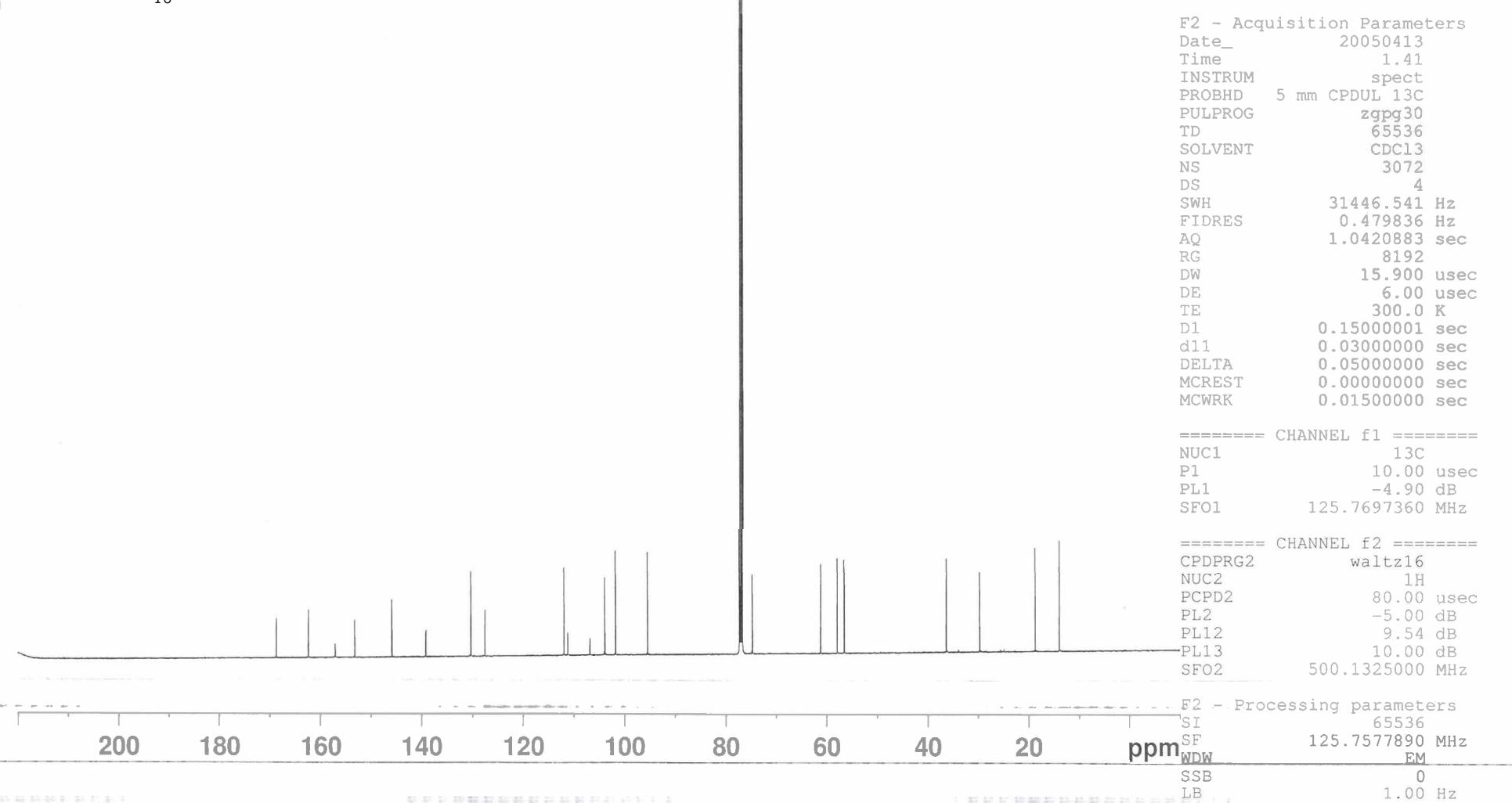
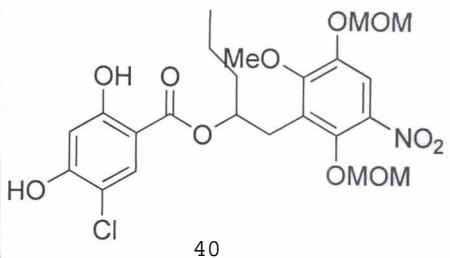


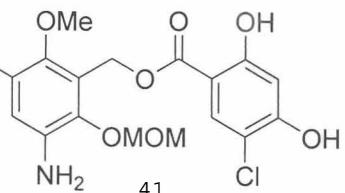
Current Data Parameters
 NAME sg439
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050411
 Time 2.04
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 322.5
 DW 104.400 usec
 DE 5.50 usec
 TE 297.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

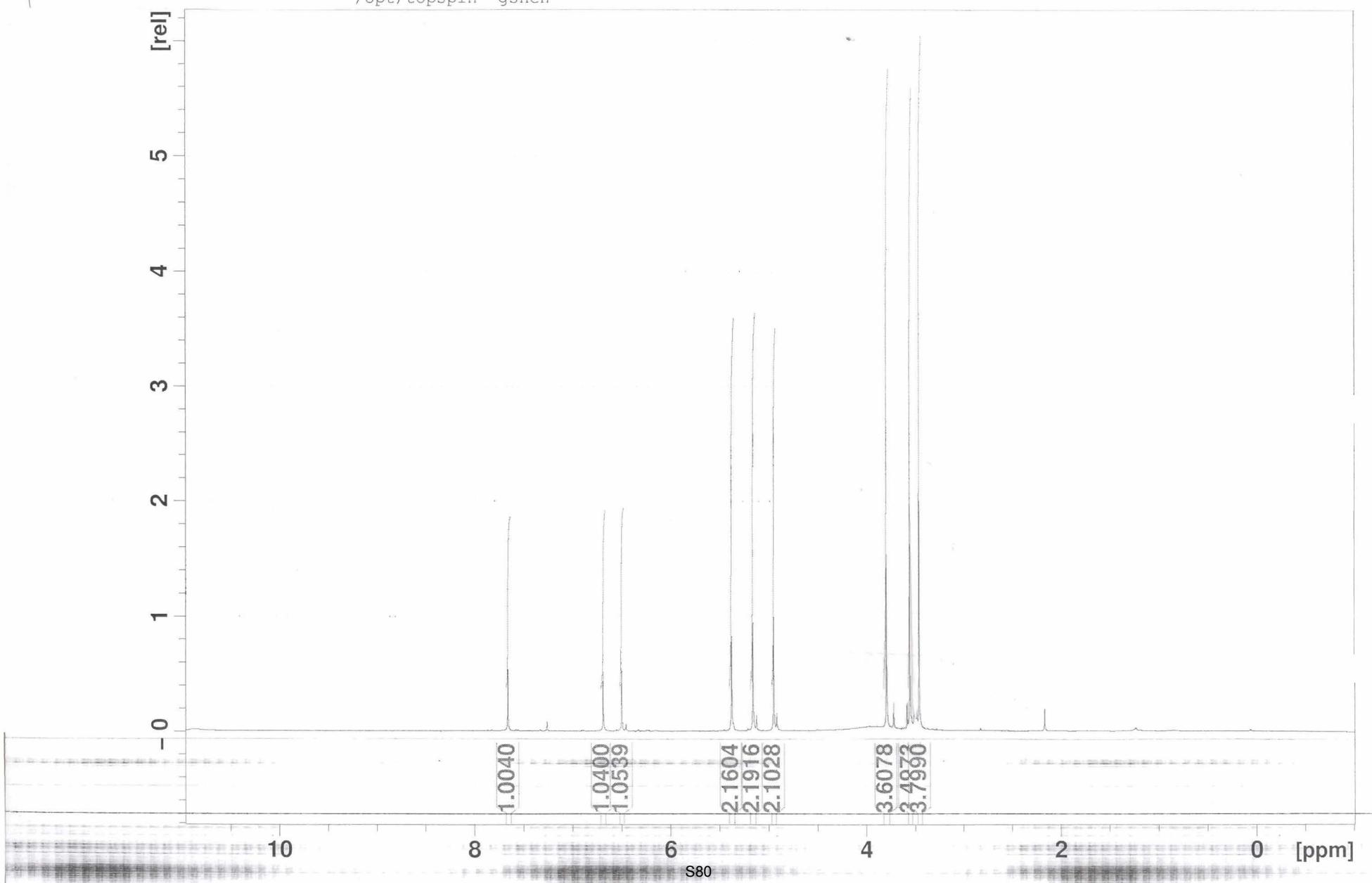
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

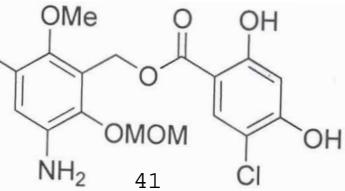
F2 - Processing parameters
 SI 32768
 SF 400.13000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





/opt/topspin gshen





41 /opt/toplevel gshen

[rel]

4

3

2

1

0

200

150

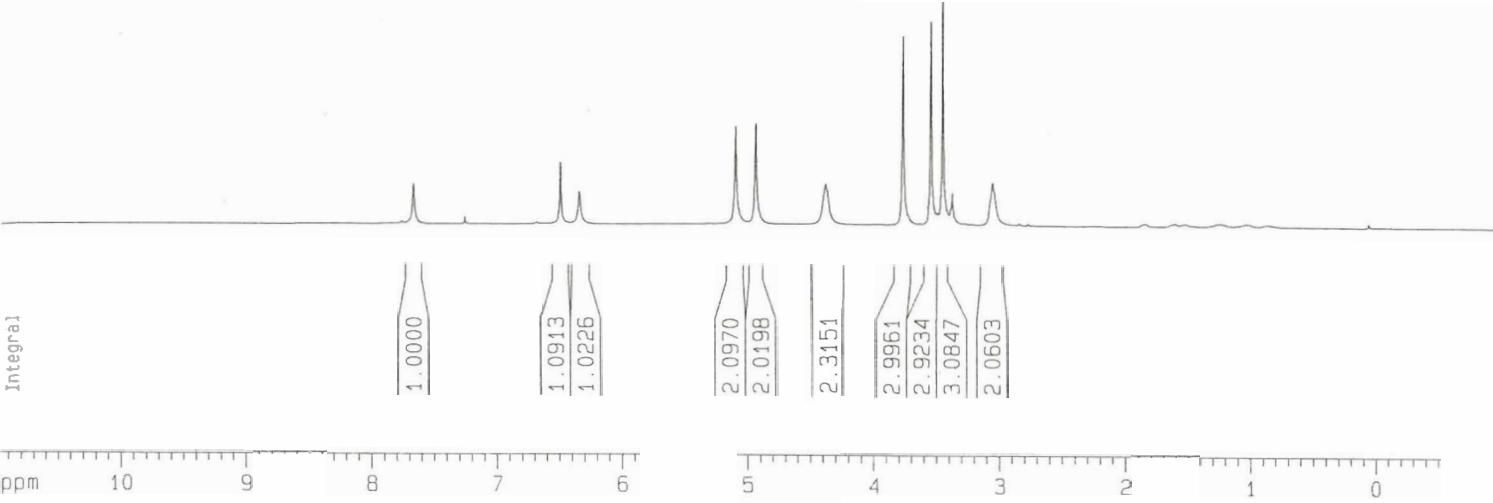
s81

100

50

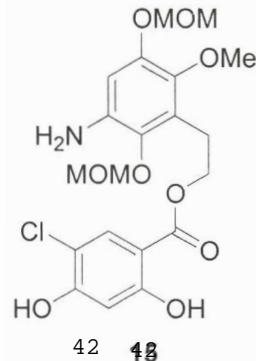
[ppm]

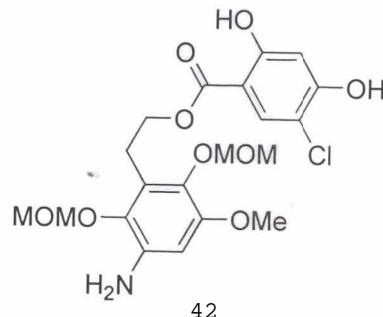
Integral



ppm

S82





Current Data Parameters
 NAME sg330
 EXPNO 1
 PROCNO 1

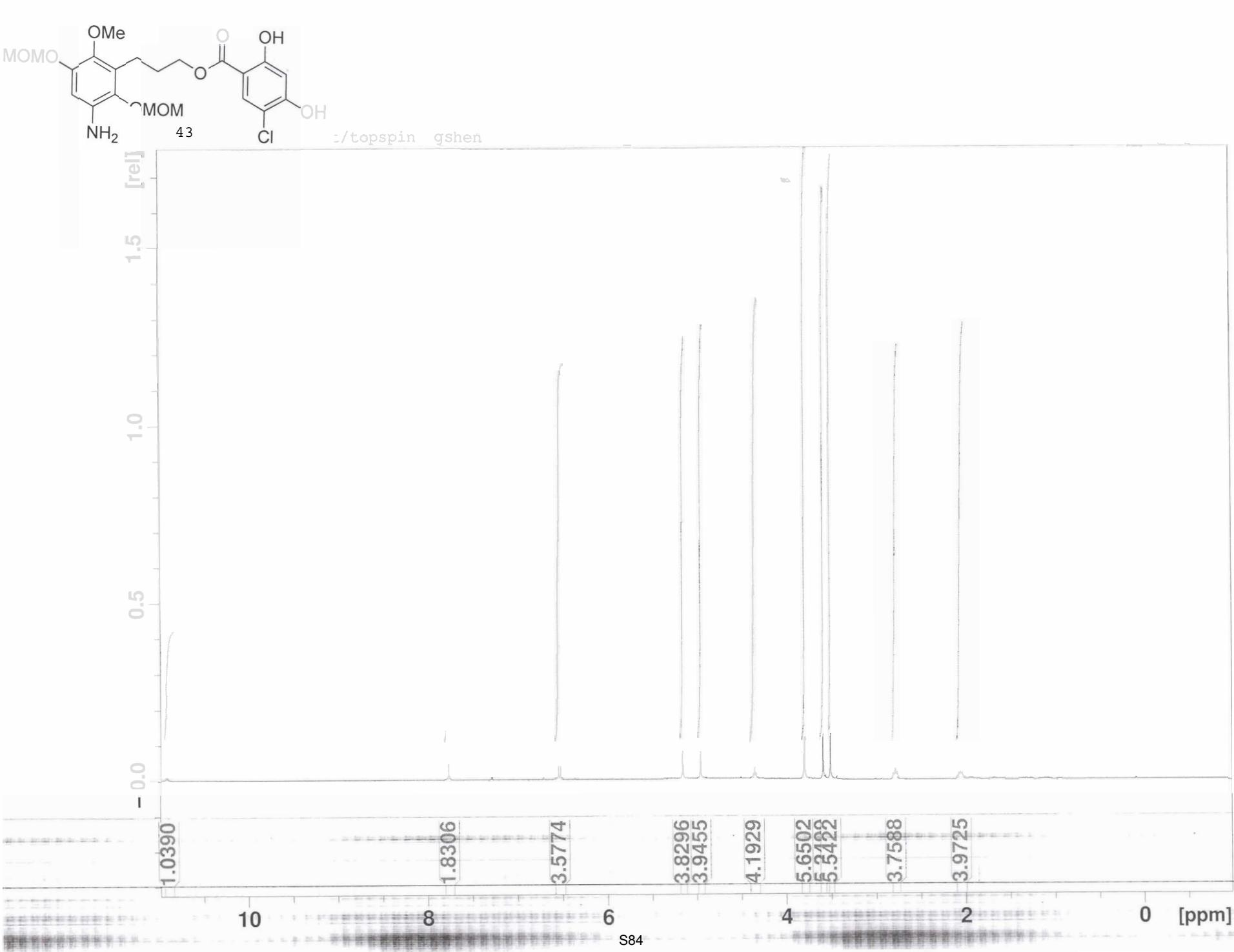
F2 - Acquisition Parameters
 Date_ 20040414
 Time 6.08
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 2517
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 512
 DW 21.600 usec
 DE 5.50 usec
 TE 1809.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

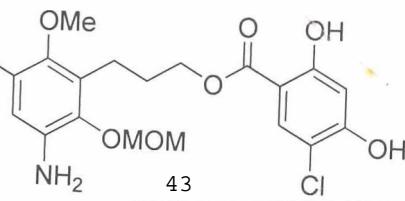
===== CHANNEL f1 ======
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 ======
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 0.40







43

/topspin gshen

[rel]

30

20

10

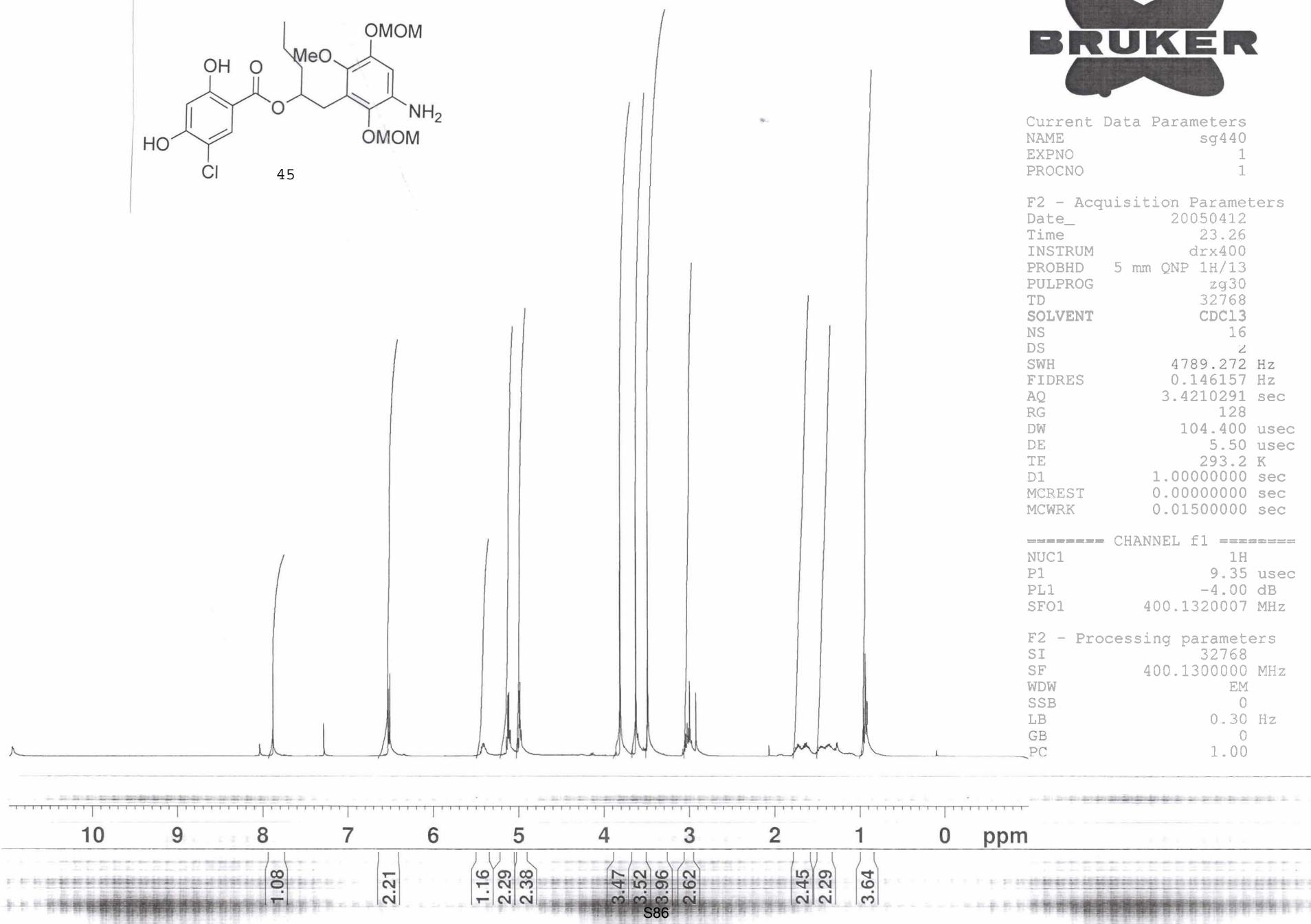
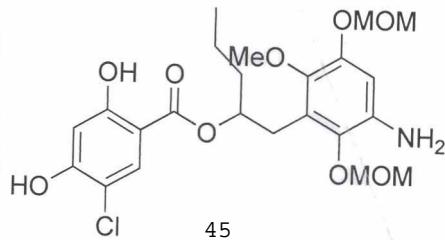
0

200

150 S85 100

50

[ppm]



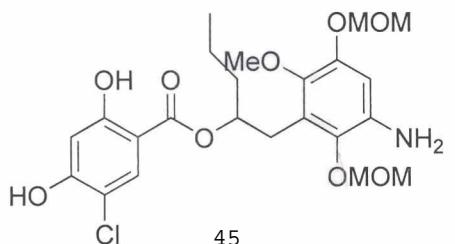
Current Data Parameters
 NAME sg440
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050412
 Time 23.28
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 183
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

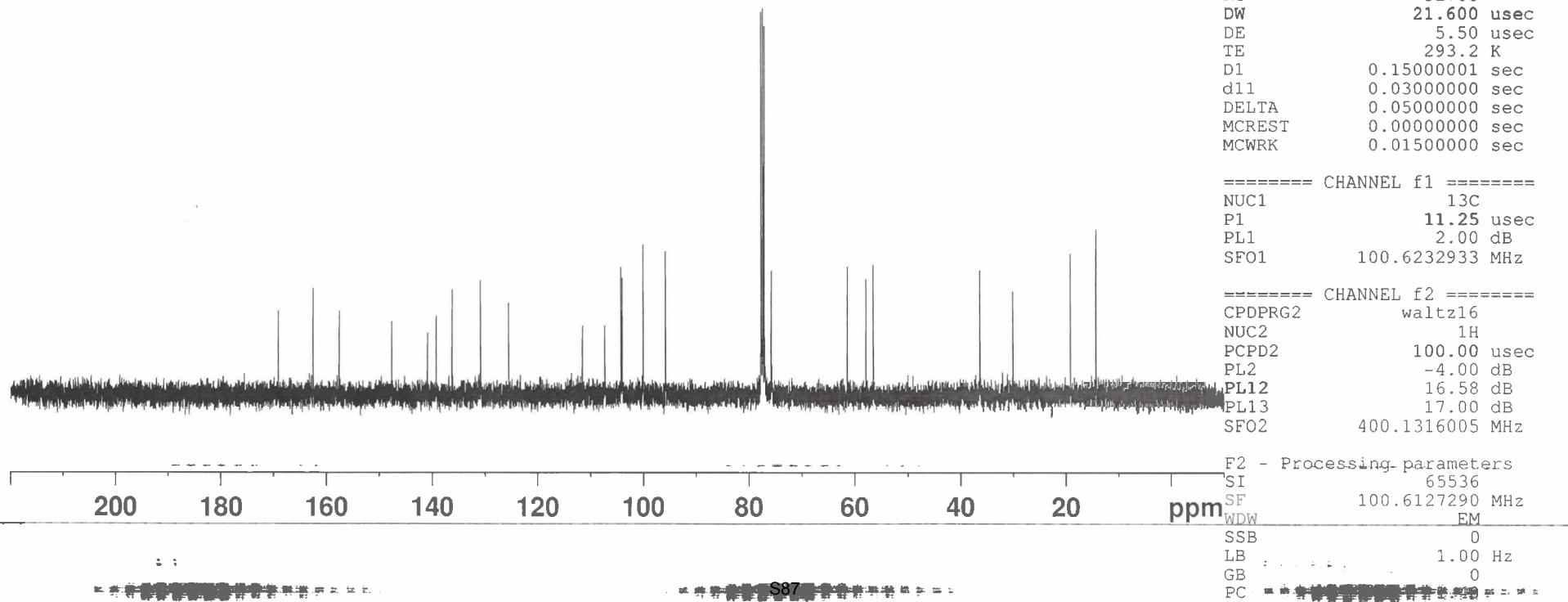
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

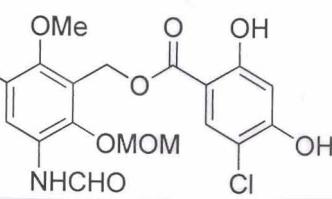
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing- parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC

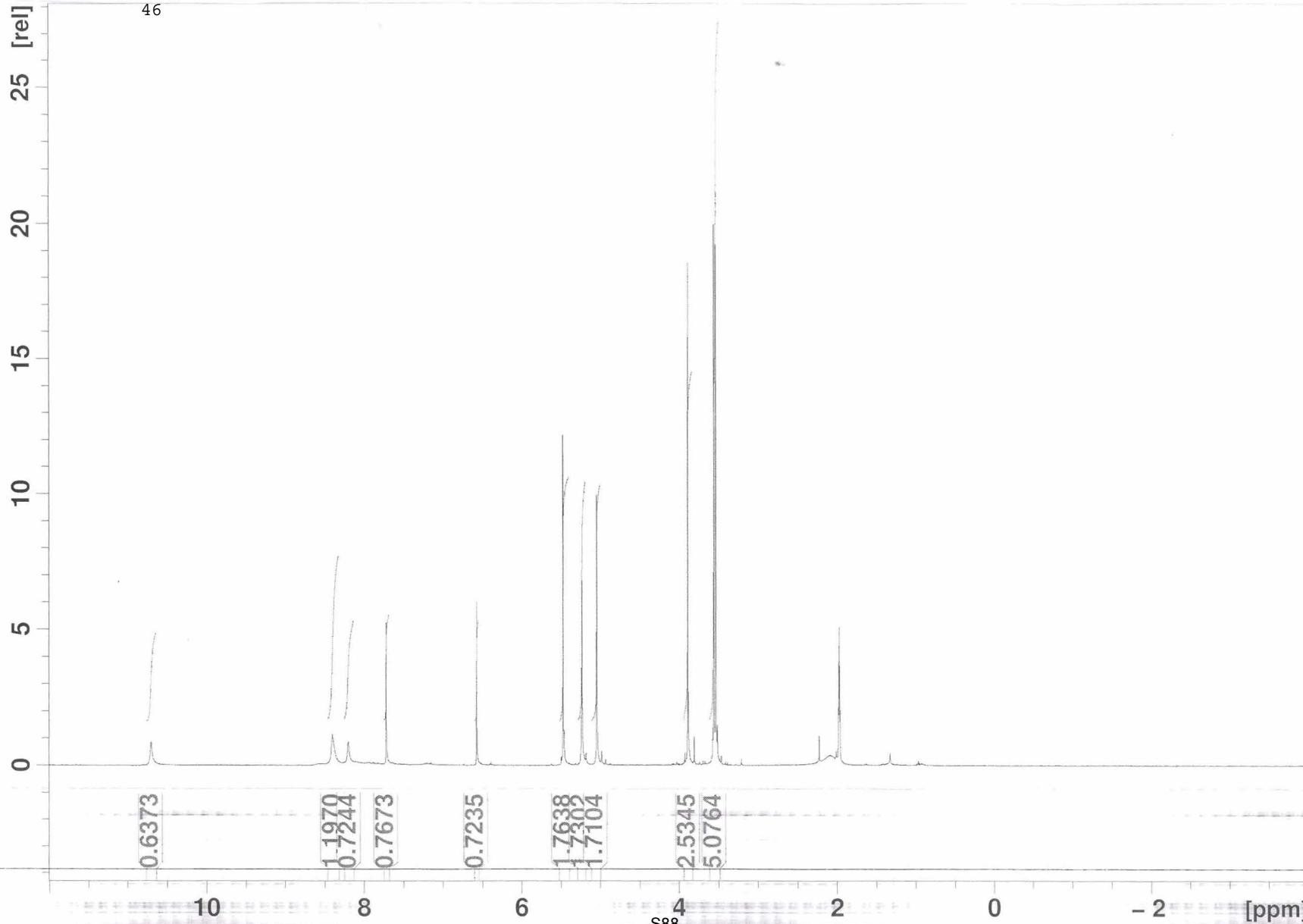


45





/opt/topspin gshen





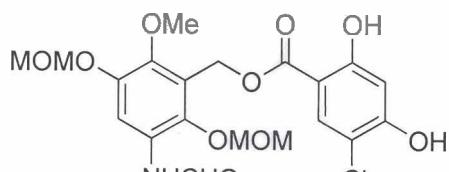
Current Data Parameters
 NAME lcmmomnhcho
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20060406
 Time 13.48
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 18432
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 295.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

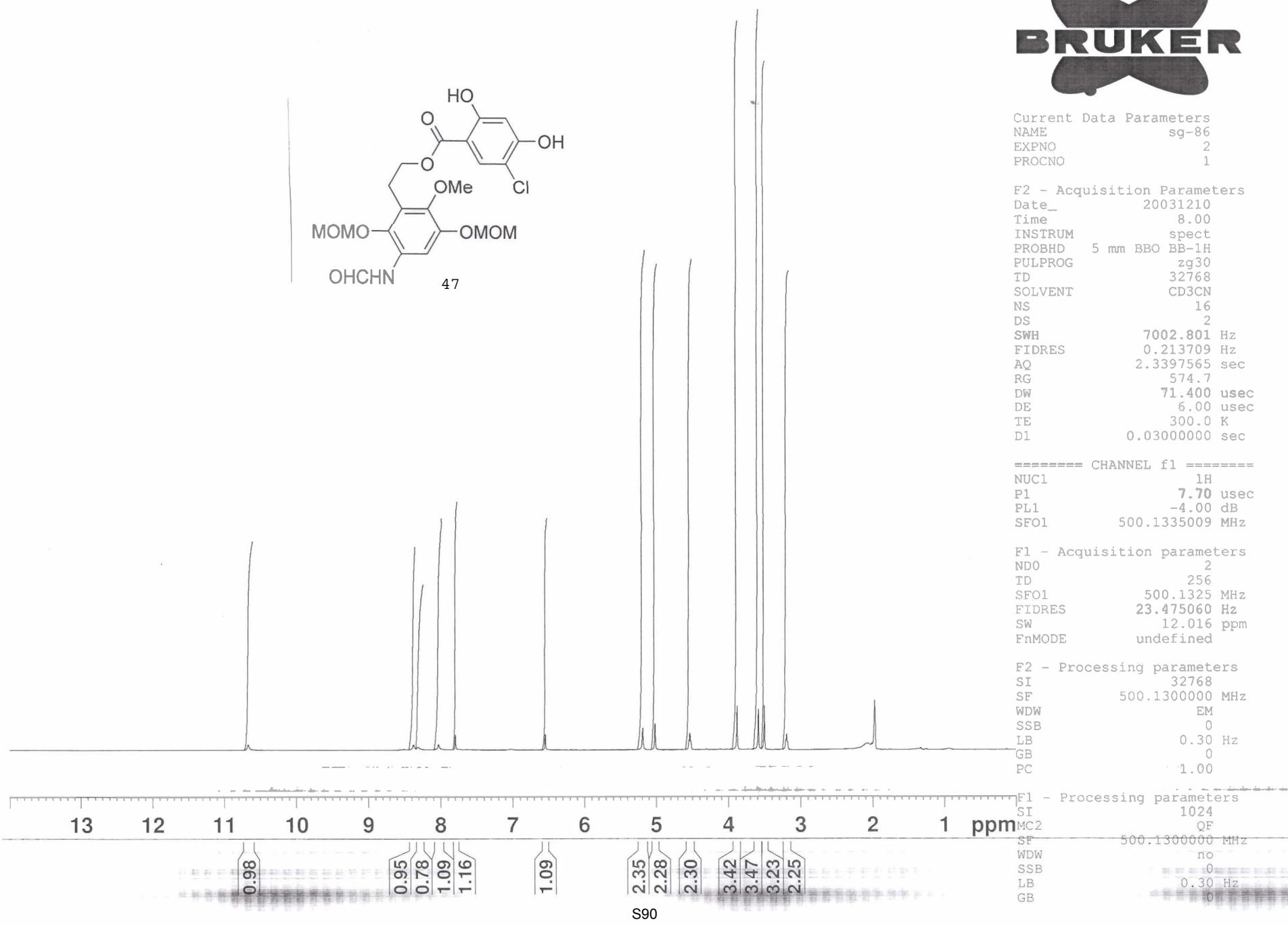
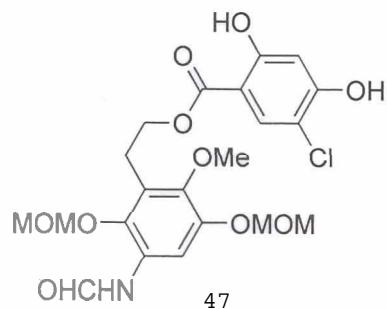
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB
 DC



46

200 180 160 140 120 100 80 60 40 20 ppm





Current Data Parameters
NAME sg-86
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20031210
Time 10.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 8192
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 2048
DW 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.0000200 sec

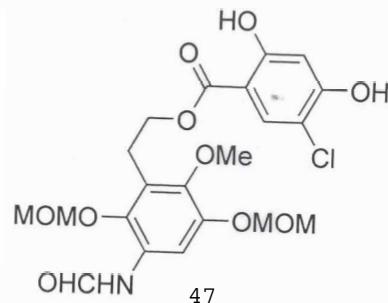
===== CHANNEL f1 =====
NUC1 13C
P1 6.50 usec
PL1 5.00 dB
SFO1 125.7719472 MHz

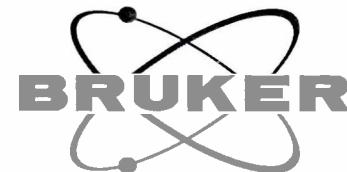
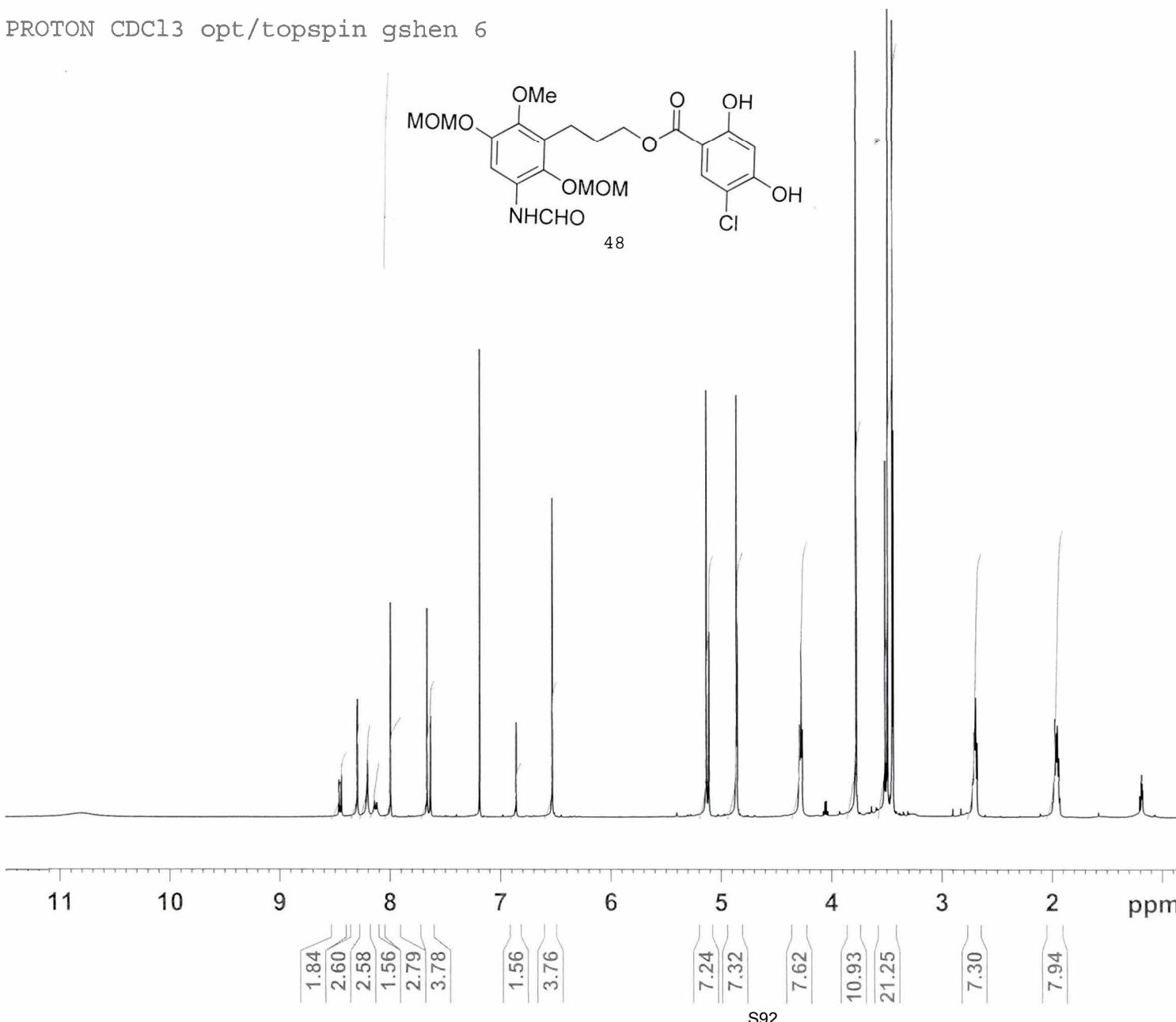
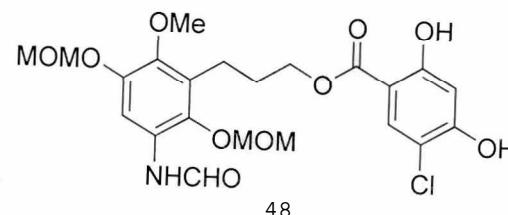
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 95.00 usec
PL2 -4.00 dB
PL12 19.00 dB
PL13 30.00 dB
SFO2 500.1325000 MHz

F1 - Acquisition parameters
ND0 2
TD 256
SFO1 500.1325 MHz
FIDRES 23.475060 Hz
SW 12.016 ppm
FnMODE undefined

F2 - Processing parameters
SI 65536
SF 125.7578008 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300000 MHz
WDW no
SSB 0



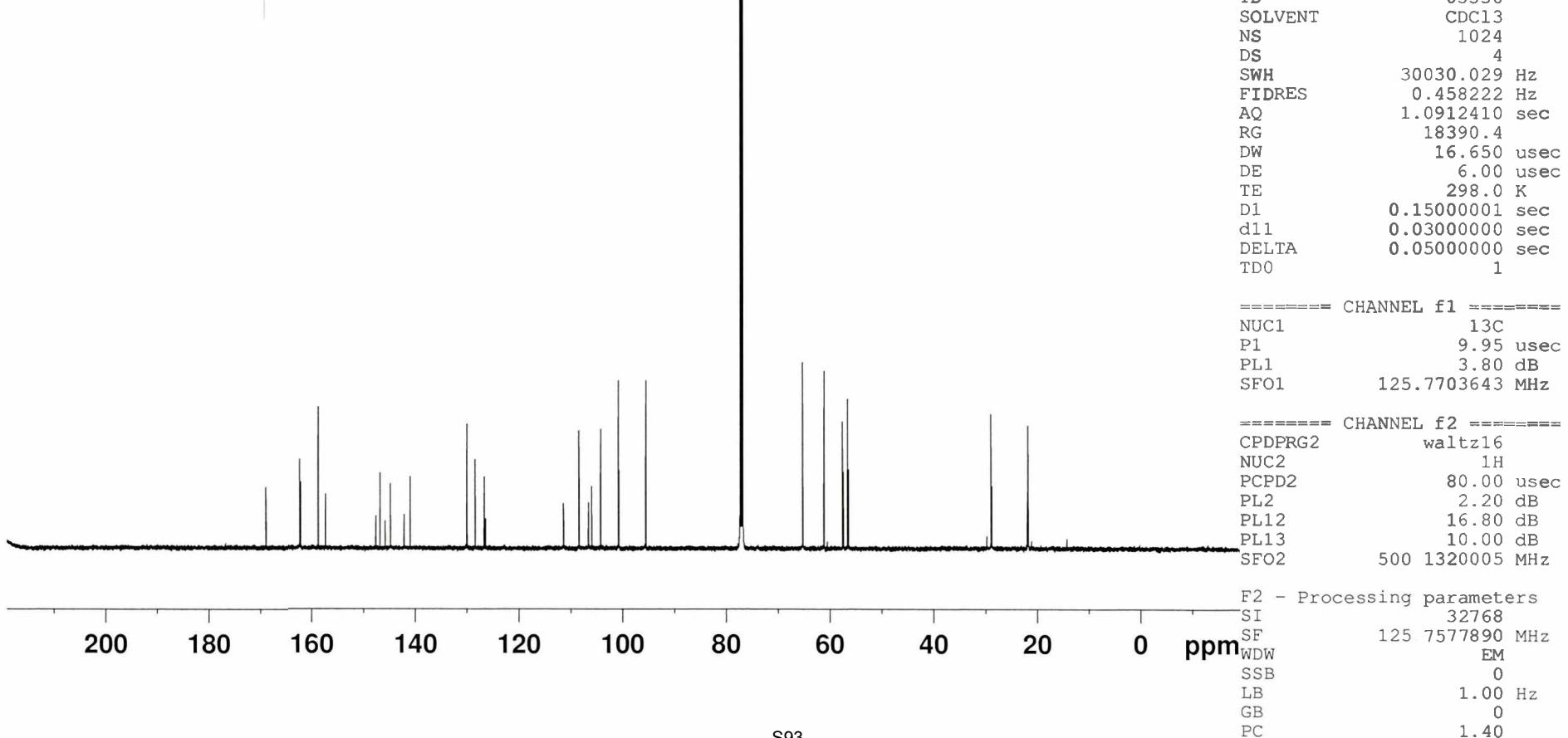
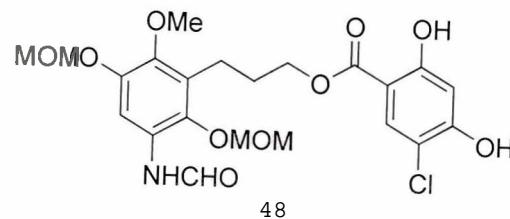


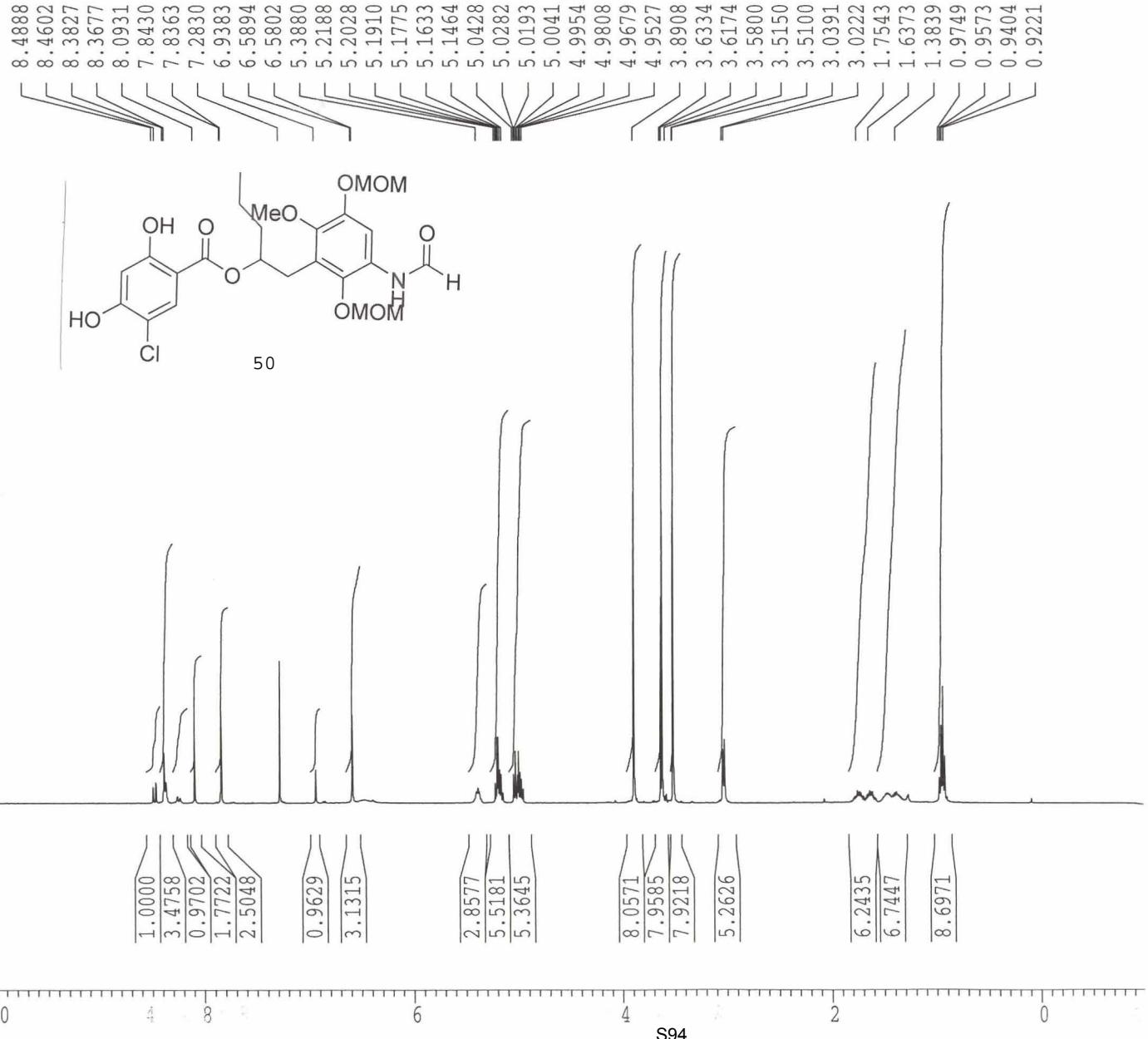
Current Data Parameters
 NAME gang04
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060503
 Time 16.01
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 181
 DW 48.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 ======
 NUC1 1H
 P1 14.90 usec
 PL1 2.20 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300469 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



ppm
10.9141

Current Data Parameters
 NAME sg443
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050415
 Time 10.26
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 228.1
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.00 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Current Data Parameters
 NAME sg442
 EXPNO 2
 PROCNO 1

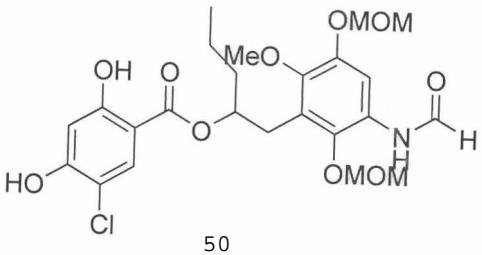
F2 - Acquisition Parameters
 Date_ 20050414
 Time 16.01
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.35213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

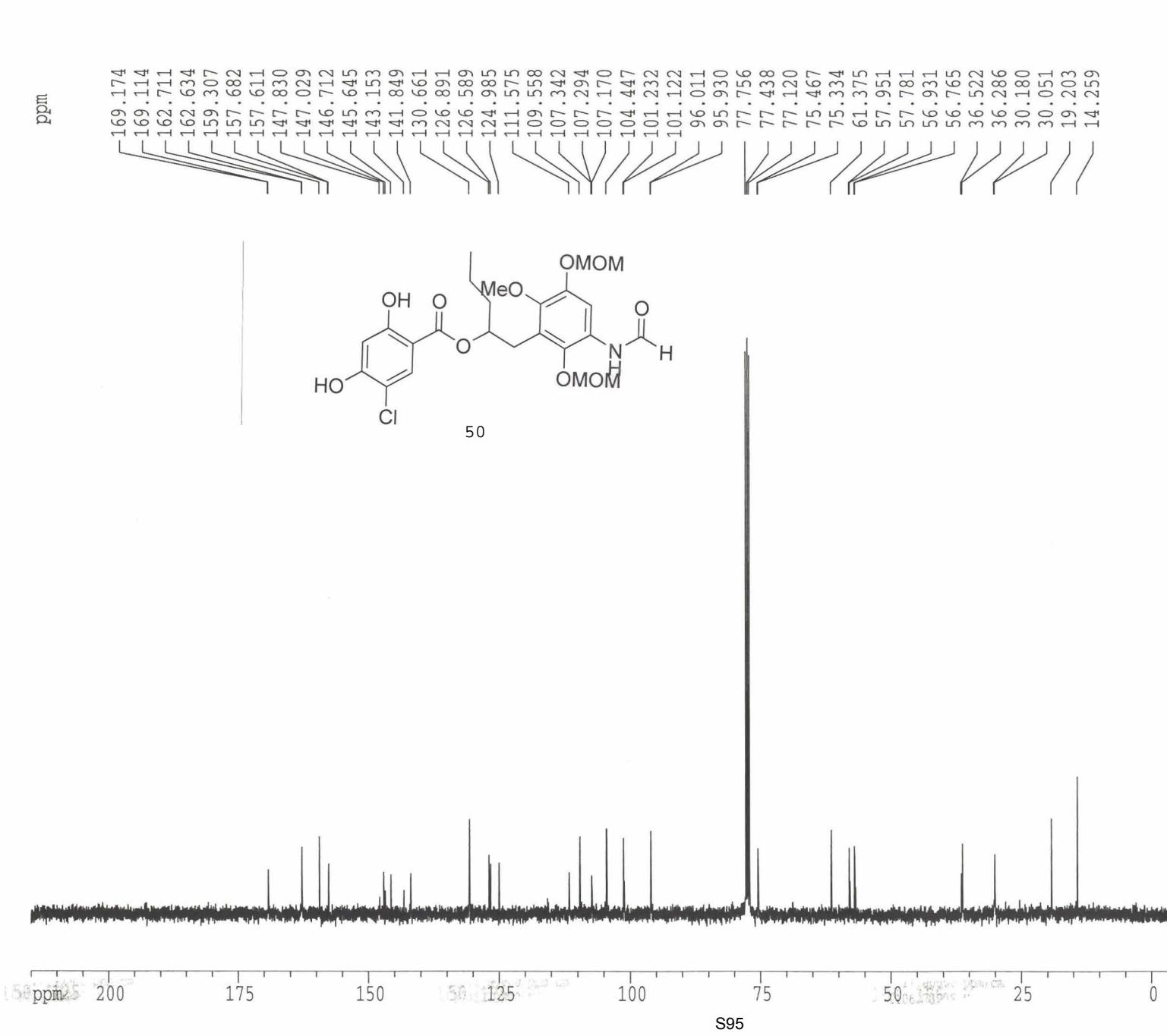
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SP 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

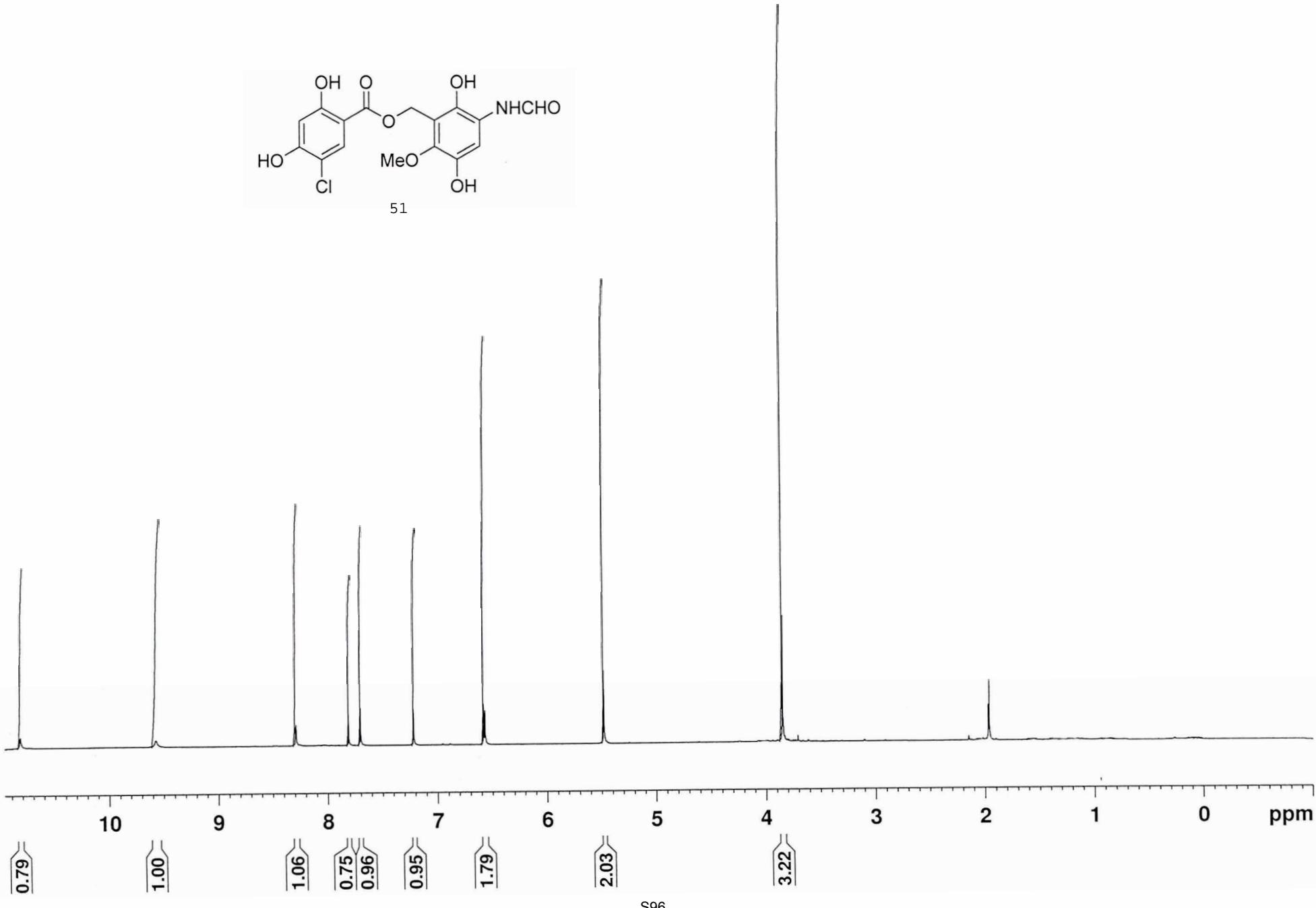
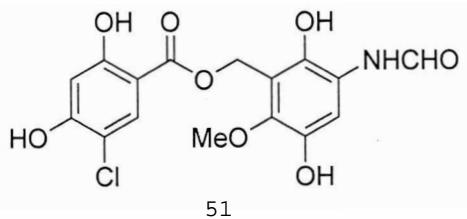
1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMMT 11.00000 ppm/cm
 HZCM 1106178999 Hz/cm

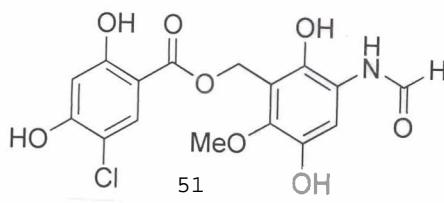


50

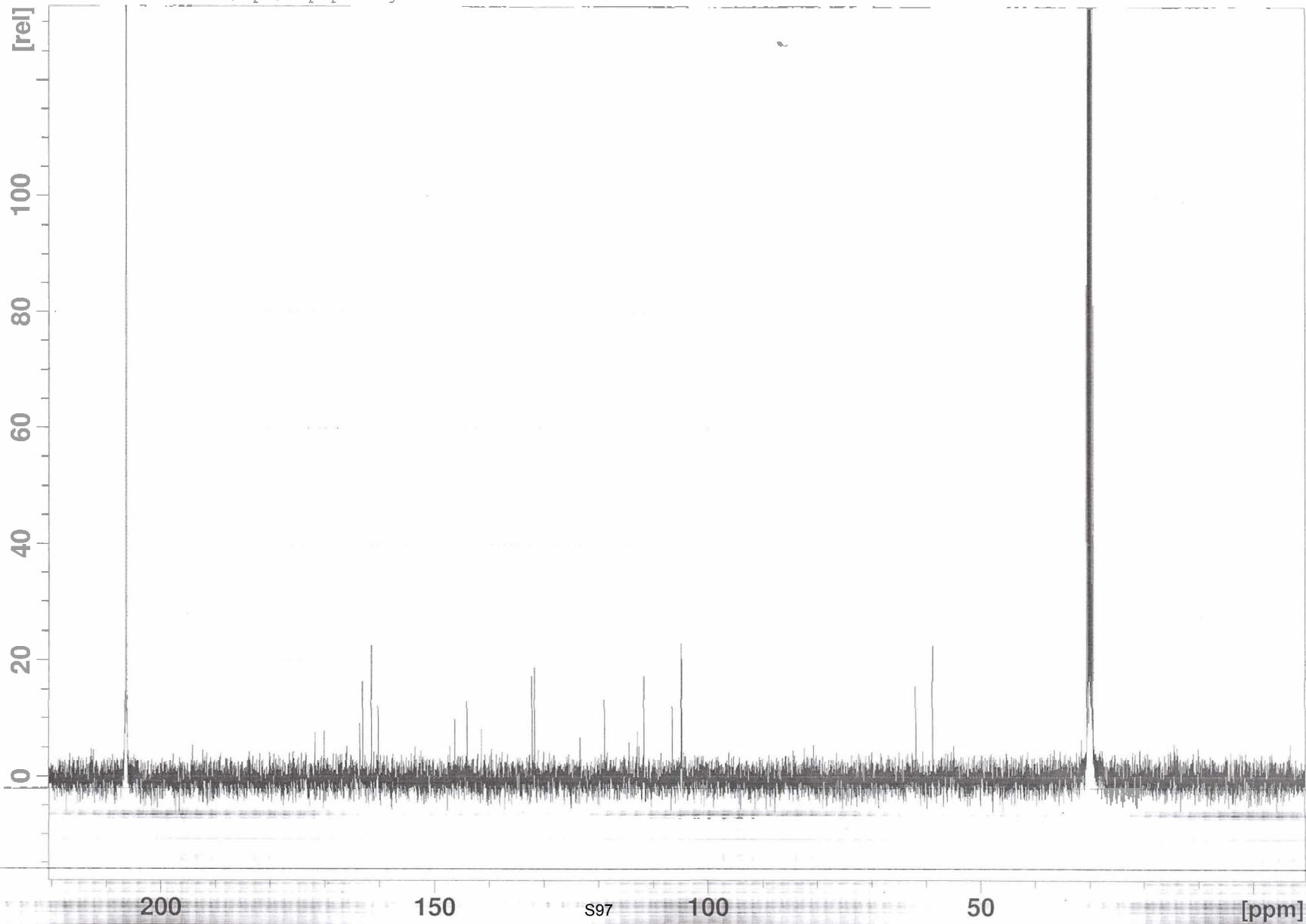


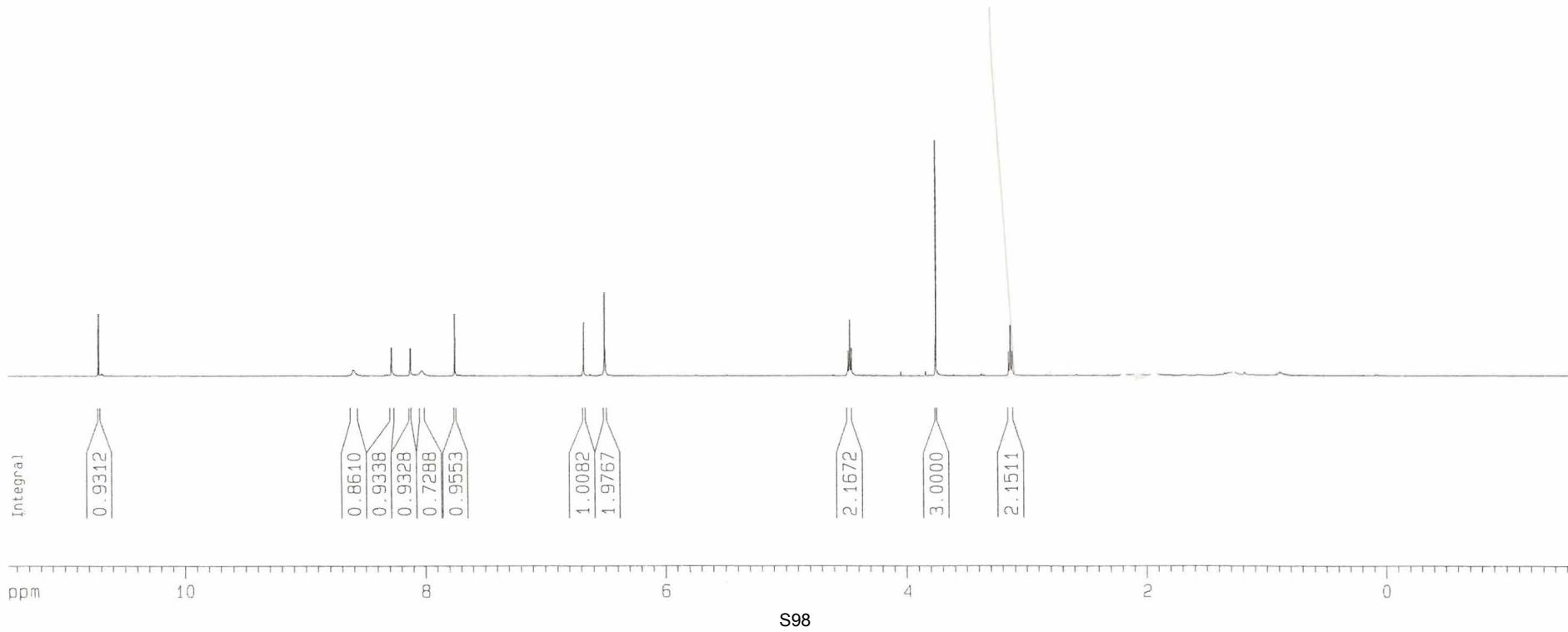
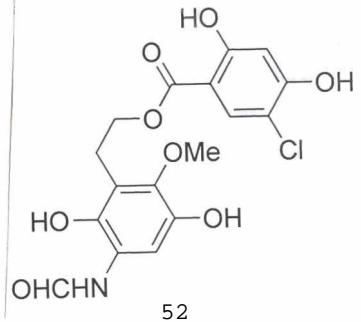
S95

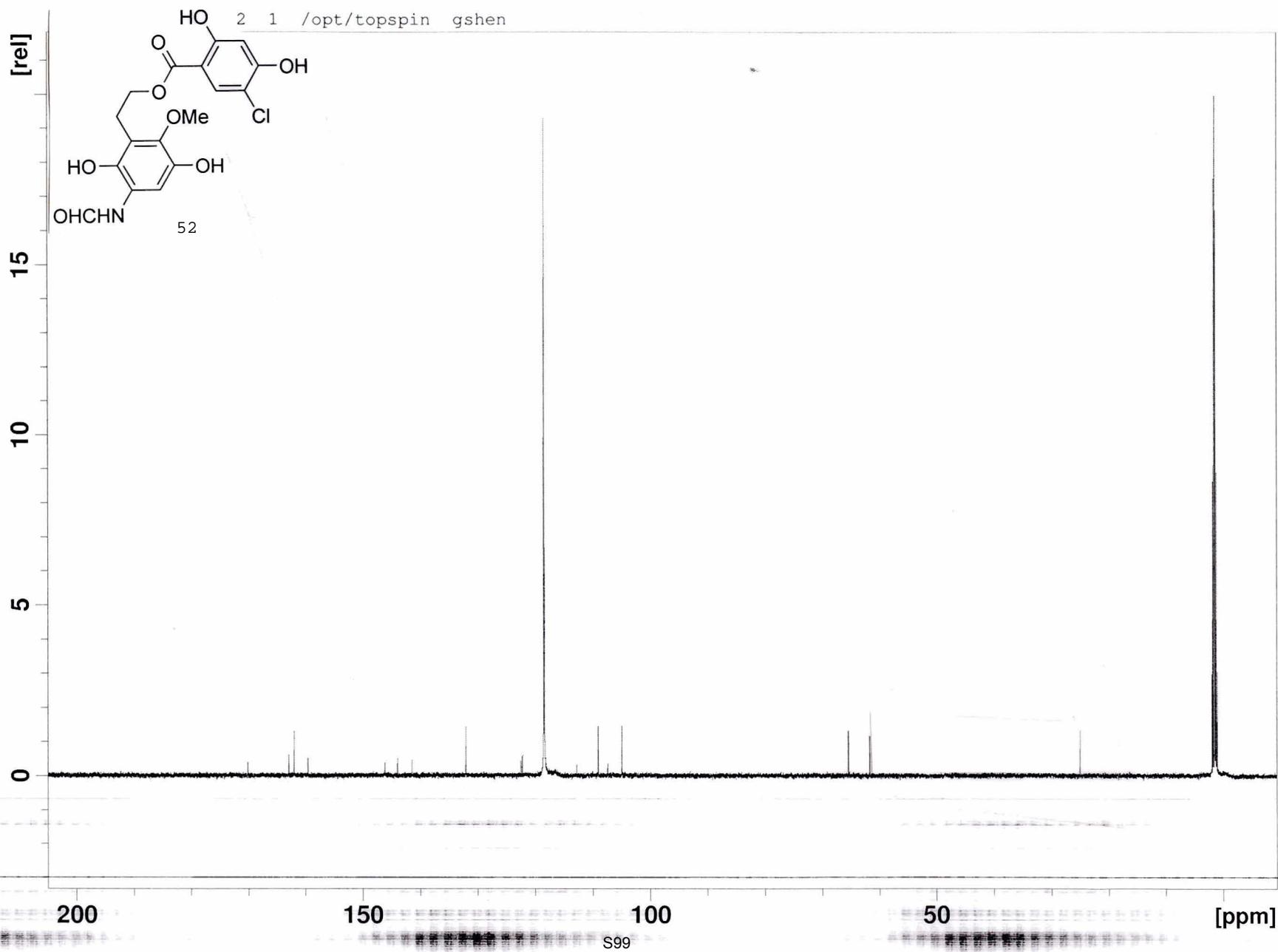


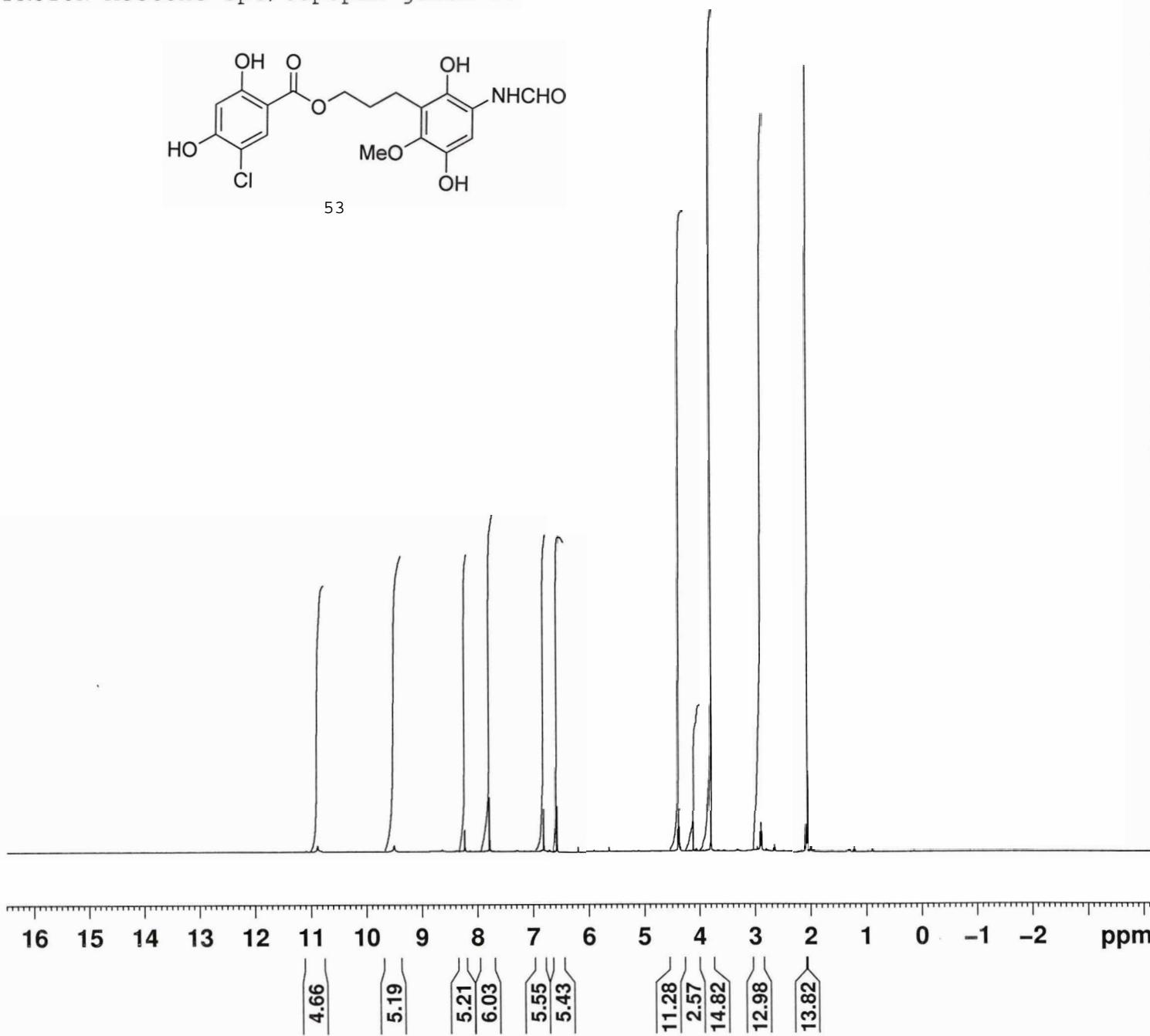
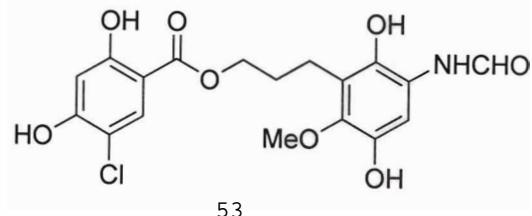


/opt/topspin gshen







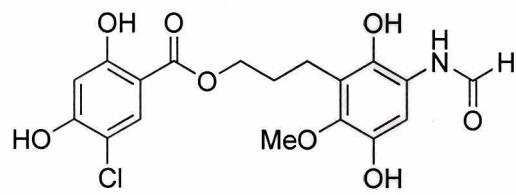


Current Data Parameters
 NAME 3c-nhcho
 EXPNO 1
 PROCNO 1

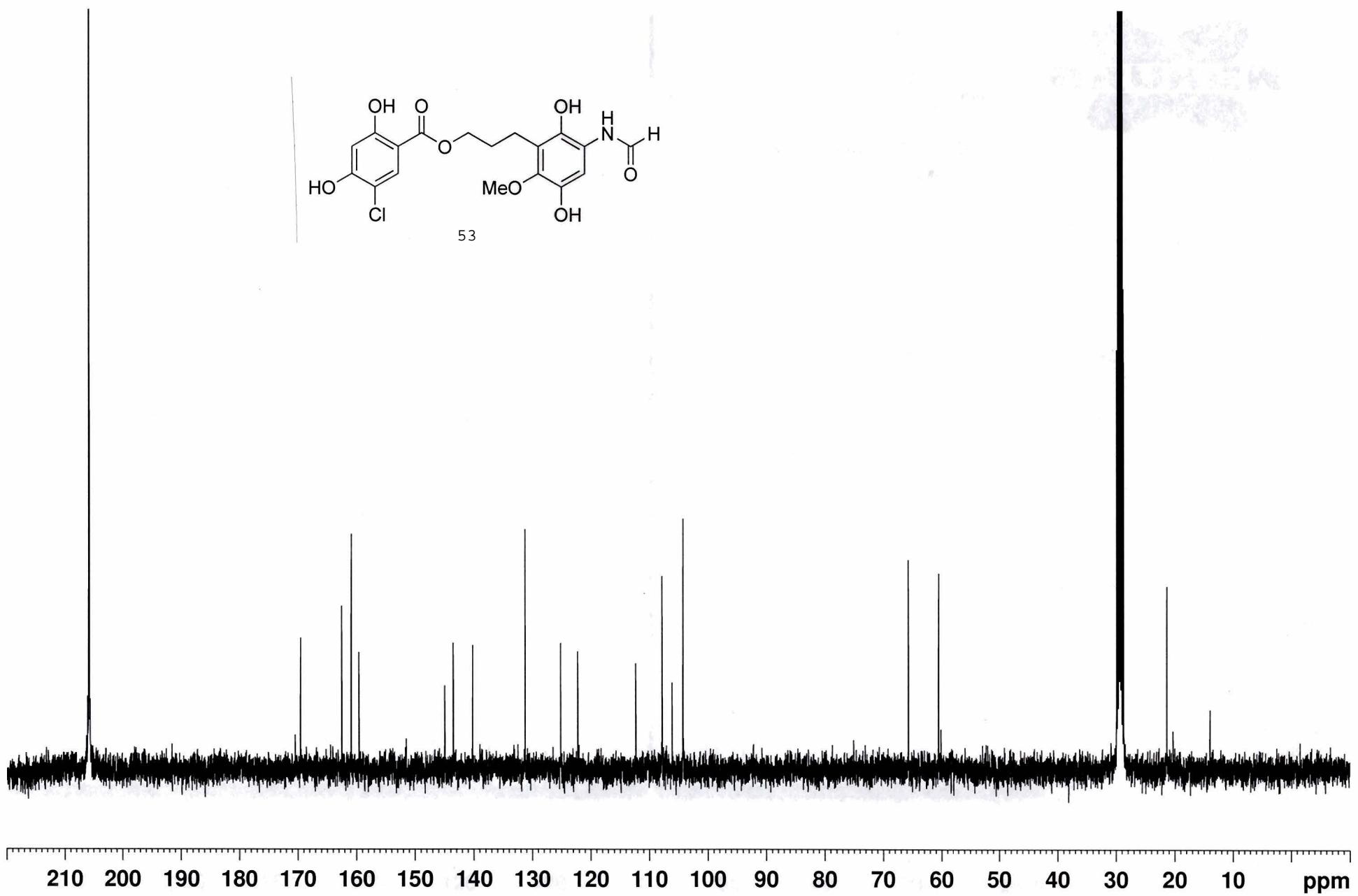
F2 - Acquisition Parameters
 Date 20060407
 Time 22.50
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 114
 DW 48.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.90 usec
 PL1 2.20 dB
 SFO1 500.13300885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.13000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



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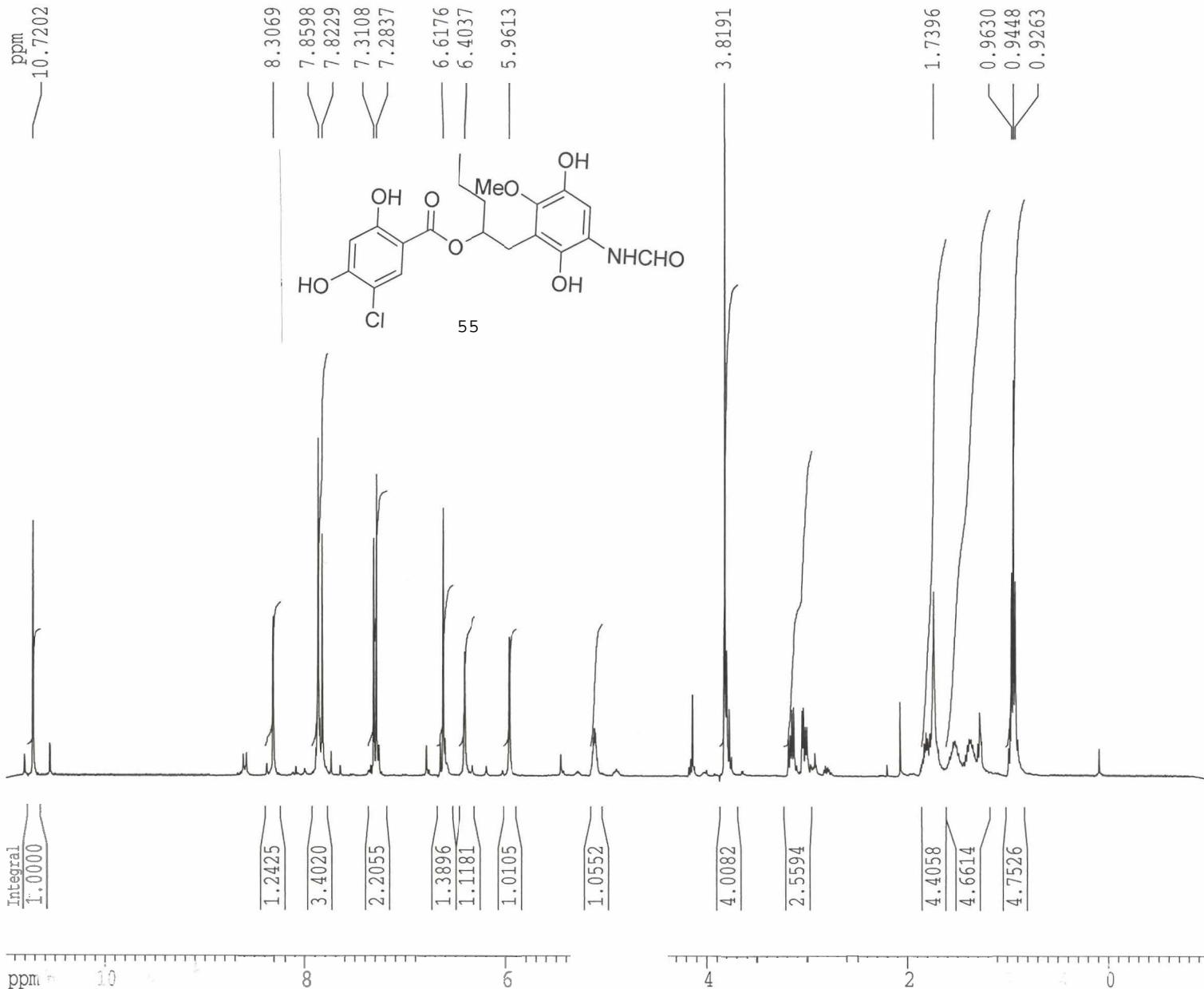
Current Data Parameters
 NAME sg447
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20050421
 Time 10.19
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 256
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

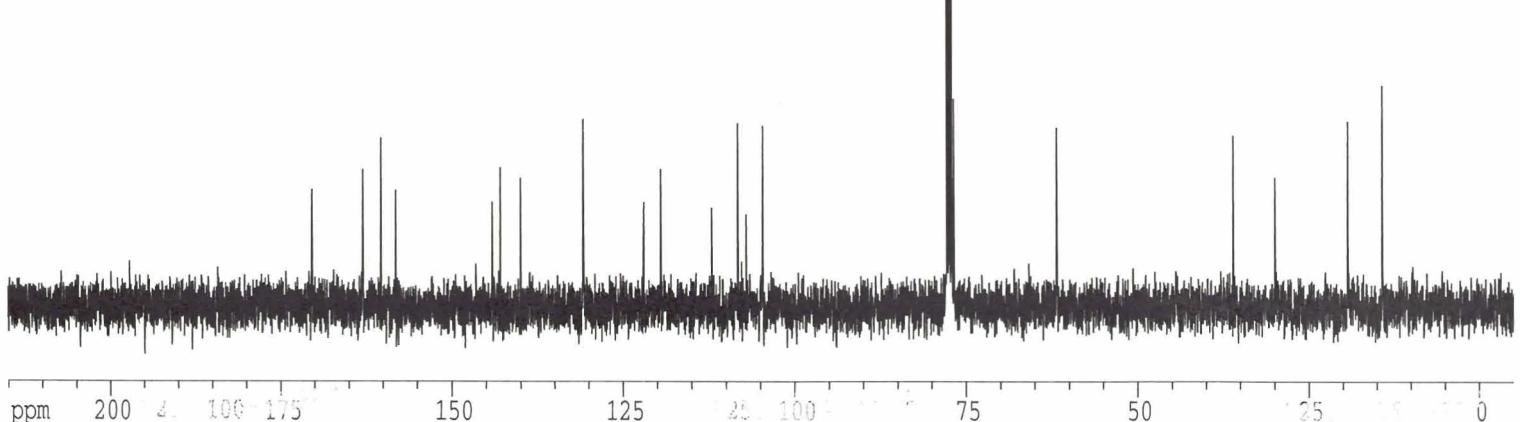
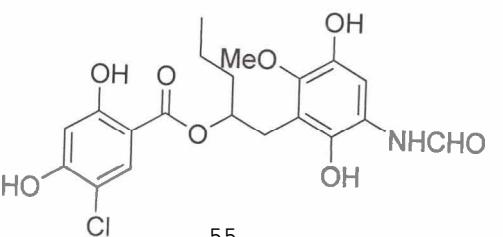
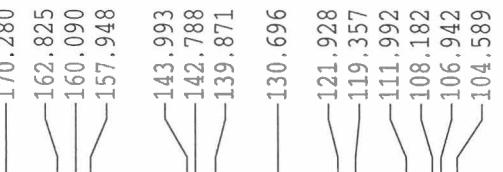
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400 1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400 1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm



ppm



Current Data Parameters
 NAME sg447
 EXPNO 2
 PROCN0 1

F2 - Acquisition Parameters

Date 20050421
 Time 10.34
 INSTRUM dix400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 505
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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

NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

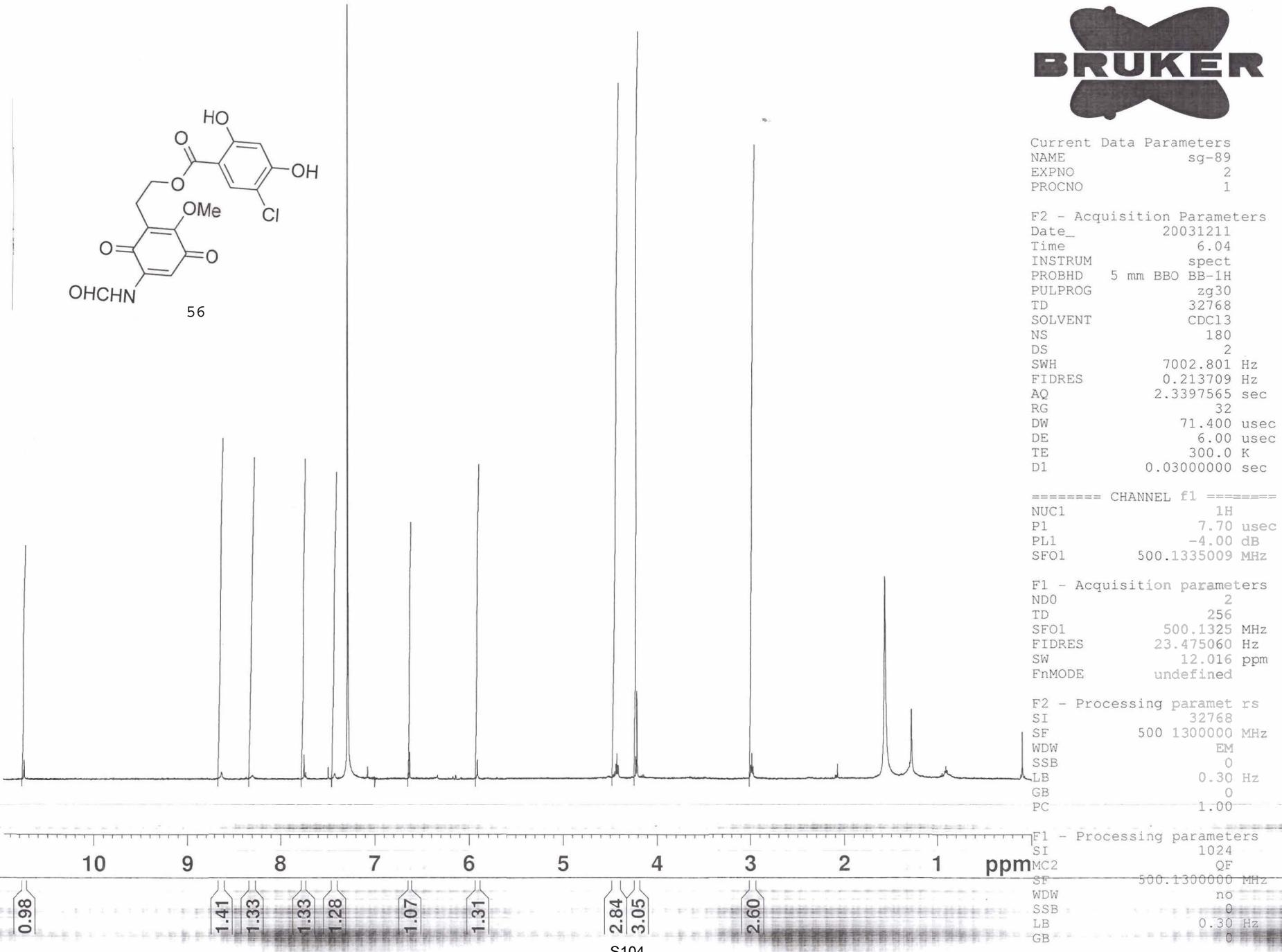
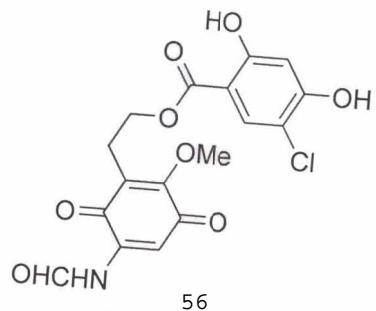
===== CHANNEL f2 =====

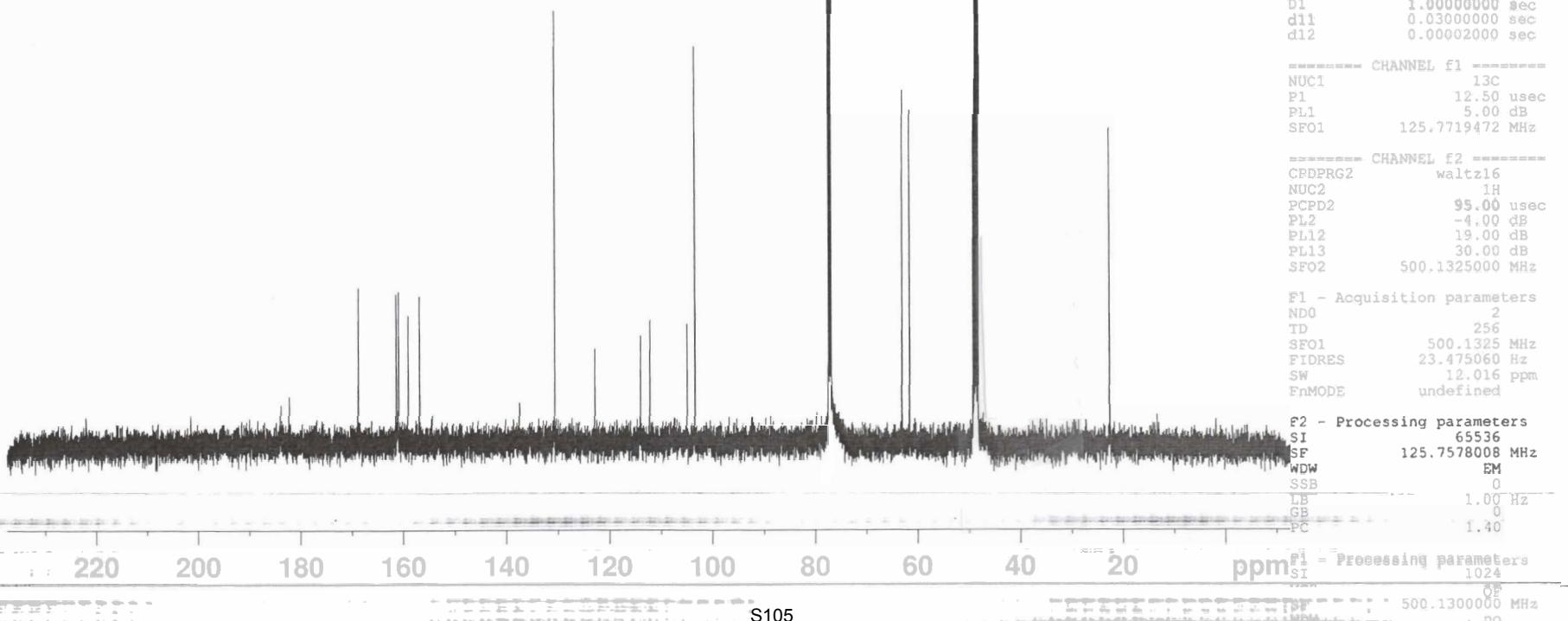
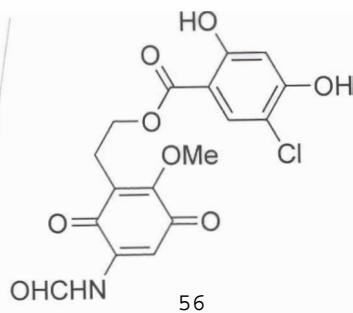
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 CY 20.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm





ppm

Integral
1.0000

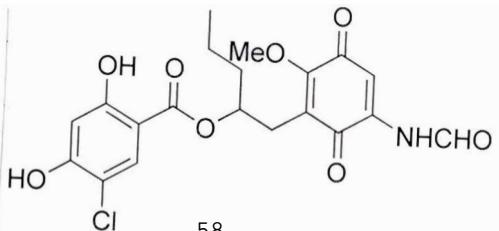
ppm

10.8020

7.7414
7.3641
7.2837

6.6025

58



4.1408

3.7762

2.8204

1.8805
1.2734
0.9944
0.9763
0.9580

1.0363

1.0762

1.0627

0.9707

1.1612

1.2111

3.1498
1.0367

2.2835

1.2847
3.3580
3.0595
3.7379

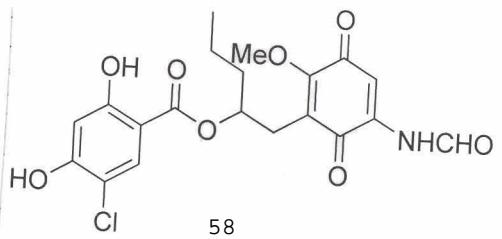
Current Data Parameters
 NAME sg448
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050422
 Time 9.50
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 406.4
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

==== CHANNEL f1 ====
 NUC1 1H
 F1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 7.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm



Current Data Parameters
 NAME sg448
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050422
 Time 18.05
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2048
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420883 sec
 RG 8192
 DW 15.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

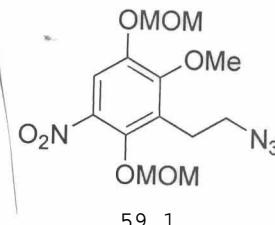
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -4.90 dB
 SFO1 125.7697360 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPDRG2 80.00 usec
 PL2 -5.00 dB
 PL12 9.54 dB
 PL13 10.00 dB
 SFO2 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

200 180 160 140 120 100 80 60 40 20

ppm

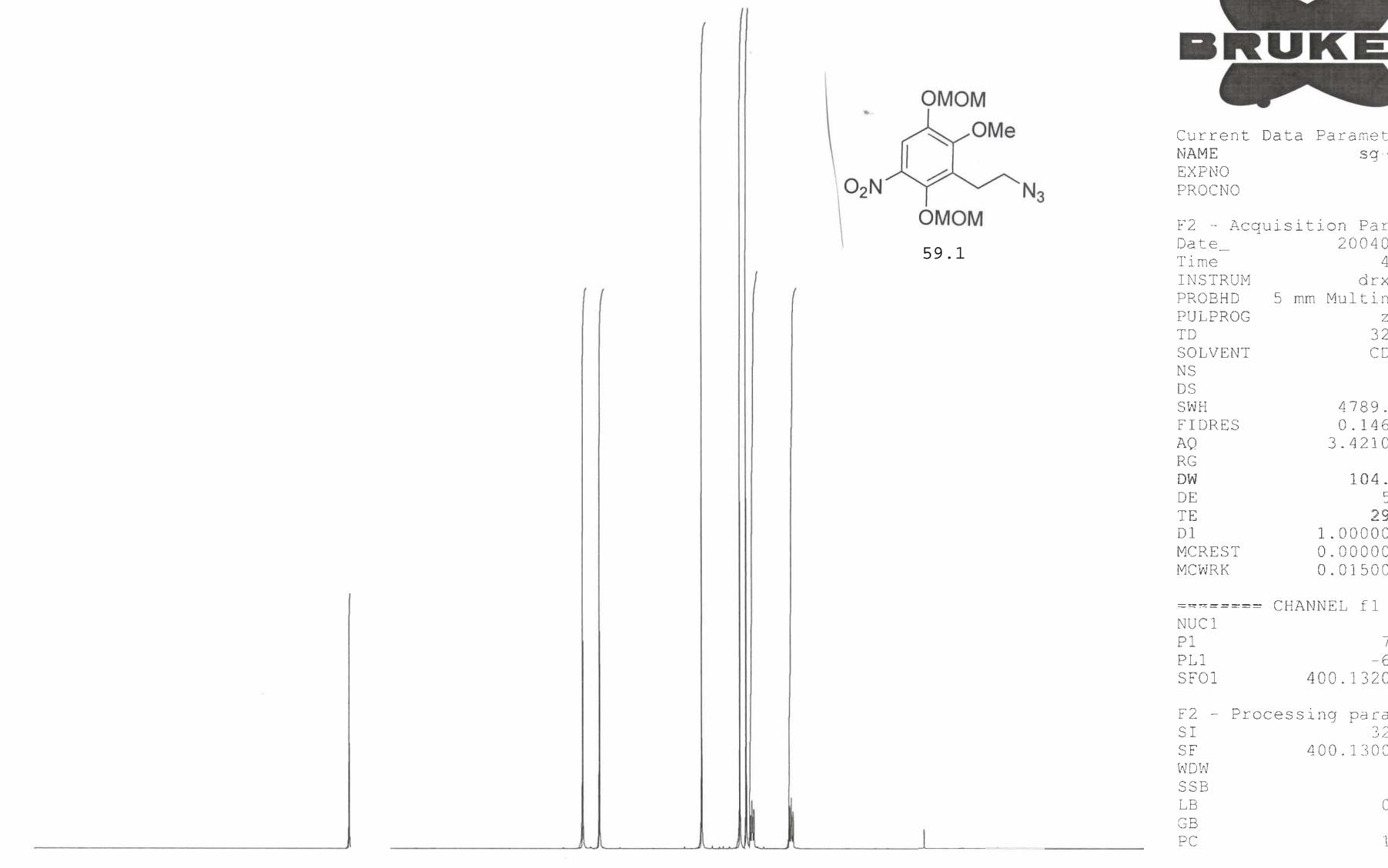


Current Data Parameters
NAME sg·471
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040819
Time 4.59
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 64
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



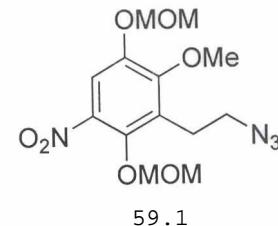
10 9 8 7 6 5 4 3 2 1 0 ppm

1.00 2.09 2.08 3.07 3.12 3.12 3.15 2.09

S108



Current Data Parameters
 NAME sg-472
 EXPNO 1
 PROCNO 1



F2 - Acquisition Parameters
 Date_ 20040819
 Time 5.01
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 43
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

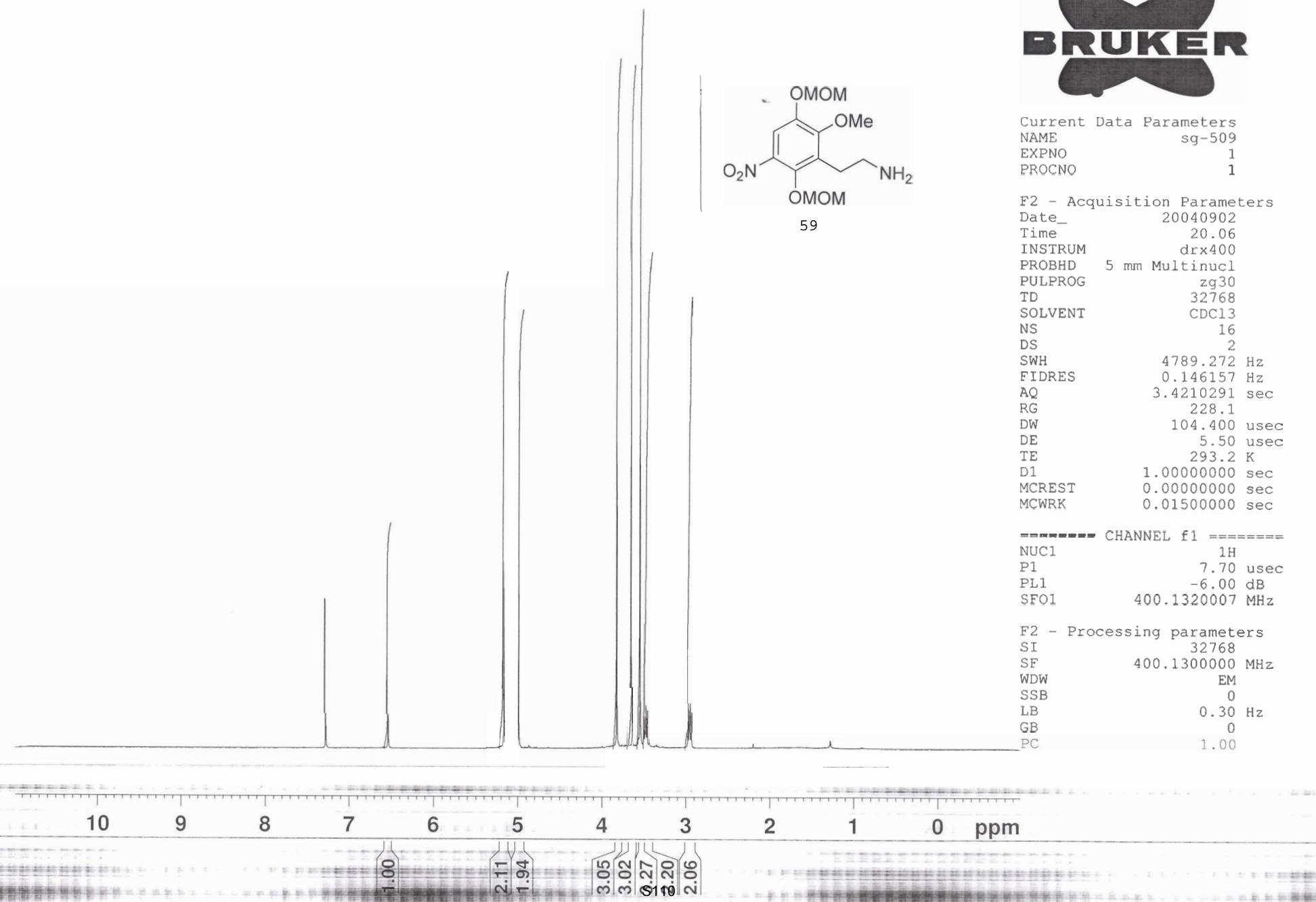
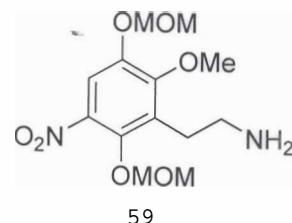
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz

200 180 160 140 120 100 80 60 40 20

ppm





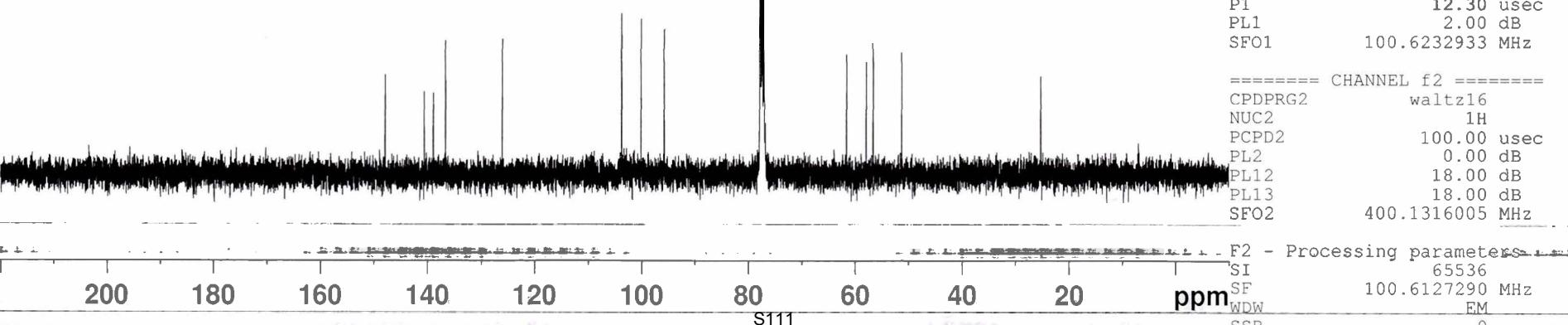
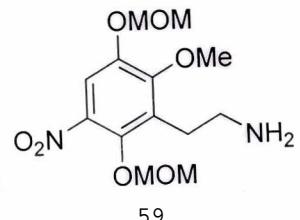
Current Data Parameters
NAME sg-513
EXPNO 1
PROCNO 1

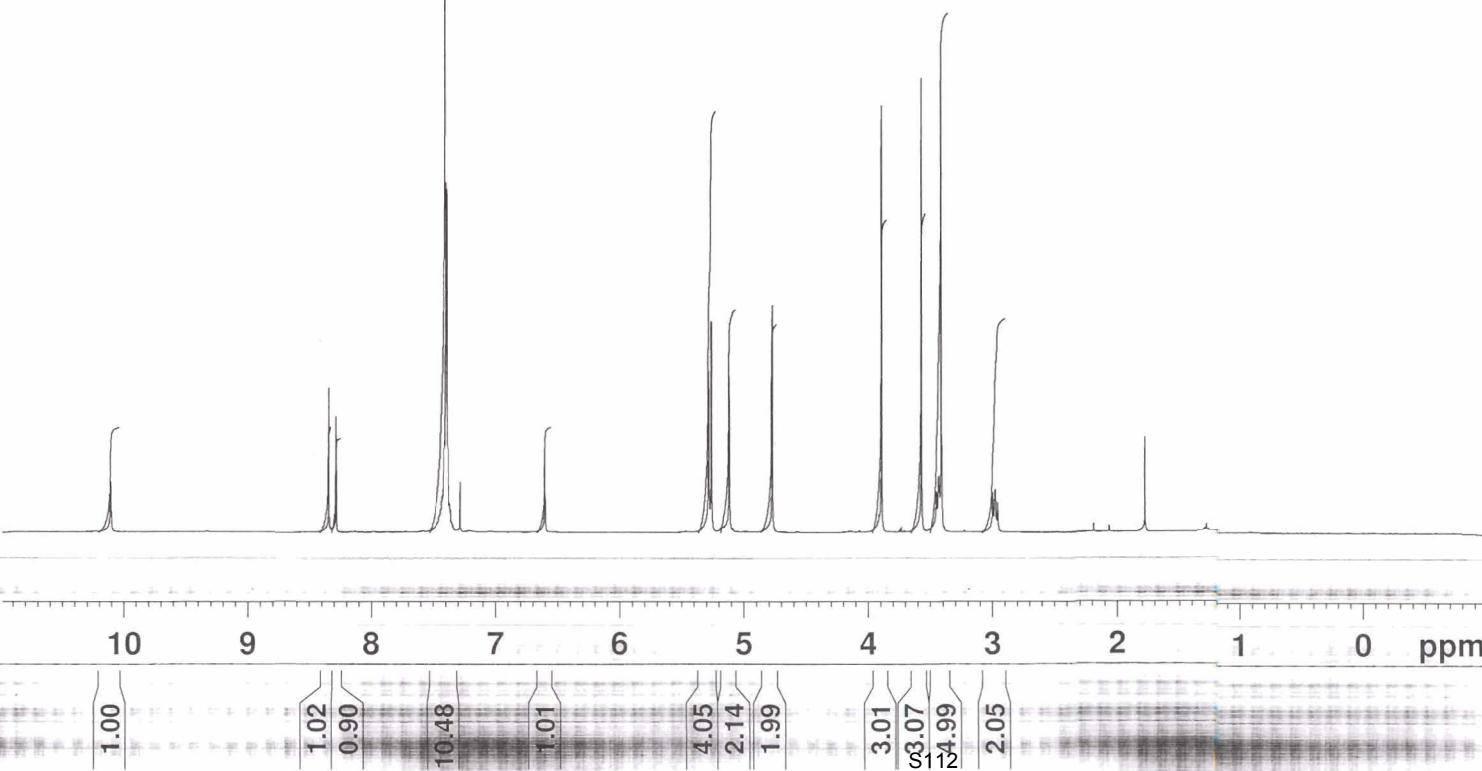
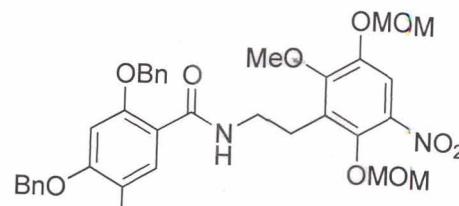
F2 - Acquisition Parameters
Date_ 20040907
Time 4.17
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2124
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 2298.8
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.30 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0



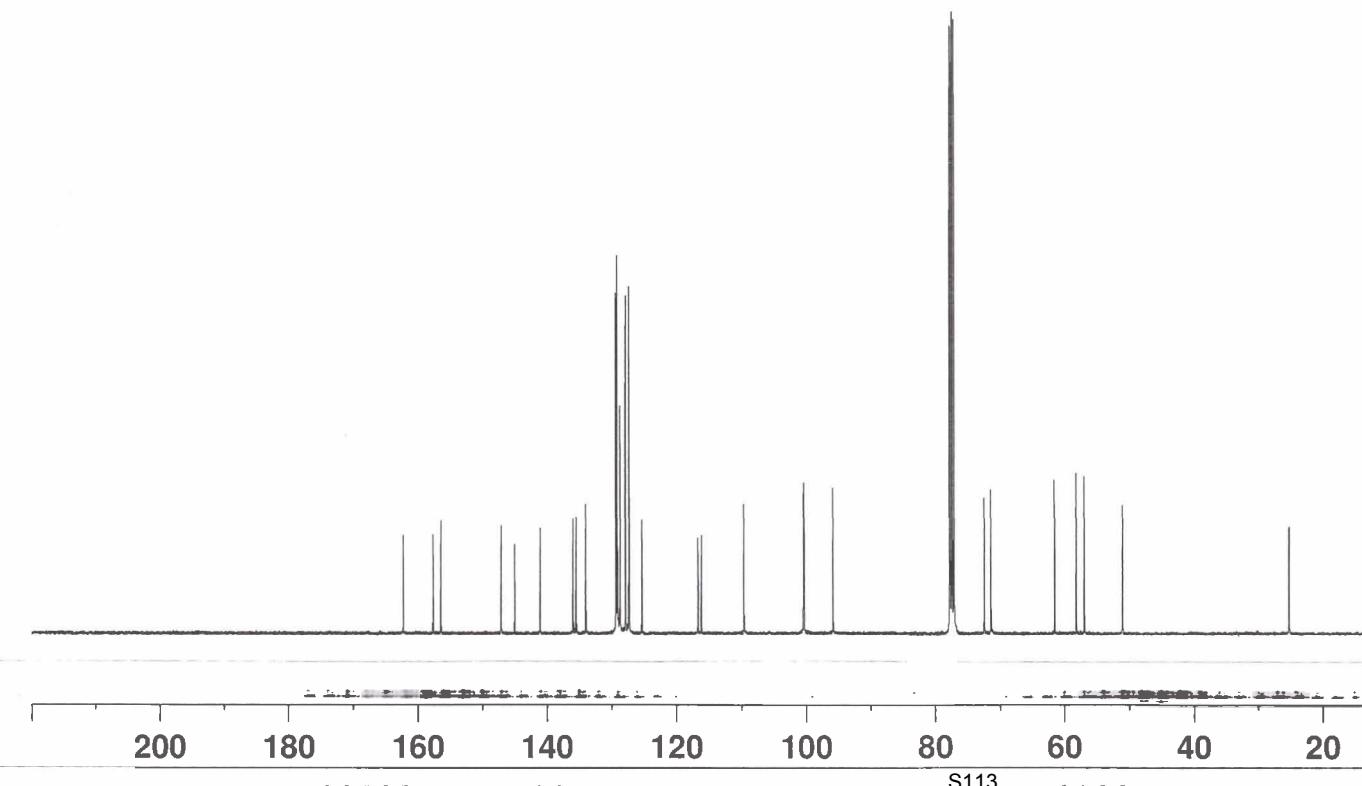
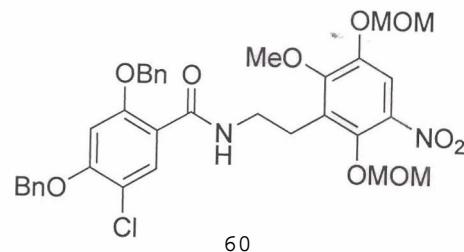


Current Data Parameters
 NAME sg-522
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040912
 Time 6.50
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 9
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



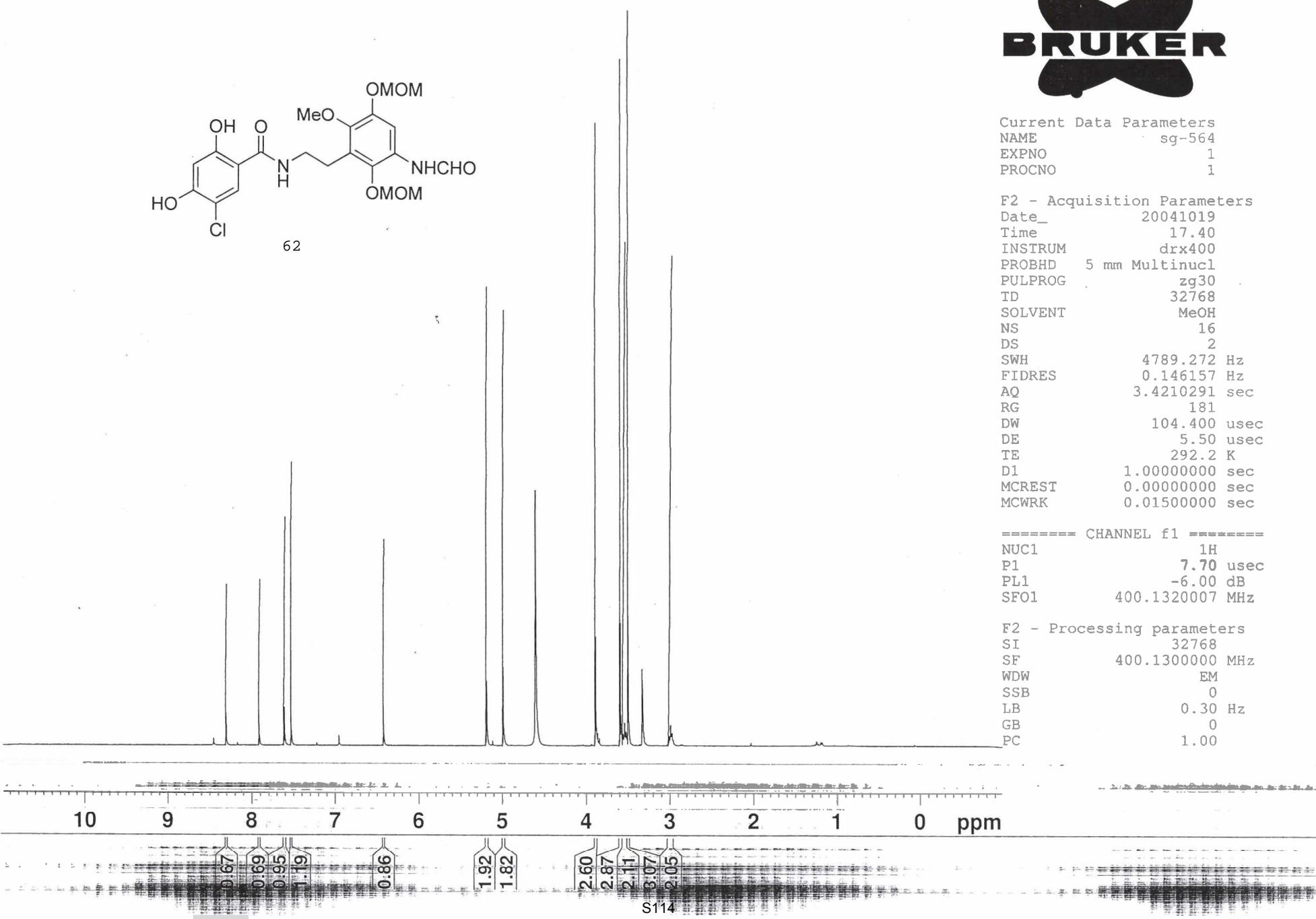
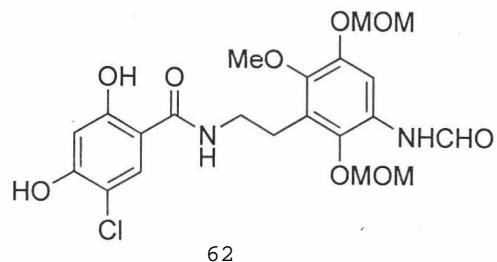
Current Data Parameters
 NAME sg-522
 EXPNO 2
 PROCNO 1

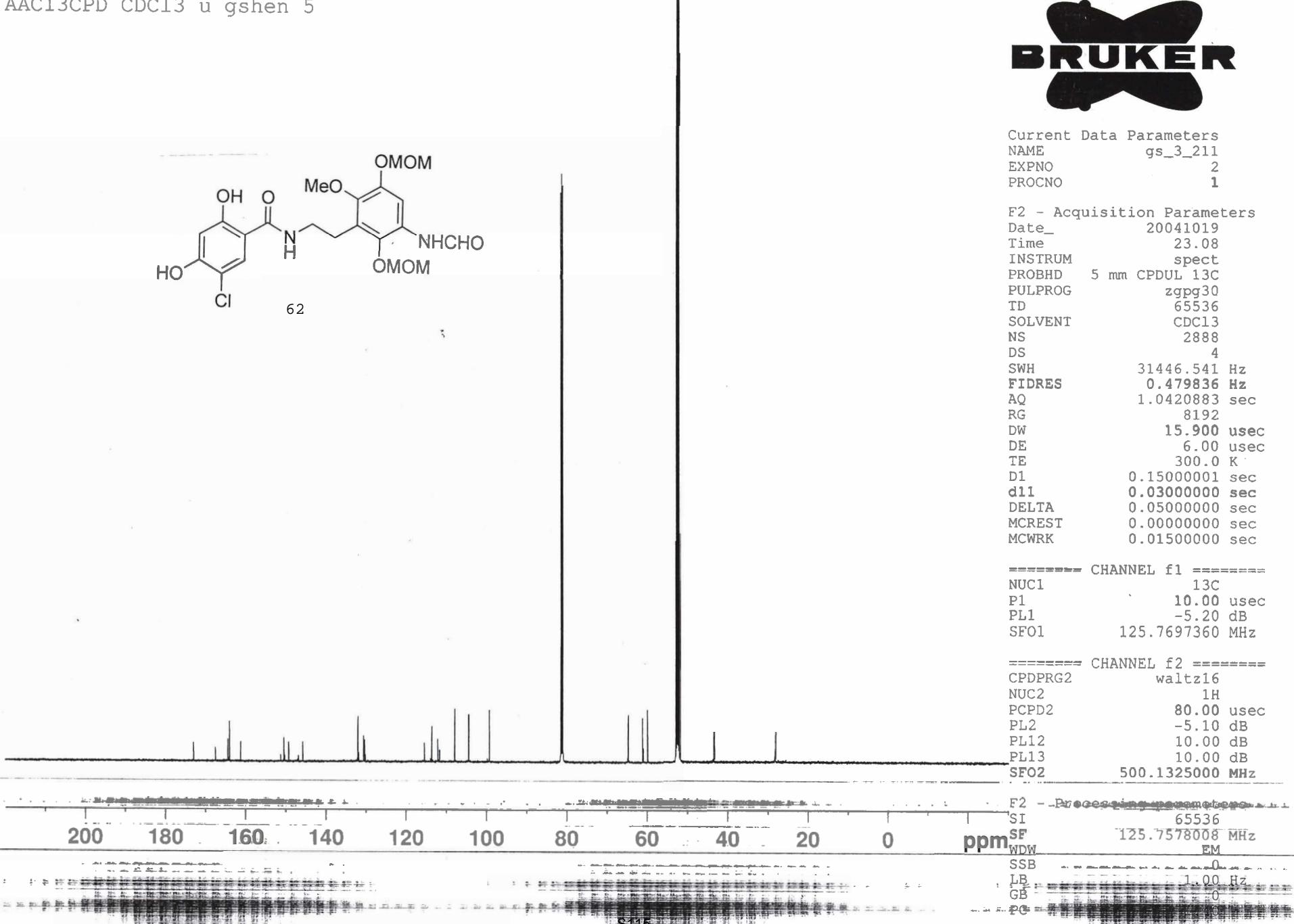
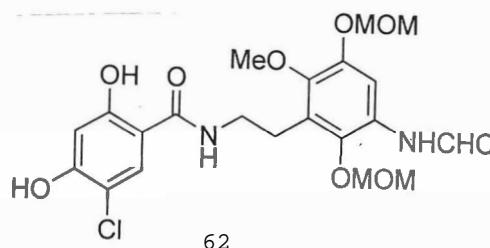
F2 - Acquisition Parameters
 Date_ 20040912
 Time 15.46
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 9216
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 645.1
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

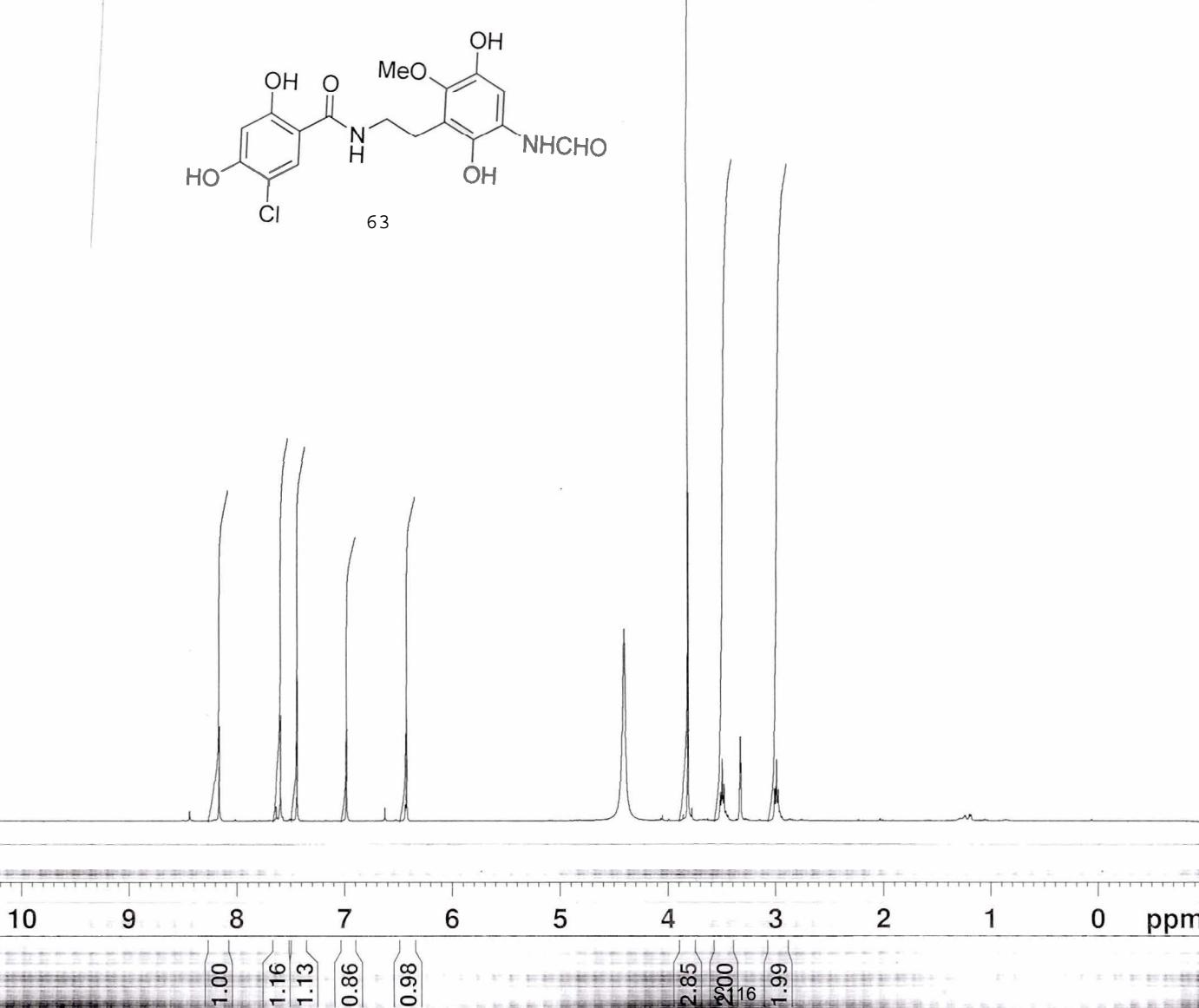
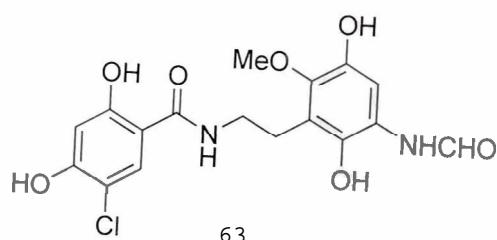
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0





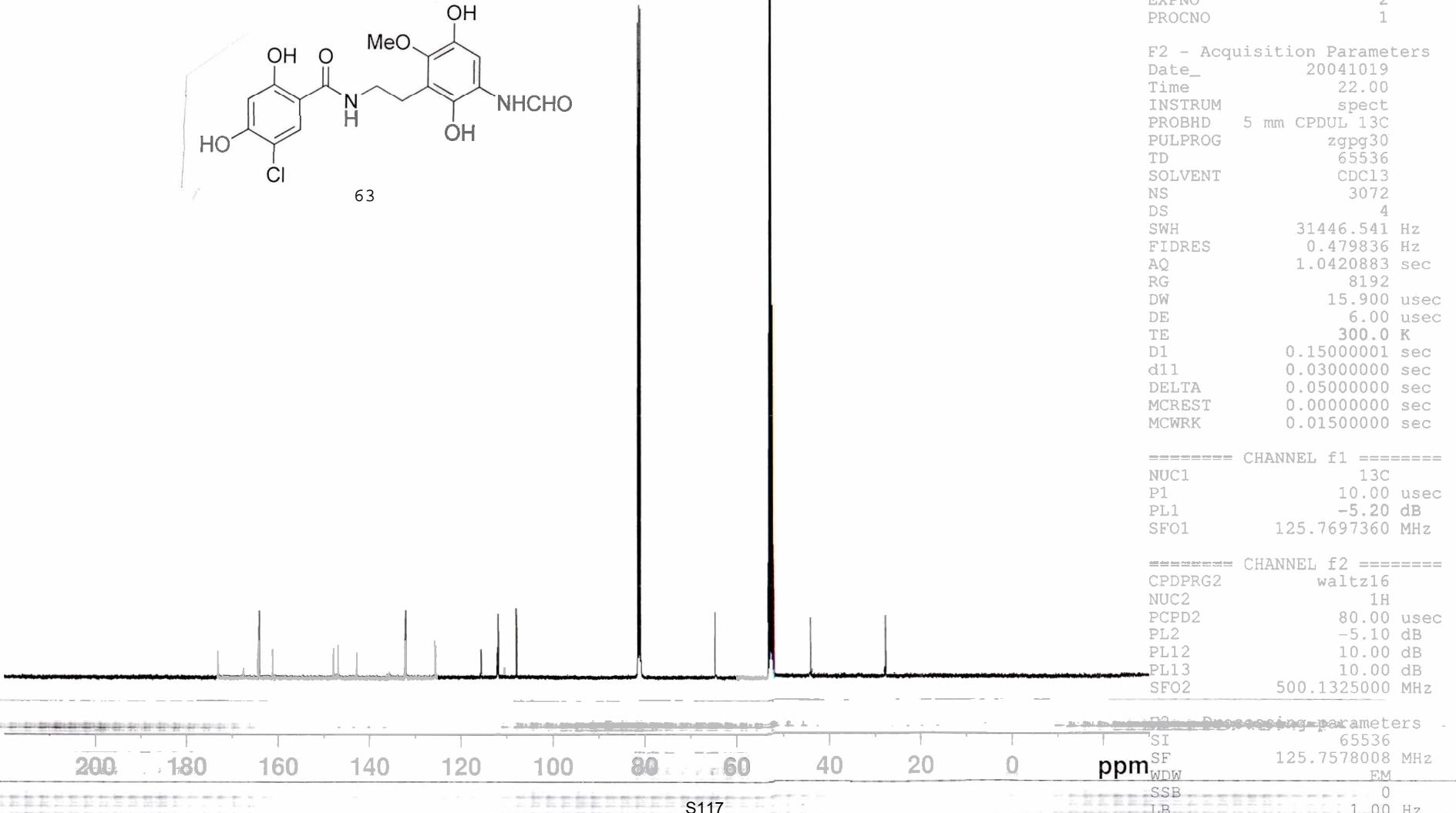
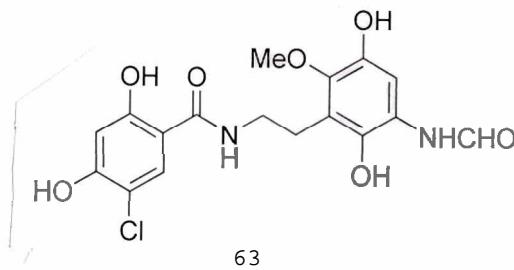


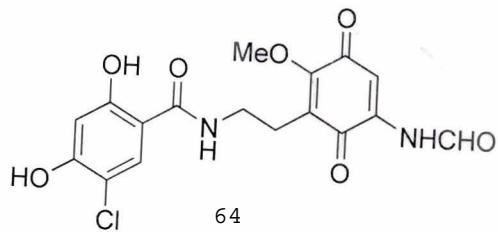
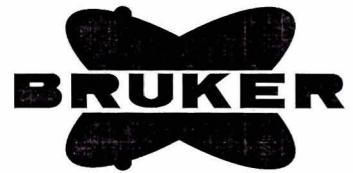
Current Data Parameters
NAME sg-565
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041019
Time 17.47
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT MeOH
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 181
DW 104.400 usec
DE 5.50 usec
TE 292.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

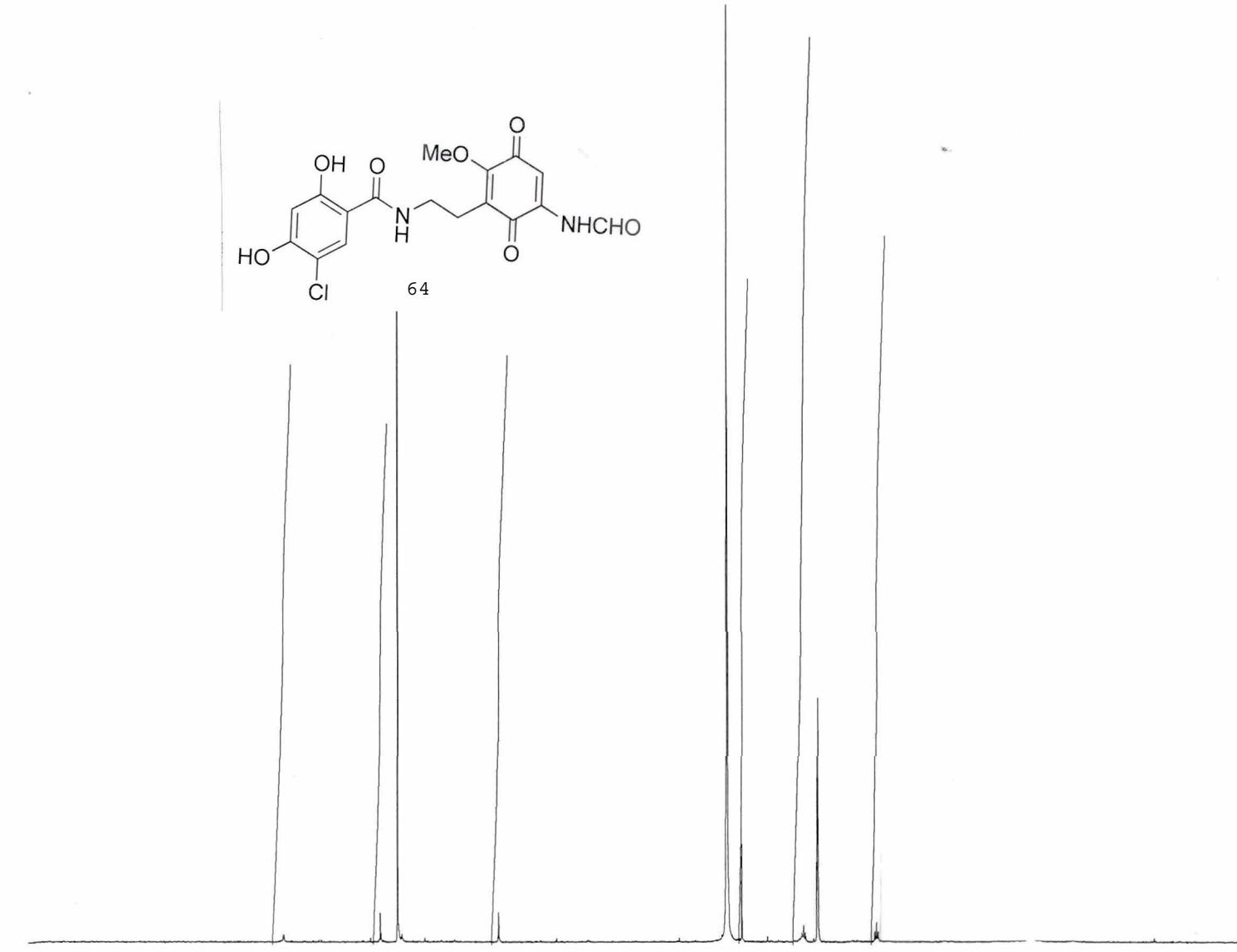
===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





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Current Data Parameters
NAME sg-566 amide-quinone
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041022
Time 16.51
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT MeOH
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 256
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1
P1 7.70 usec
PL1 -6.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 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

1.00

0.90

1.02

1.15

1.56

1.22

S118

Current Data Parameters
 NAME sg_3_q
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20041029
 Time 18.40
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOH
 NS 2324
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420883 sec
 RG 8192
 DW 15.900 usec
 DE 6.00 usec
 TE 301.0 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

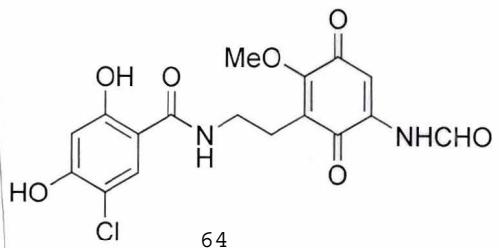
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -5.20 dB
 SF01 125.7697360 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.10 dB
 PL12 10.00 dB
 PL13 10.00 dB
 SF02 500.1325000 MHz

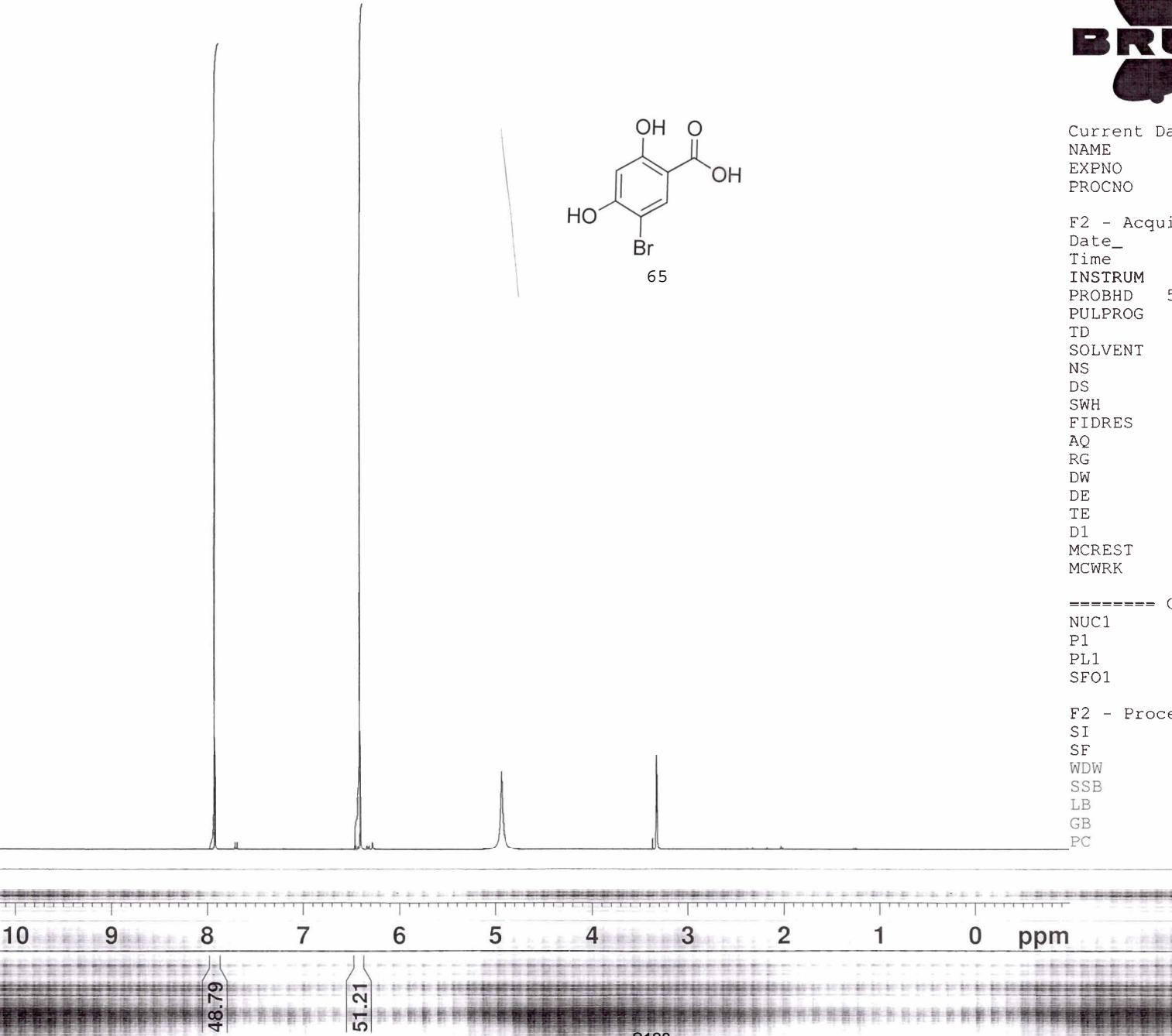
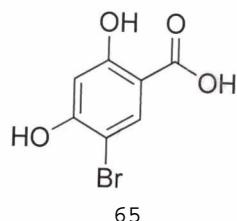
F1 - Acquisition parameters
 NDO 2
 TD 256
 SF01 500.1325 MHz
 FIDRES 23.475060 Hz
 SW 12.016 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 65536
 SF 125.7578008 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SL 1024
 MC2 QF
 SE 500.1300000 MHz
 SP 1.0000000 sec
 F 1.0000000 sec
 NO : 1



200 180 160 140 120 100 80 60 40 20 0 ppm

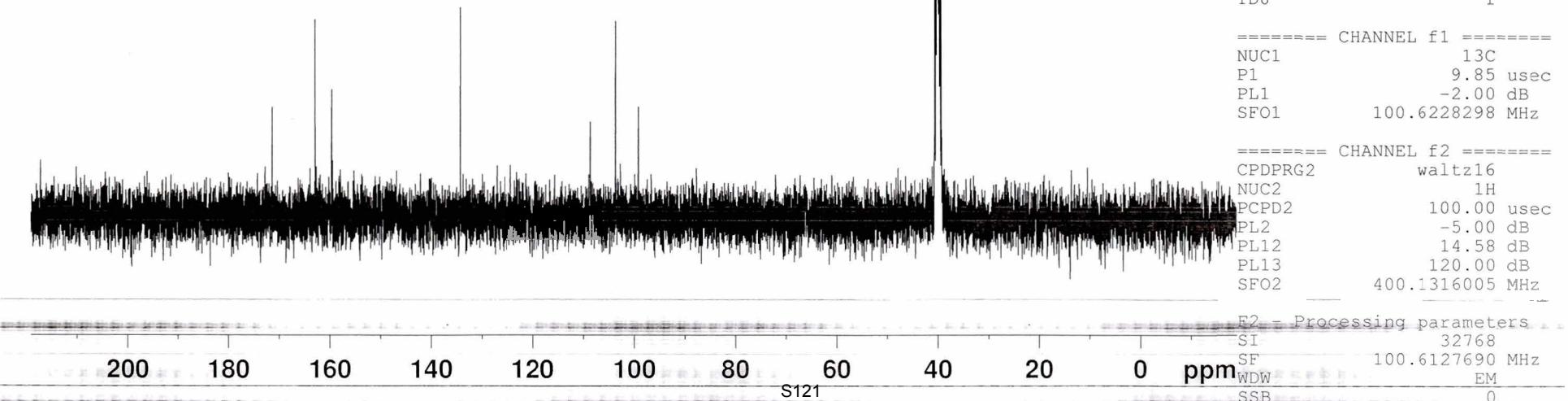
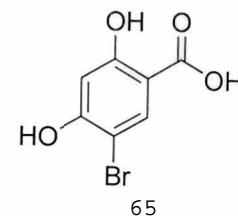


Current Data Parameters
 NAME sg454
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050608
 Time 2.00
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT MeOH
 NS 12
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 456.1
 DW 104.400 usec
 DE 5.50 usec
 TE 295.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 ======
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



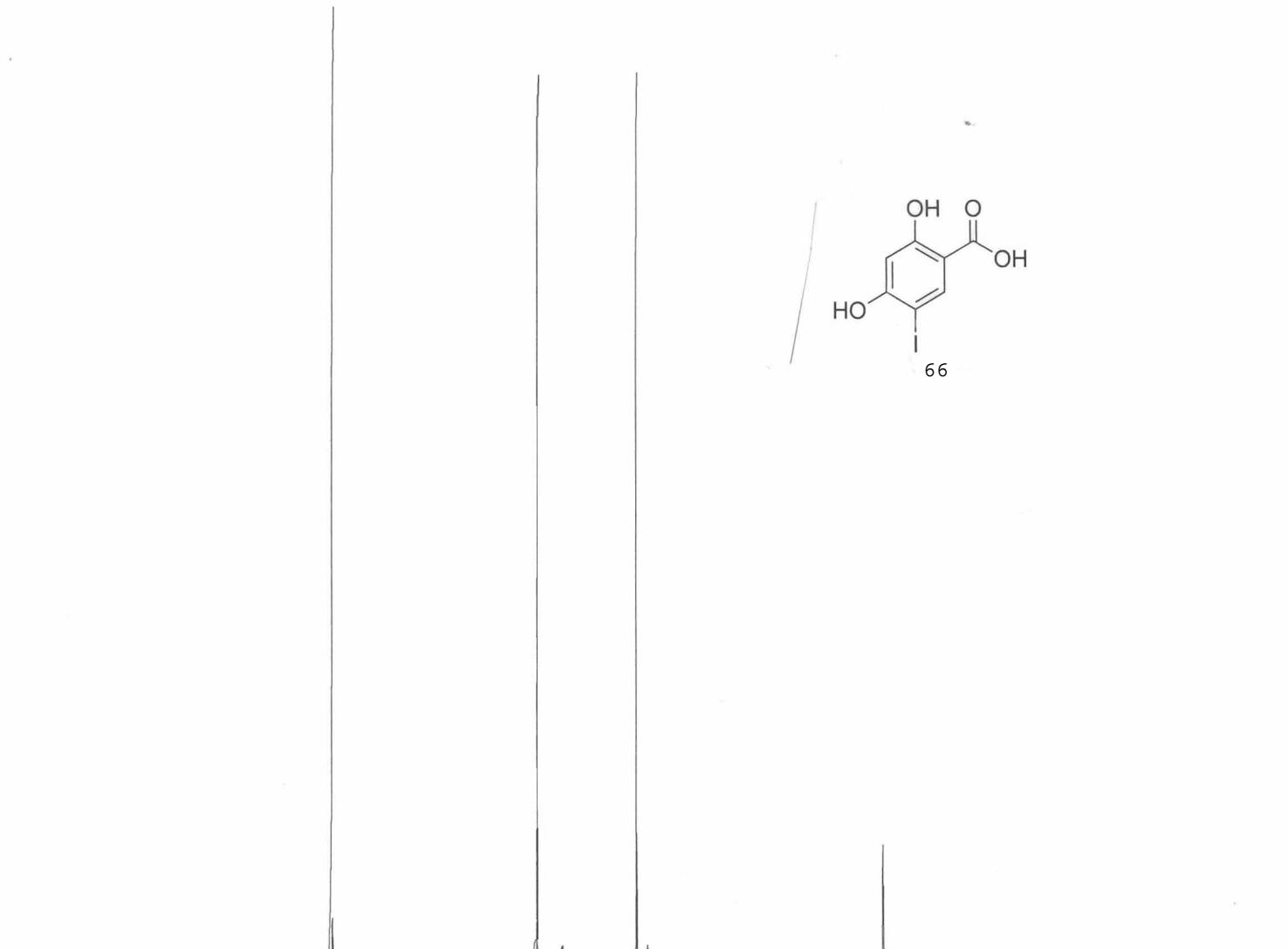
Current Data Parameters
NAME gang04
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20060415
Time 0.24
INSTRUM drx400
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 253
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.85 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 14.58 dB
PL13 120.00 dB
SFO2 400.1316005 MHz

E2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0



Current Data Parameters
NAME gang05
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060415
Time 1.03
INSTRUM drx400
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 13
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 456.1
DW 60.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PL1 -5.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

38.49

35.75

35.84



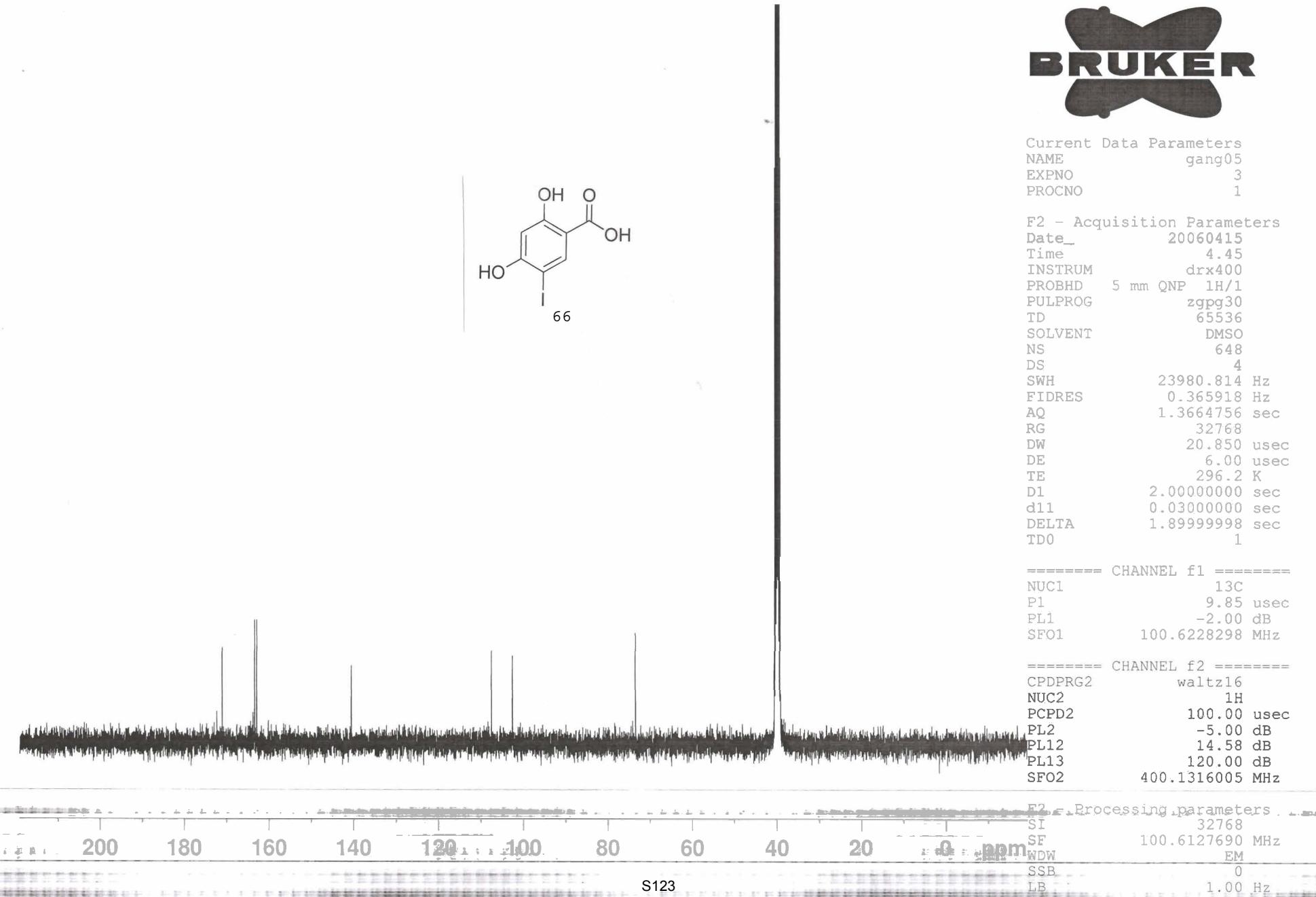
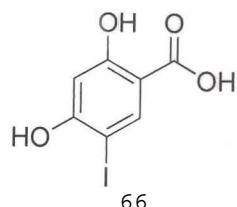
Current Data Parameters
NAME gang05
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060415
Time 4.45
INSTRUM drx400
PROBHD 5 mm QNP 1H/1
PULPROG zpg30
TD 65536
SOLVENT DMSO
NS 648
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.85 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 14.58 dB
PL13 120.00 dB
SFO2 400.1316005 MHz

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



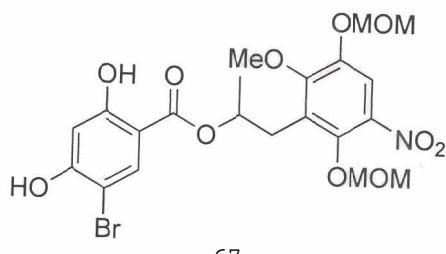


Current Data Parameters
NAME sg464
EXPNO 1
PROCNO 1

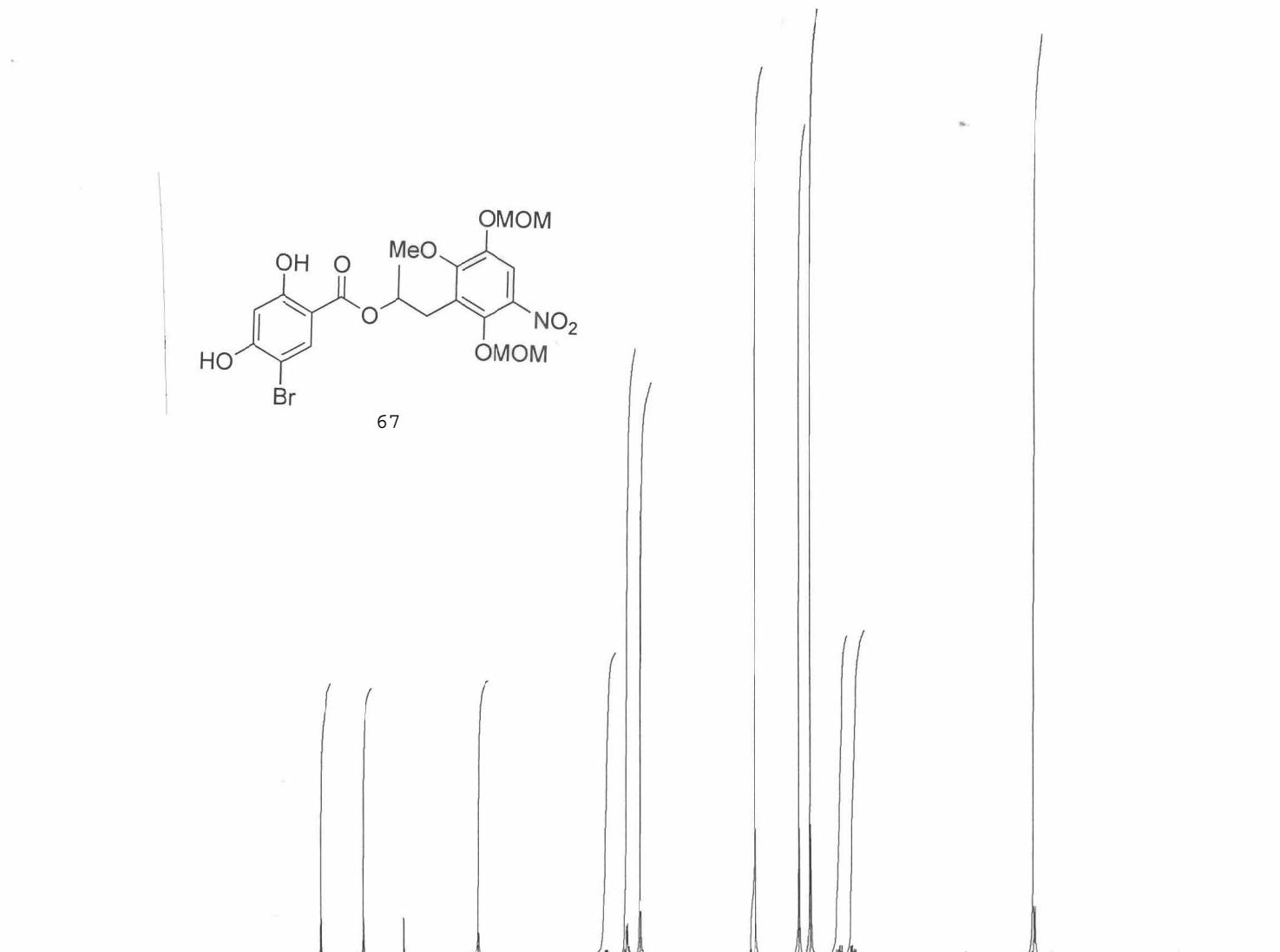
F2 - Acquisition Parameters
Date_ 20050709
Time 5.51
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 287.4
DW 104.400 usec
DE 5.50 usec
TE 295.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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

0.97

0.96

0.98

1.09
2.18
2.06

3.20
2.99
3.41
1.14
1.17

3.32

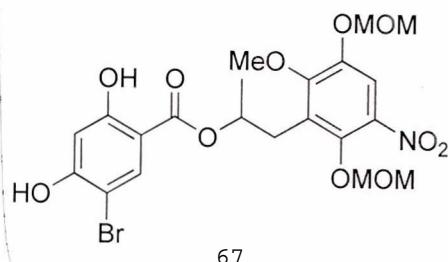
Current Data Parameters
 NAME sg464
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050709
 Time 15.37
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 21504
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 295.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

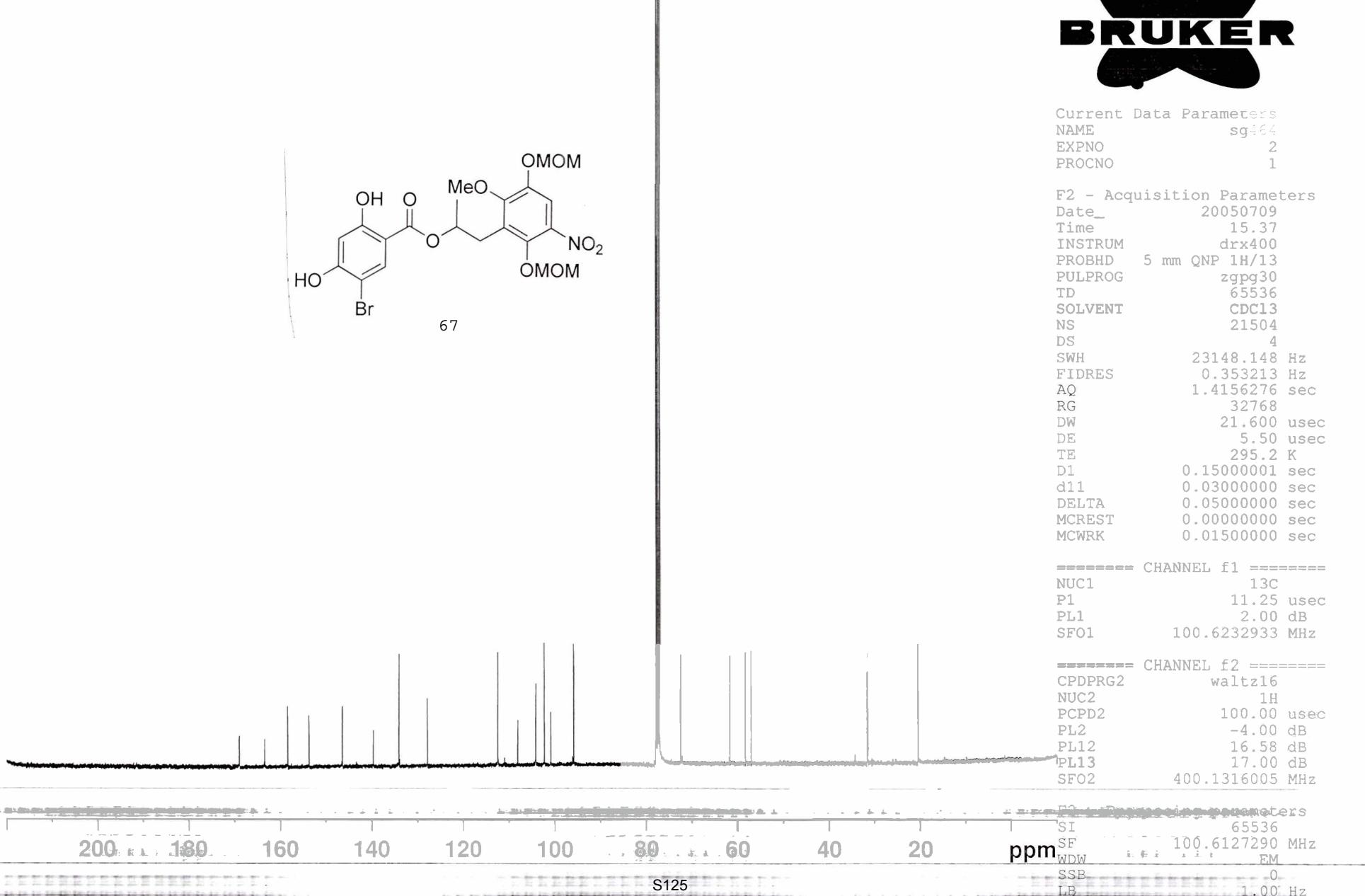
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz



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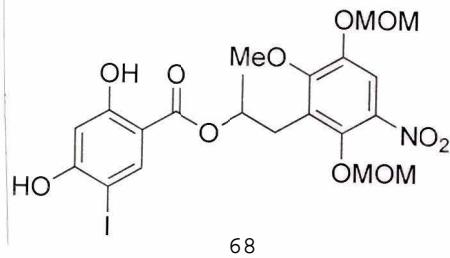


Current Data Parameters
NAME sg457
EXPNO 1
PROCNO 1

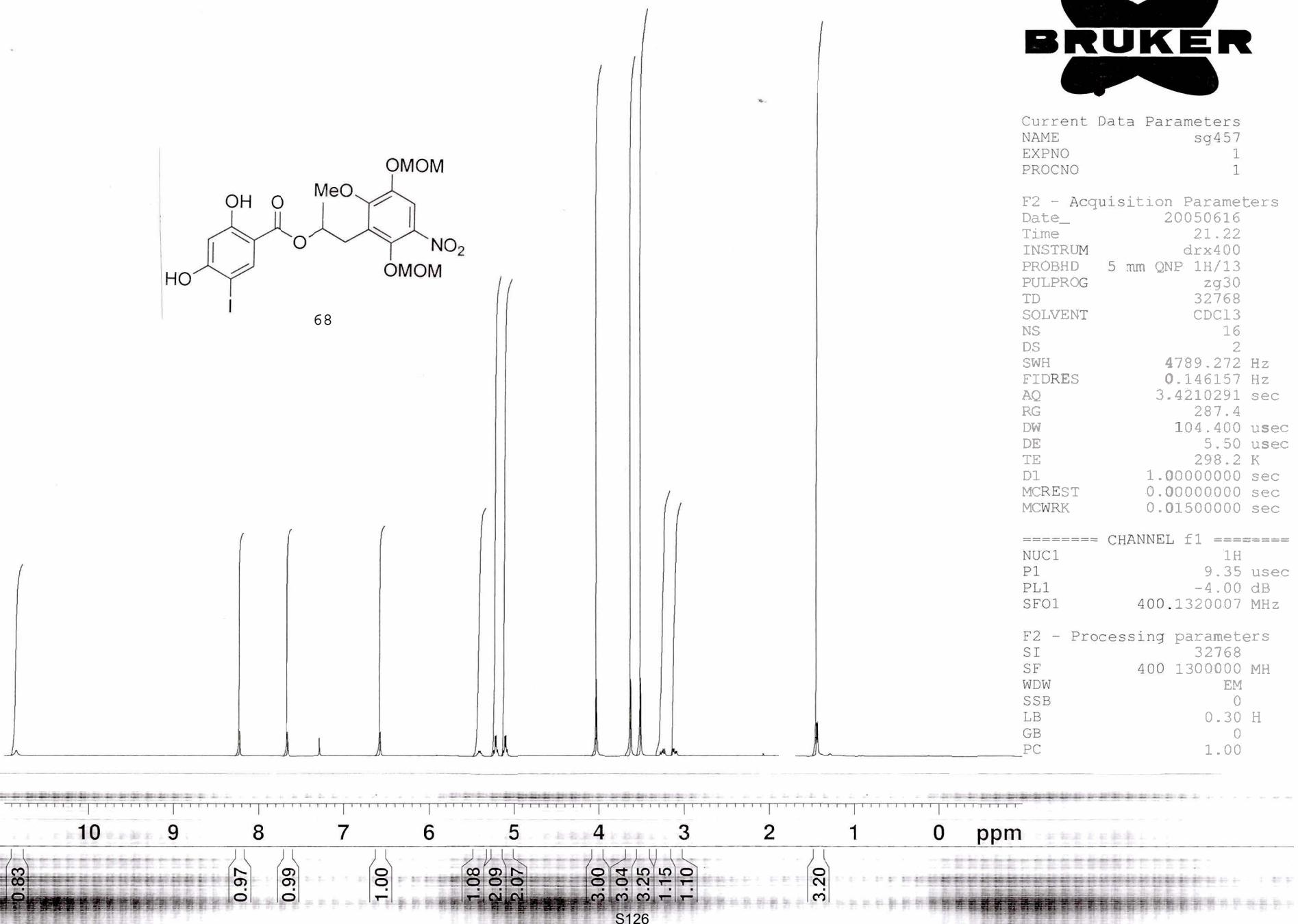
F2 - Acquisition Parameters
Date 20050616
Time 21.22
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 287.4
DW 104.400 usec
DE 5.50 usec
TE 298.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SF01 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400 1300000 MH
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00



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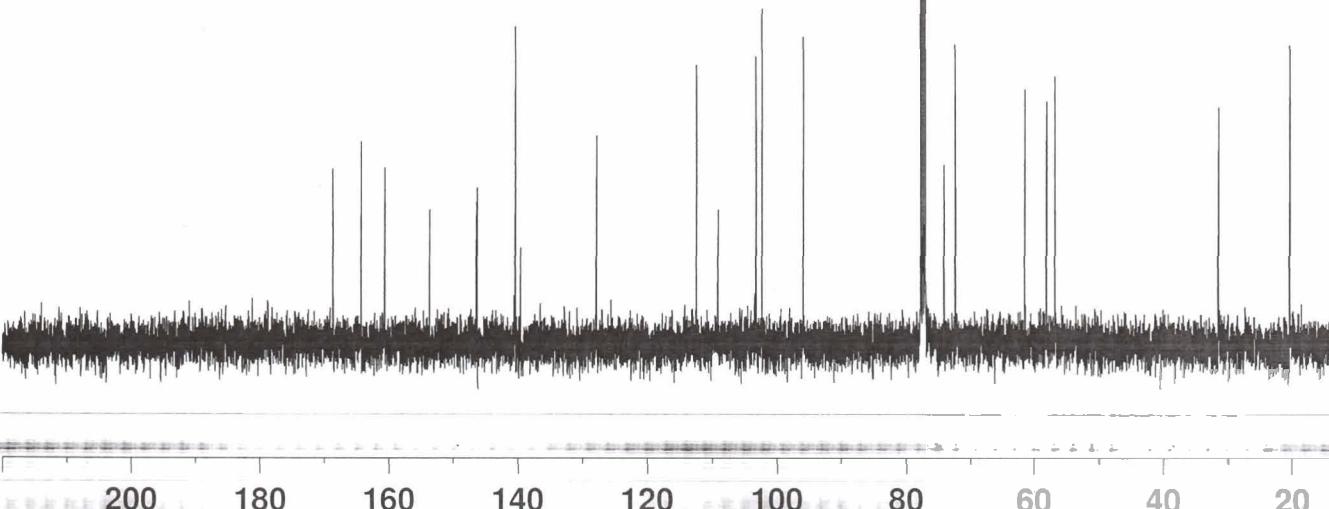
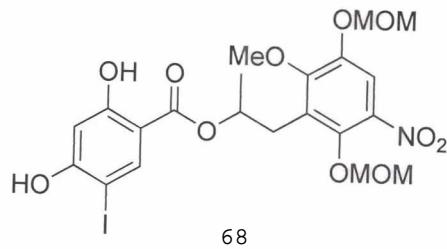
Current Data Parameters
 NAME sg457
 EXPNO 2
 PROCNO 1

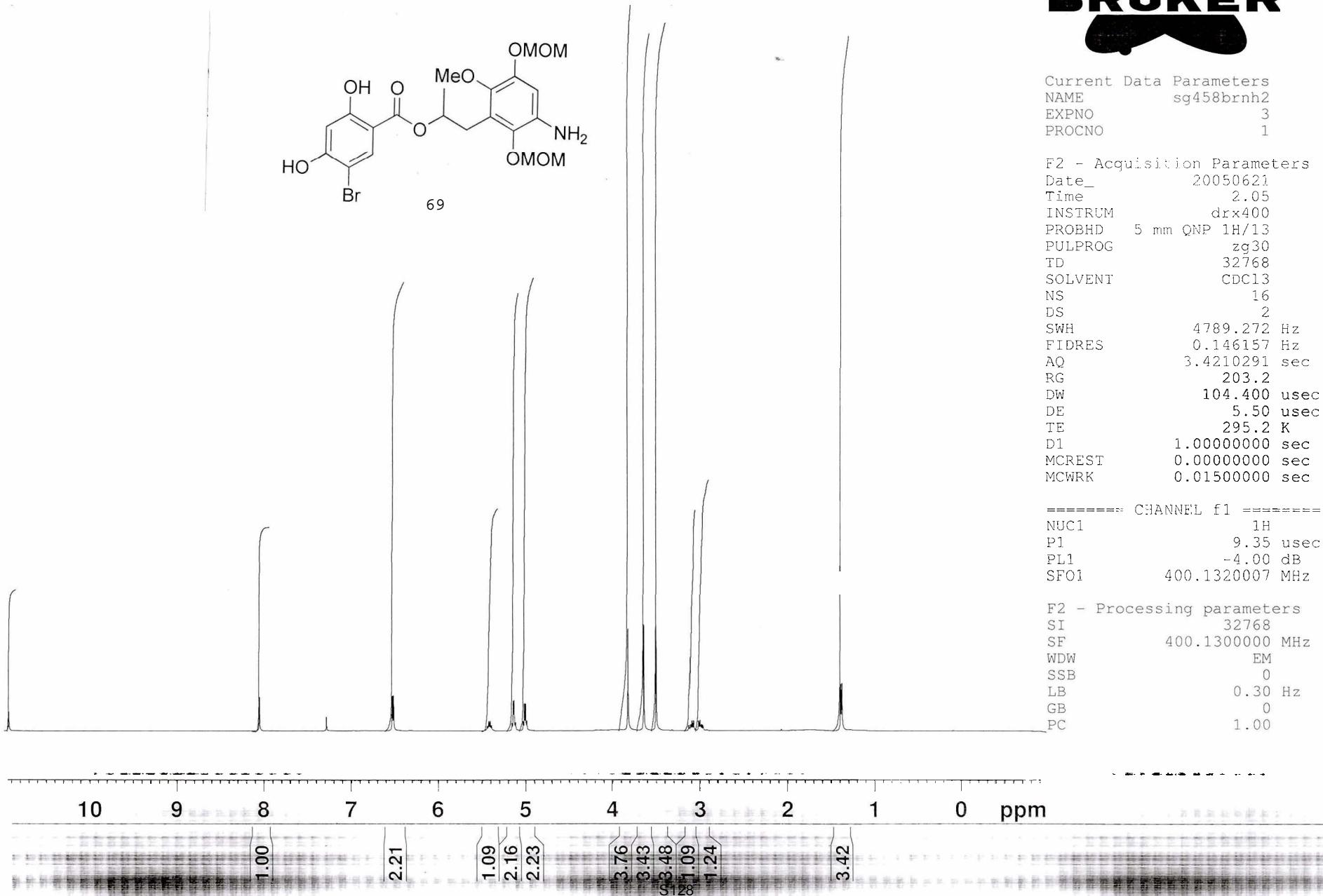
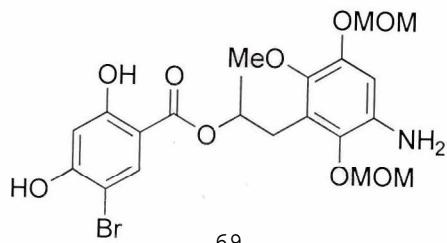
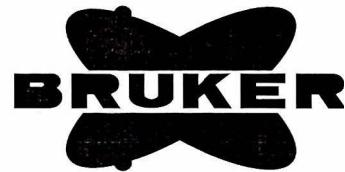
F2 - Acquisition Parameters
 Date_ 20050616
 Time 21.36
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 645
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 298.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 'SI' 65536
 'SF' 100.6127290 MHz
 'WDW' FM
 'SSB' 0
 'LB' 1.00 Hz



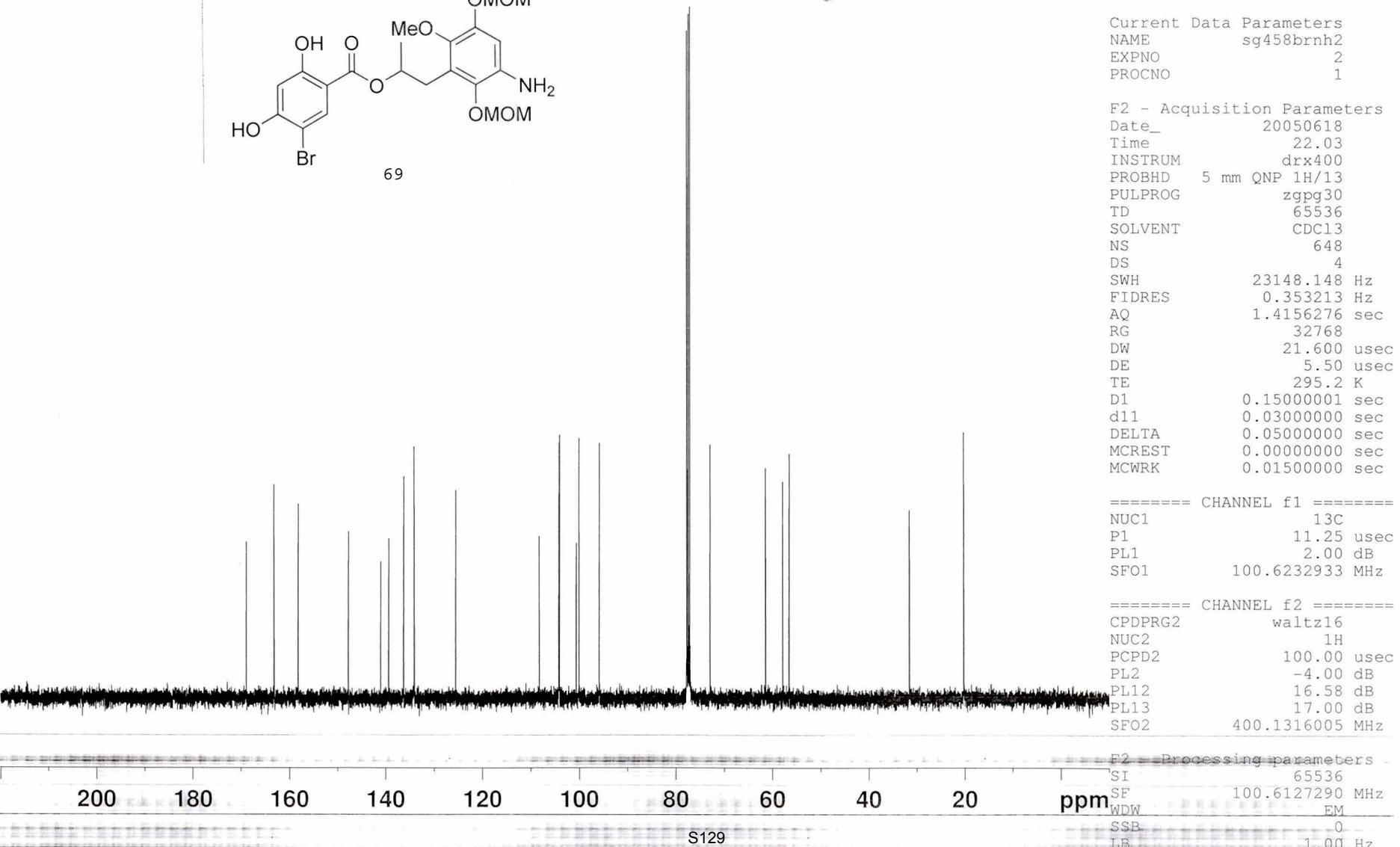
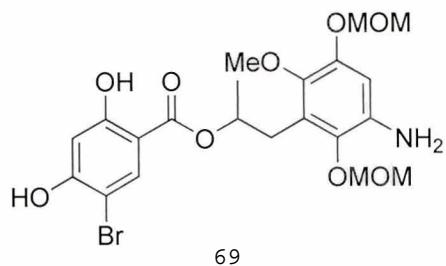


Current Data Parameters
NAME sg458brnh2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050621
Time 2.05
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 203.2
DW 104.400 usec
DE 5.50 usec
TE 295.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

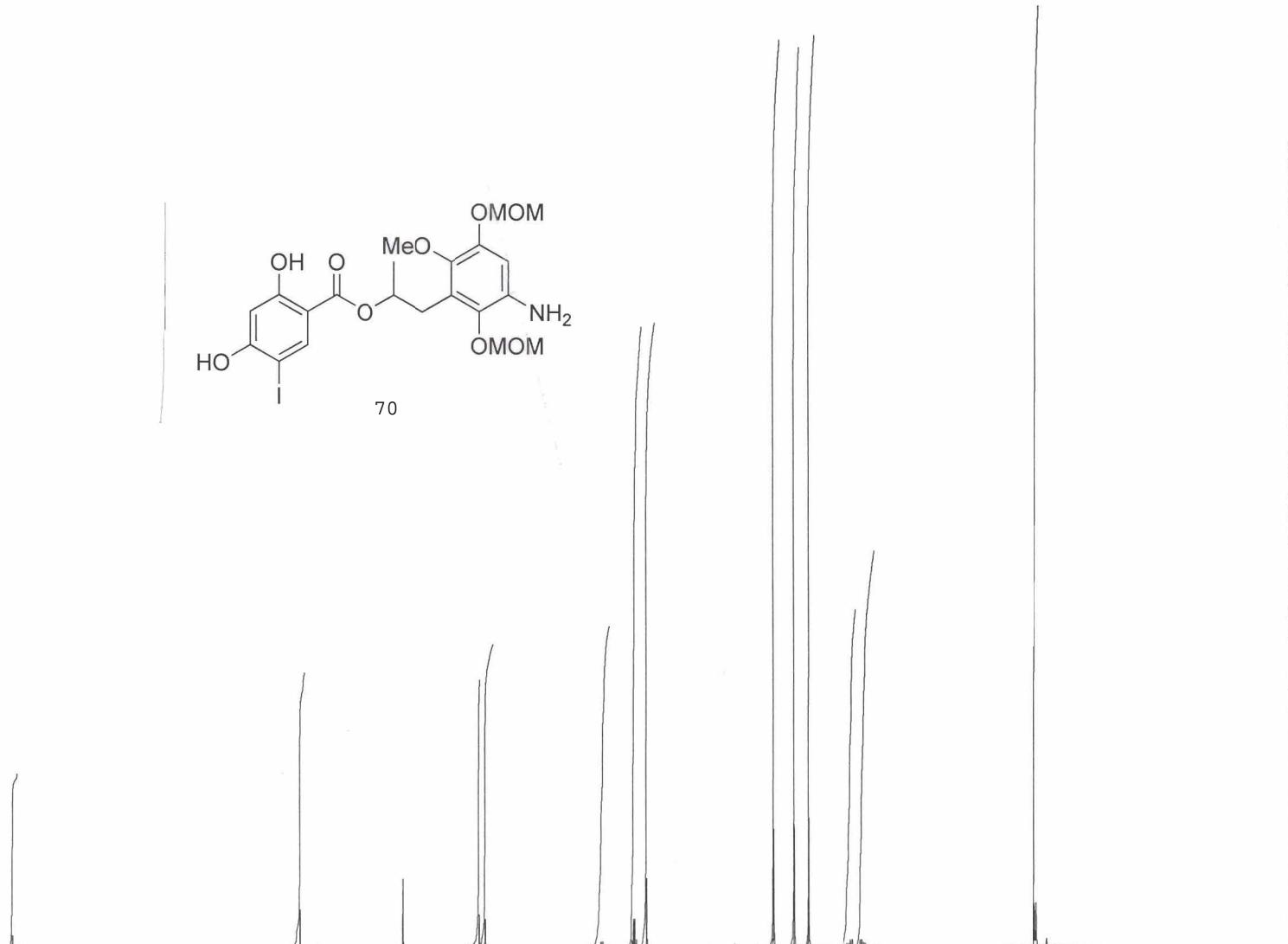
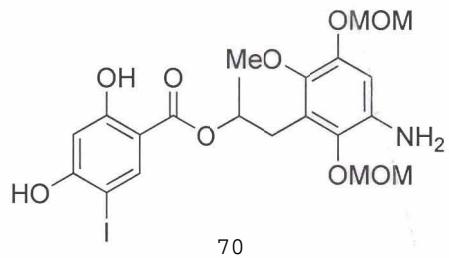


Current Data Parameters
 NAME sg461.inh2
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050626
 Time 5.11
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 362
 DW 104.400 usec
 DE 5.50 usec
 TE 310.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 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

0.97

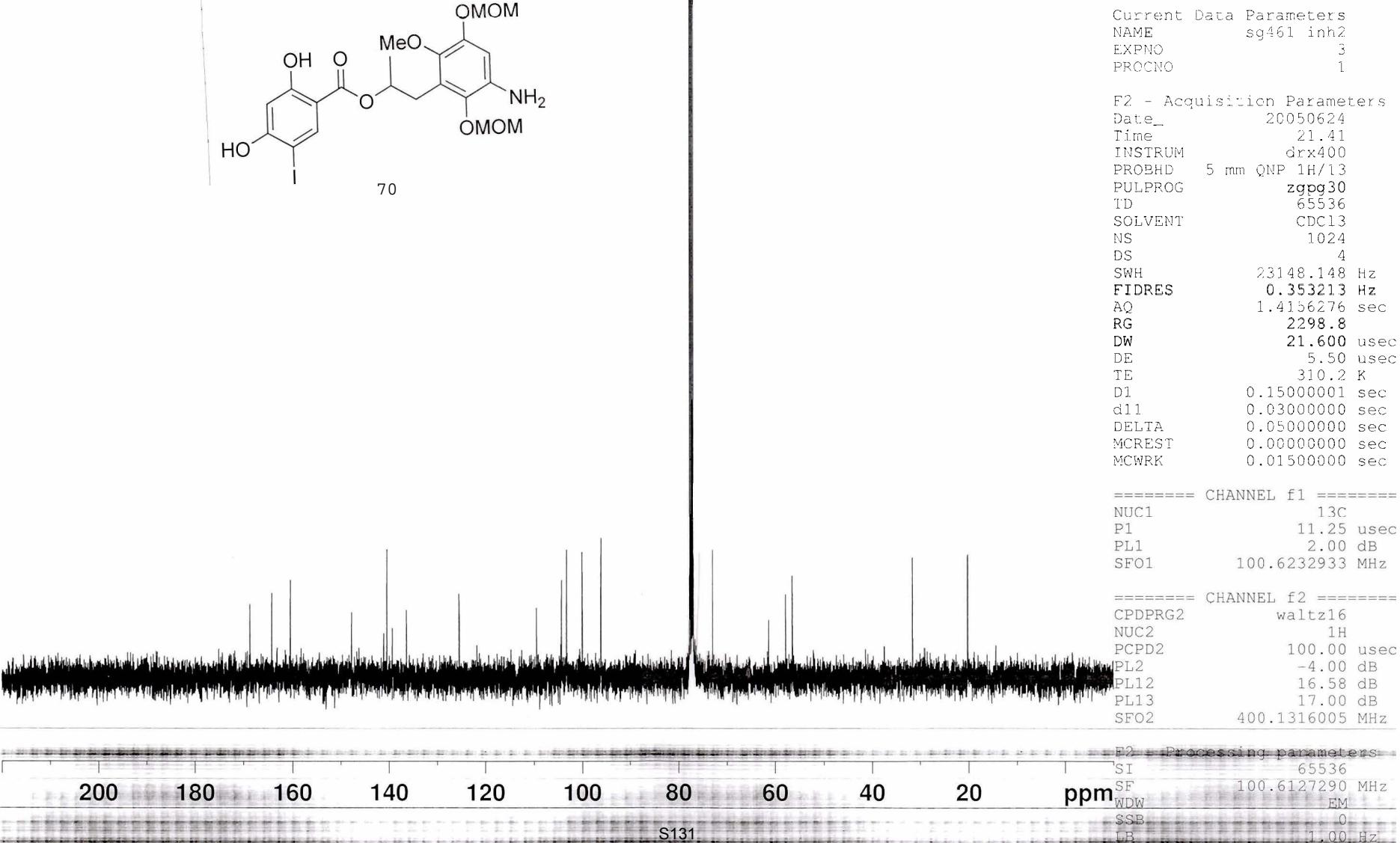
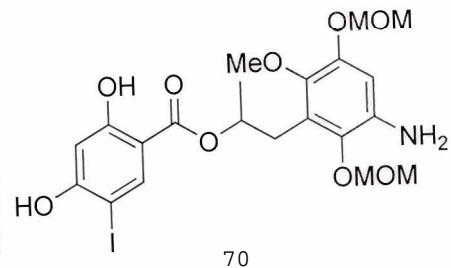
0.94
1.07

1.13
2.19
2.20

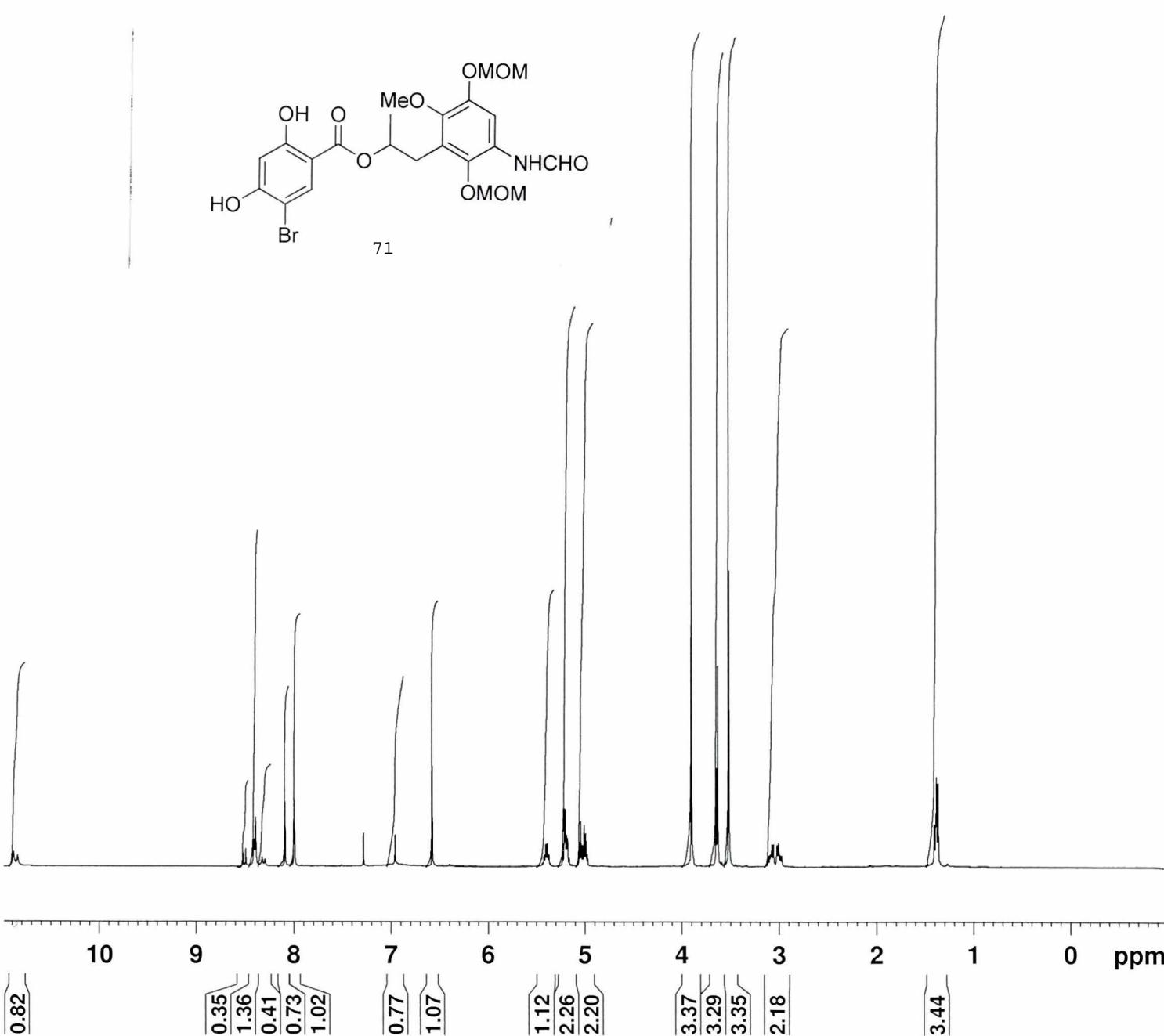
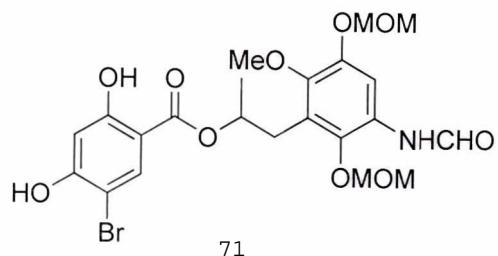
3.19
3.17
3.21
1.19
1.40

3.32

S130



200 180 160 140 120 100 80 60 40 20 ppm



Current Data Parameters
 NAME sg460_Brcoupling
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050623
 Time 20.17
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 161.3
 DW 104.400 usec
 DE 5.50 usec
 TE 296.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400 13000000 MH
 WD EM
 SS 0
 LB 0.30 Hz
 GB 0
 PC 1.00



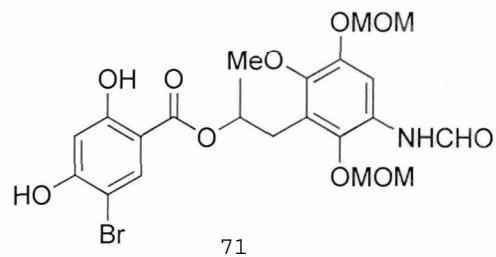
Current Data Parameters
NAME sg460_Brcoupling
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20050623
Time 20.21
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 332
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 5.50 usec
TE 296.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

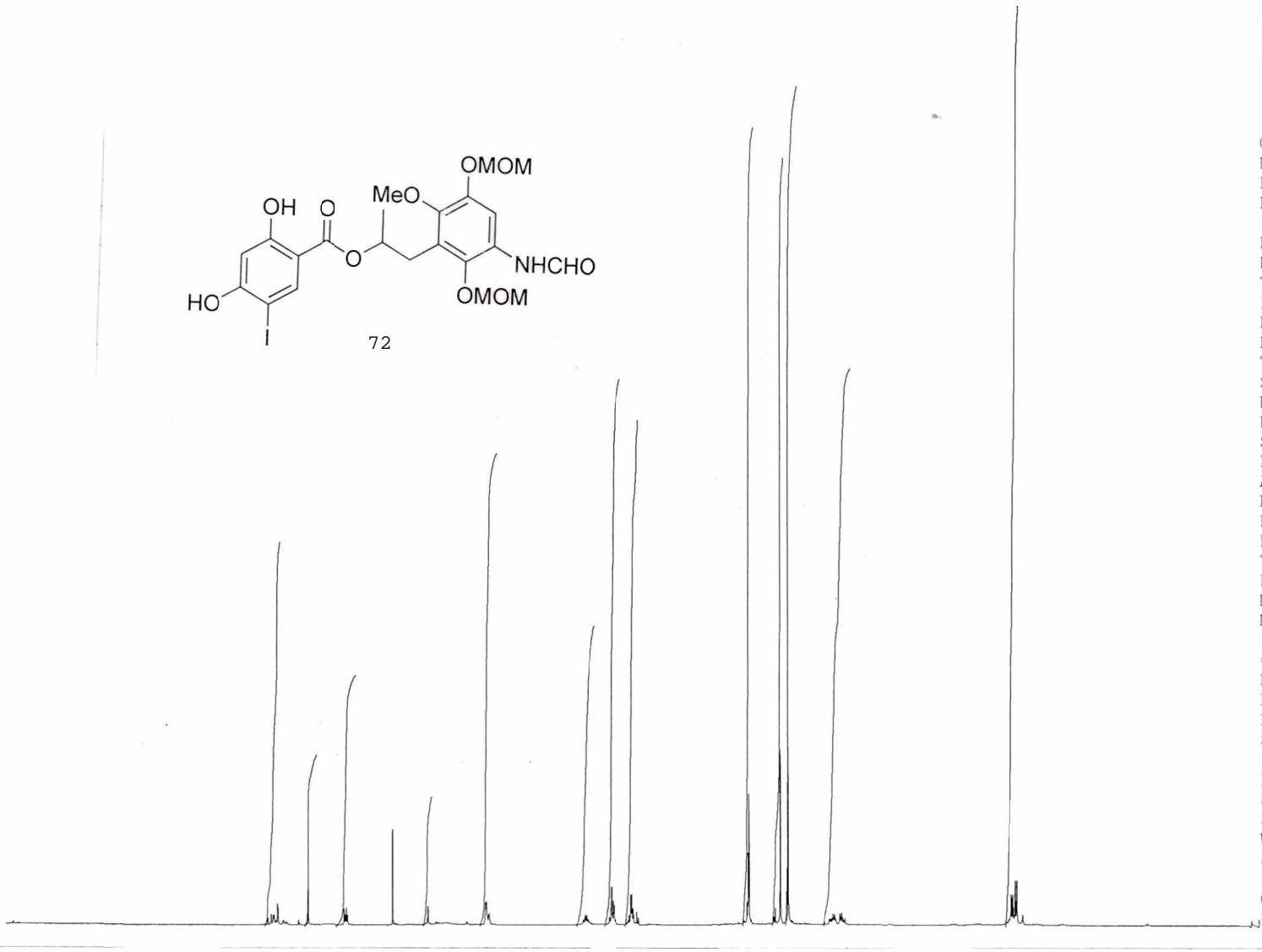
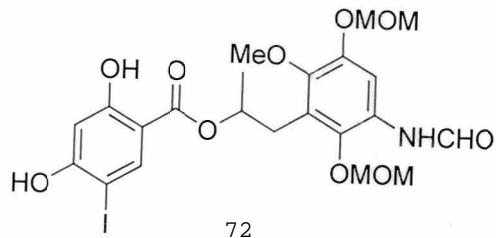
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

E2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz



200 180 160 140 120 100 80 60 40 20 ppm



Current Data Parameters
NAME sg470
EXPNO 1
PROCNO 1

F2 - Acquisition Parameter
Date 20050724
Time 2.17
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 287.4
DW 104.400 usec
DE 5.50 usec
TE 298.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SF01 400 1320007 MHz

F2 - Processing parameters
SI 32768
SF 400 1300000 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

1.50 0.67 0.98 0.51 1.85 1.18 2.14 1.98 3.13 3.01 3.29 2.18 3.61

S134



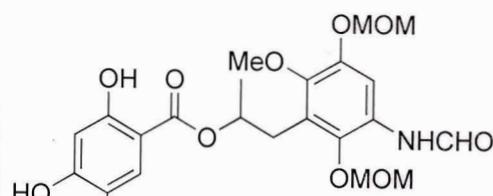
Current Data Parameters
NAME sg471
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050730
Time 1.00
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 293
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 4096
DW 21.600 usec
DE 5.50 usec
TE 296.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

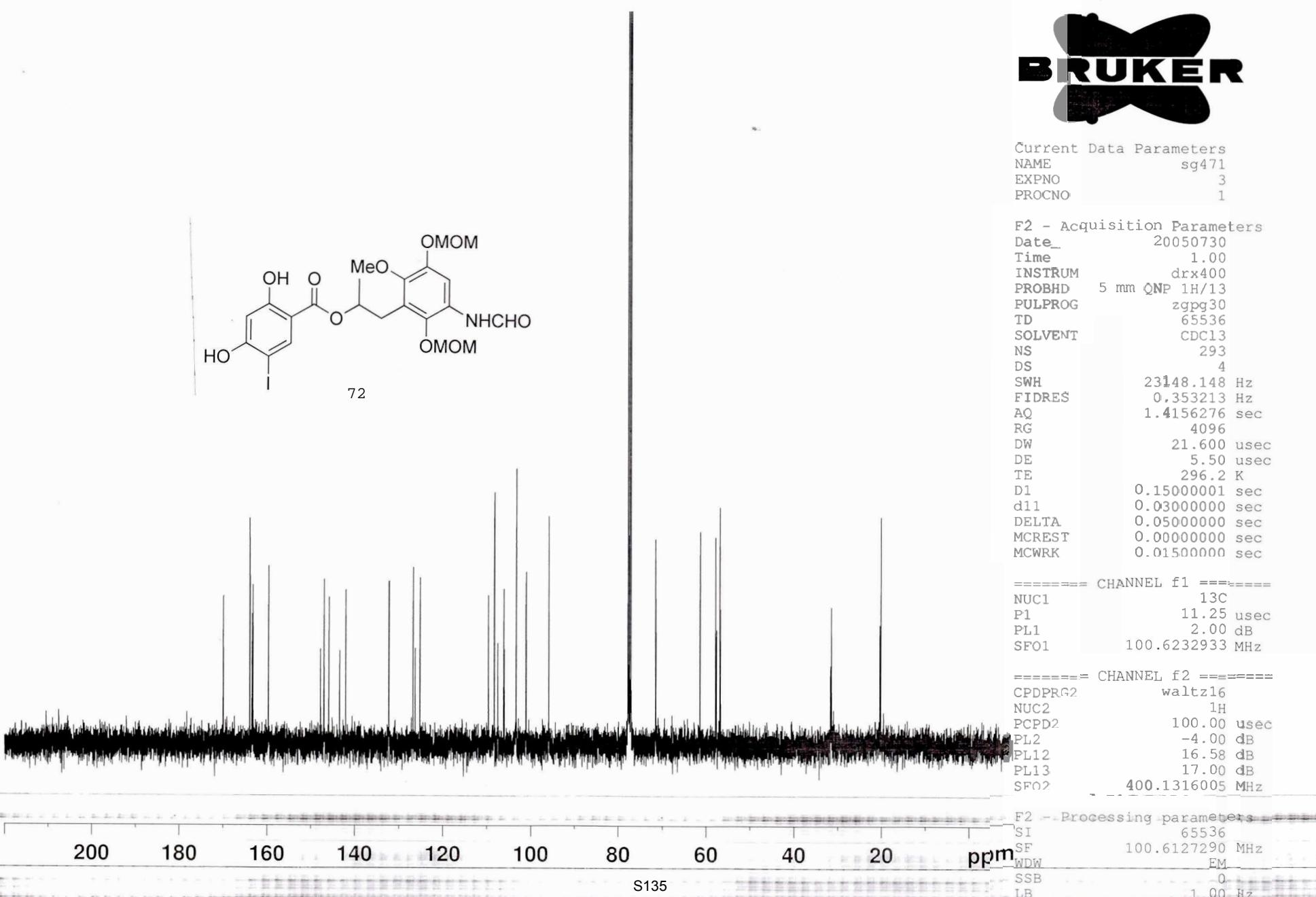
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 0
T 1.00 Hz



72



200 180 160 140 120 100 80 60 40 20 ppm

S135

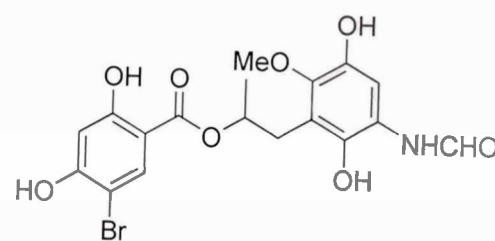


Current Data Parameters
NAME sg465
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050710
Time 23.26
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT MeOH
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 322.5
DW 104.400 usec
DE 5.50 usec
TE 295.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



73

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

0.98 1.06 0.93 1.06 1.16 3.44 1.20 1.29 3.78

S136



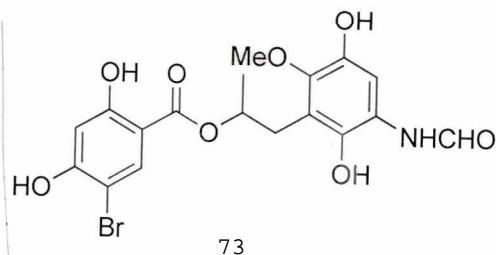
Current Data Parameters
NAME sg465
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050711
Time 0.22
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2139
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 5.50 usec
TE 295.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

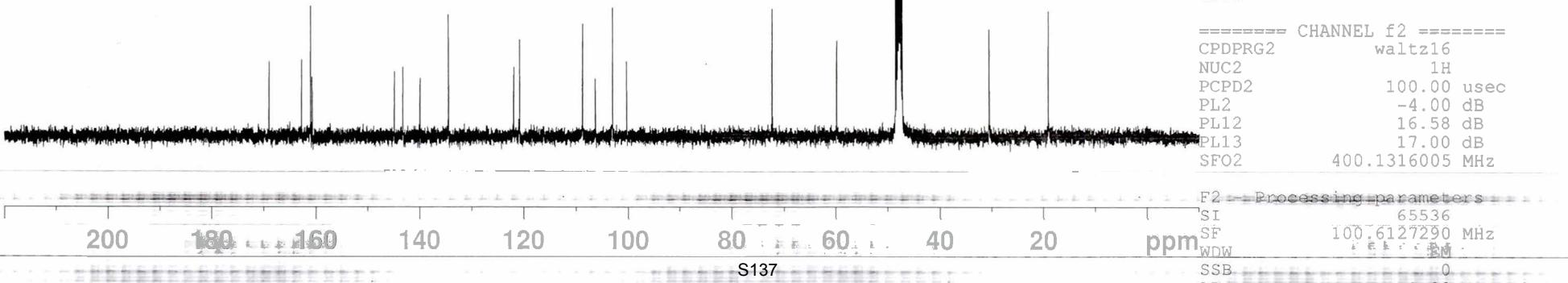
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW
SSB 0
LB 1.00
PQ



73



200

180

160

140

120

100

80

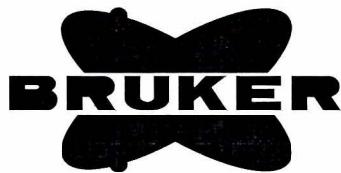
60

40

20

ppm

S137

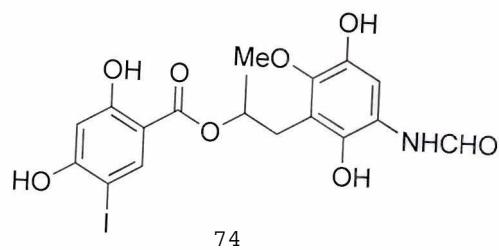


Current Data Parameters
NAME sg471
EXPNO 1
PROCNO 1

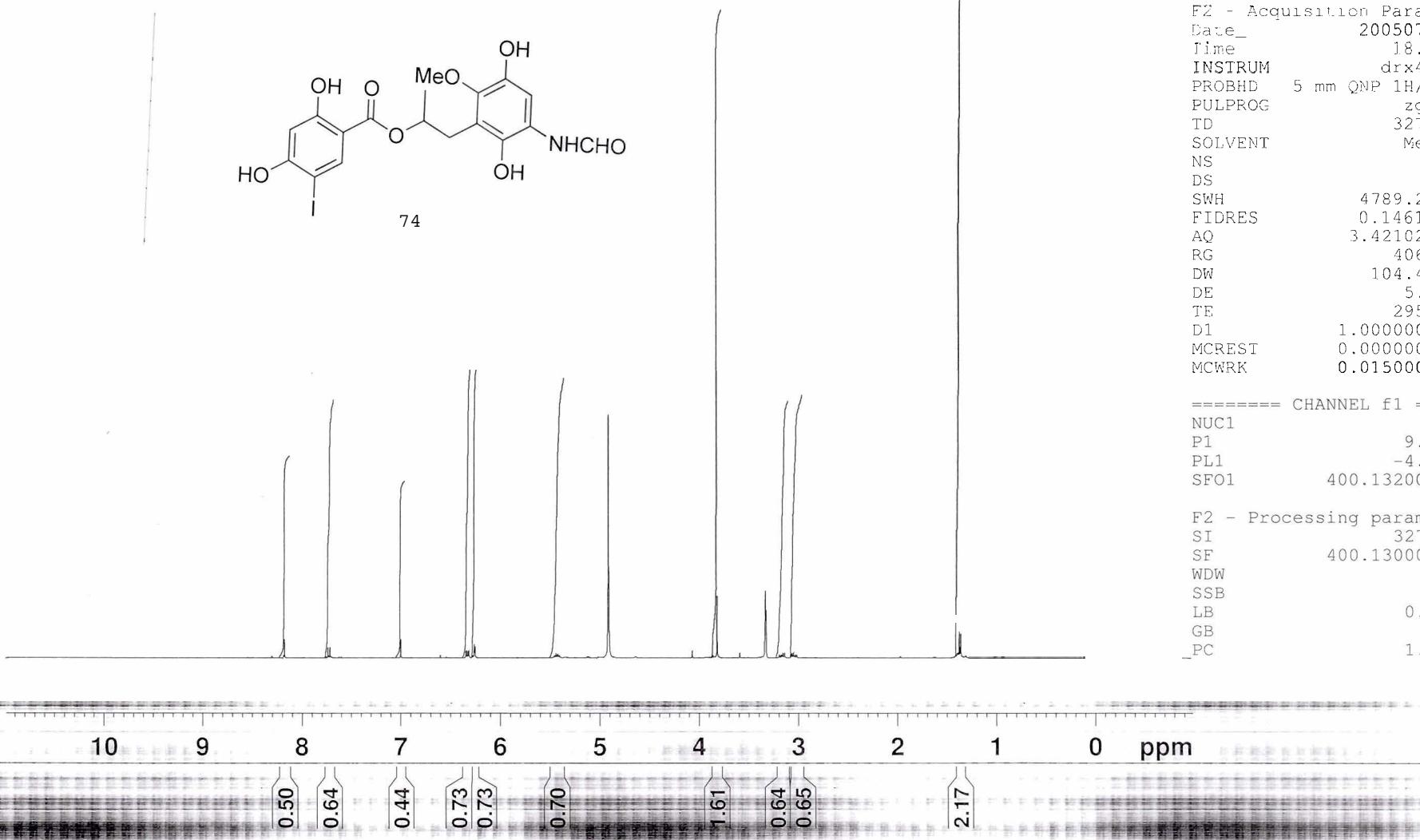
F2 - Acquisition Parameters
Date_ 20050728
Time 18.24
INSTRUM dix400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT MeOH
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 406.4
DW 104.400 usec
DE 5.50 usec
TE 295.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



74





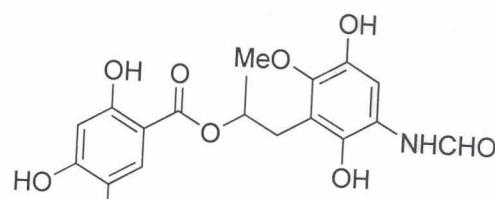
Current Data Parameters
NAME sg471
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050729
Time 5.24
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 12800
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 5.50 usec
TE 295.2 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

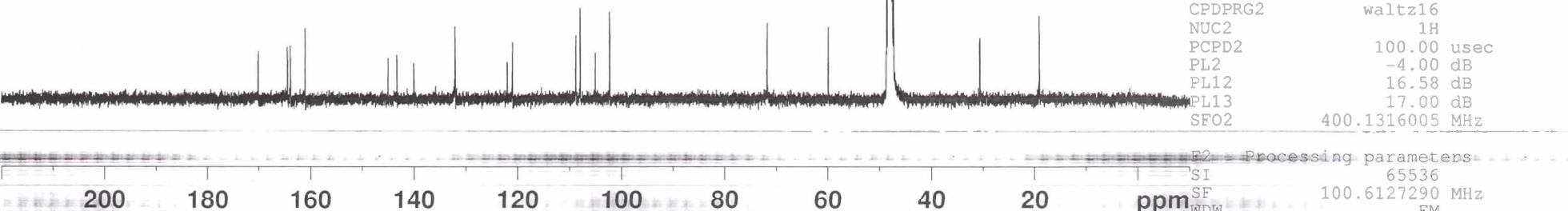
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SF01 100.6232933 MHz

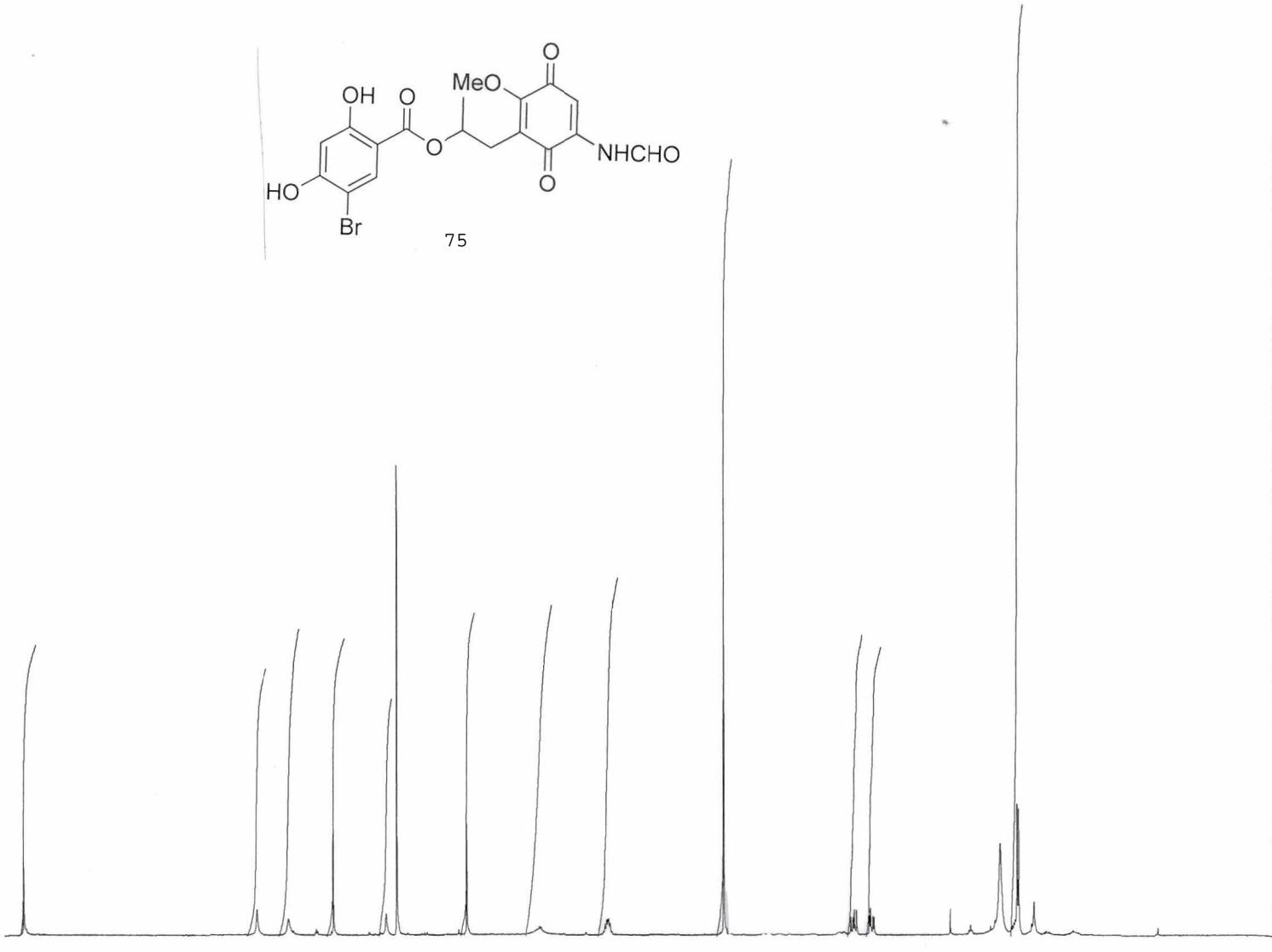
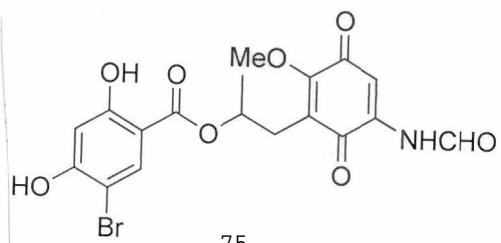
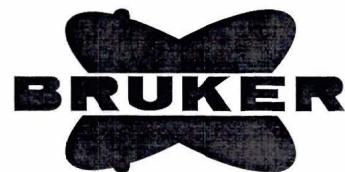
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz



74



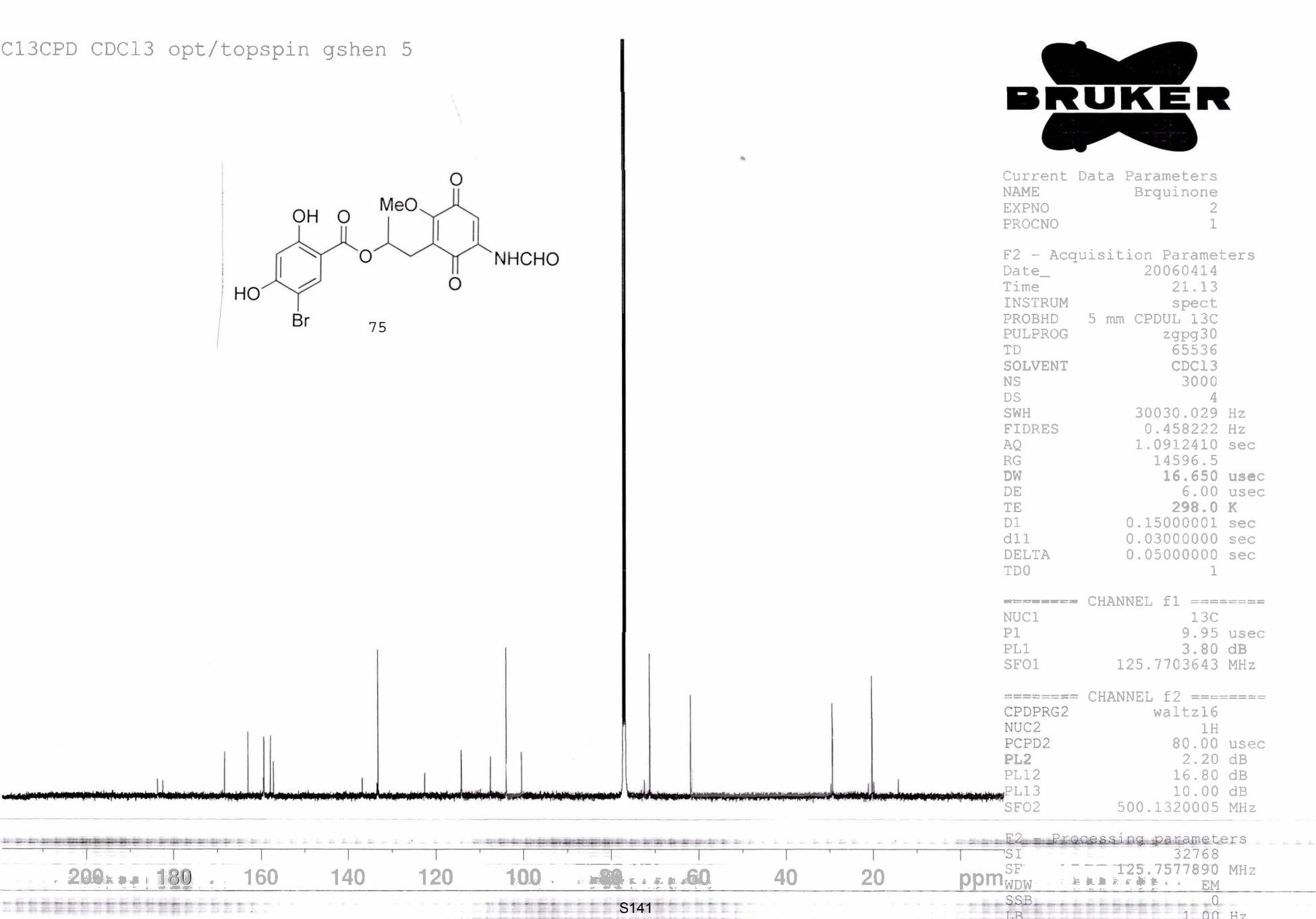
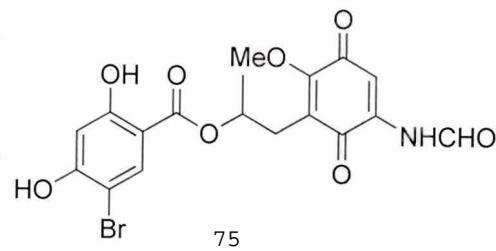


Current Data Parameters
NAME sg466
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050712
Time 2.10
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 574.7
DW 104.400 usec
DE 5.50 usec
TE 296.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

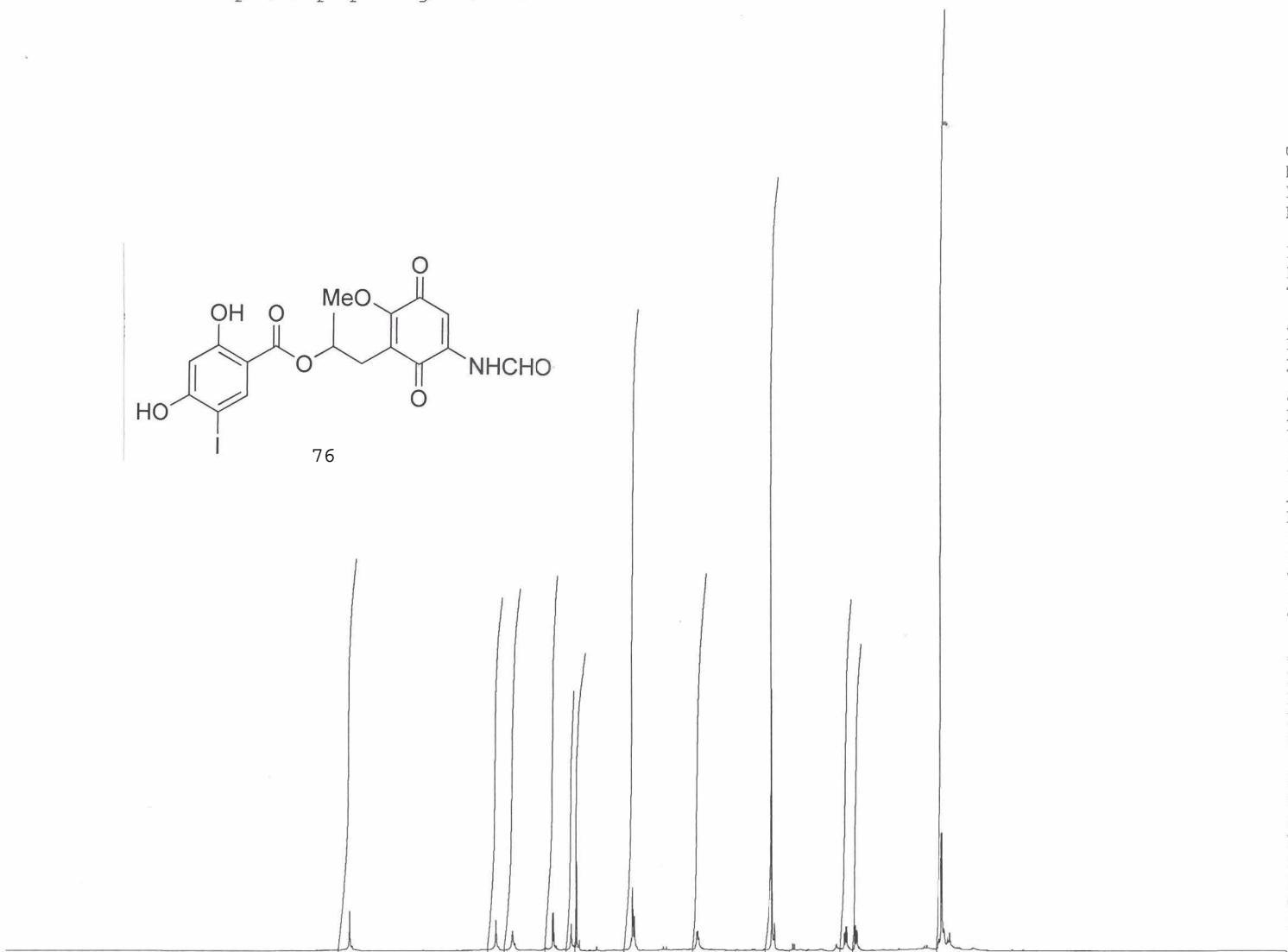
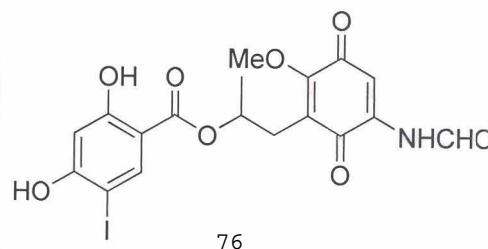
===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400 1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
 NAME 1quinone
 EXPNO 1
 PROCNO 1



16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

9.69

8.73
8.96
9.28
6.43
15.84

5.84

3.38

19.09

8.70

7.60

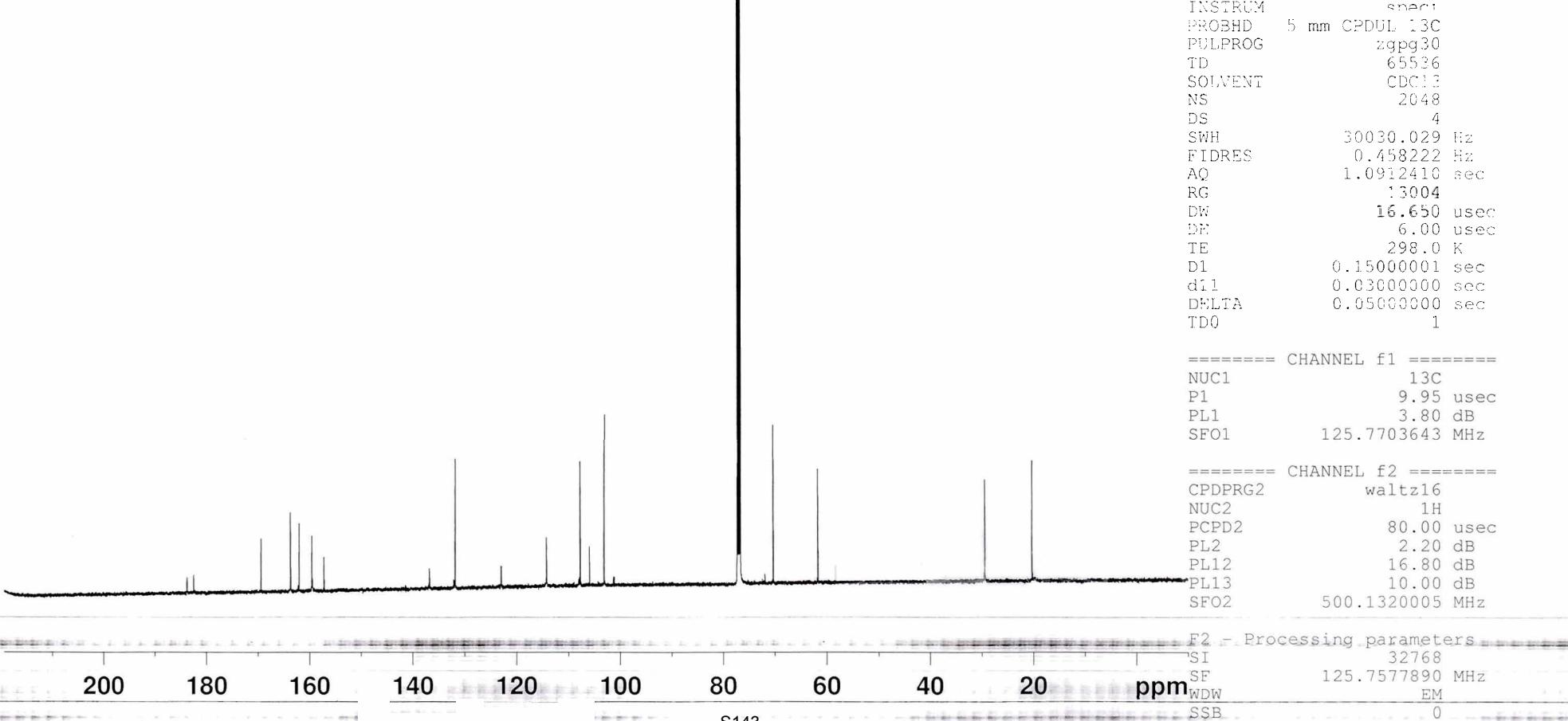
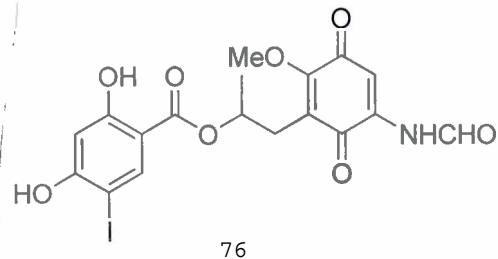
23.22

S142

F2 - Acquisition Parameters
 Date_ 20060418
 Time 0.04
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 322.5
 DW 48.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.90 usec
 PL1 2.20 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300474 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

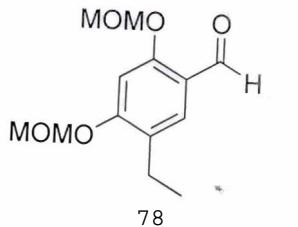
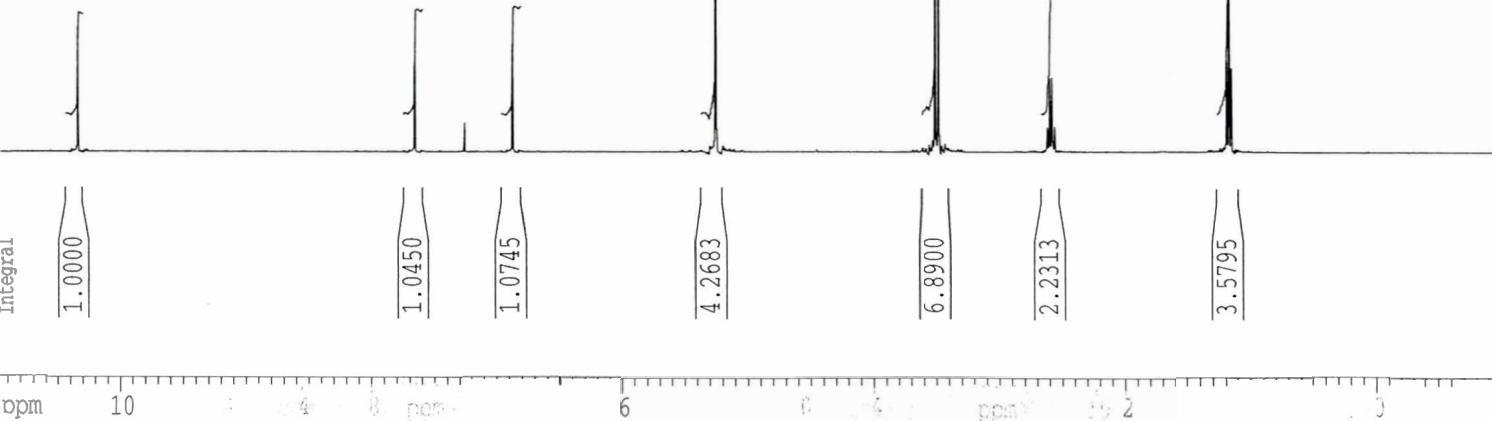


ppm

10.3423

7.6570
7.2607
6.8759

5.2609



3.5175
3.4898
2.6228
2.6040
2.5852
2.5665
1.1983
1.1797
1.1608

Current Data Parameters
NAME sg508
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060124
Time 14.59
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 161.3
DW 104.400 usec
DE 5.50 usec
TE 294.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

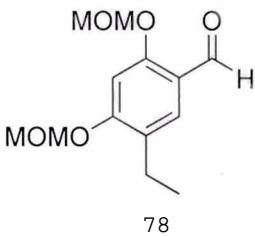
===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SF01 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 11.000 ppm
F1 4401.43 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPCM 0.60000 ppm/cm
HZCM 240.07800 Hz/cm

ppm

189.029

161.571
160.358128.857
127.637
119.963100.684
95.341
94.52677.762
77.445
77.12756.976
56.84423.067
14.457

Current Data Parameters
 NAME sg508
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060124
 Time 15.01
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 73
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.00 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPPCM 11.00000 ppm/cm
 HZCM 1106.73439 ppm/cm



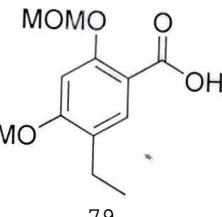
ppm

Integral

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

7.90804

6.93941

5.35610
5.237253.53150
3.46725
3.45577
2.59690
2.57815
2.55959
1.18098
1.16225
1.14338

79

1.0000

1.0504

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2.3303

3.5700

Current Data Parameters
 NAME sg509
 EXPNO 1
 PROCNO 1

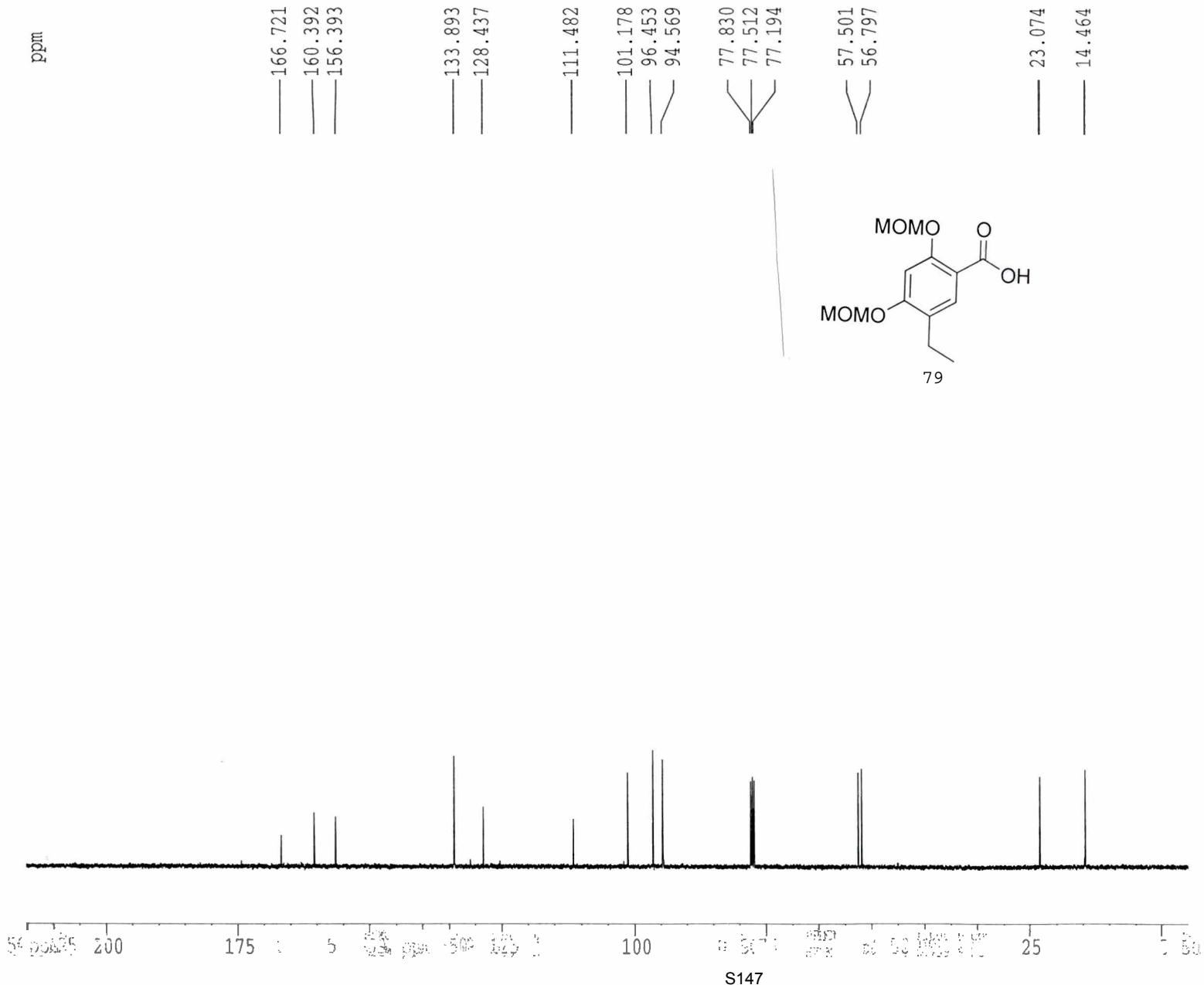
F2 - Acquisition Parameters
 Date_ 20060125
 Time 20.53
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 57
 DW 78.000 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1332010 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 3.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

ppm



Current Data Parameters
 NAME sg509
 EXPNO 2
 PROCNO 1

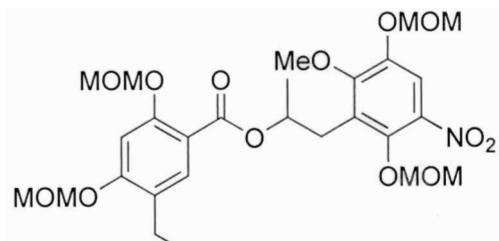
F2 - Acquisition Parameters
 Date_ 20060125
 Time 20.56
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 94
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

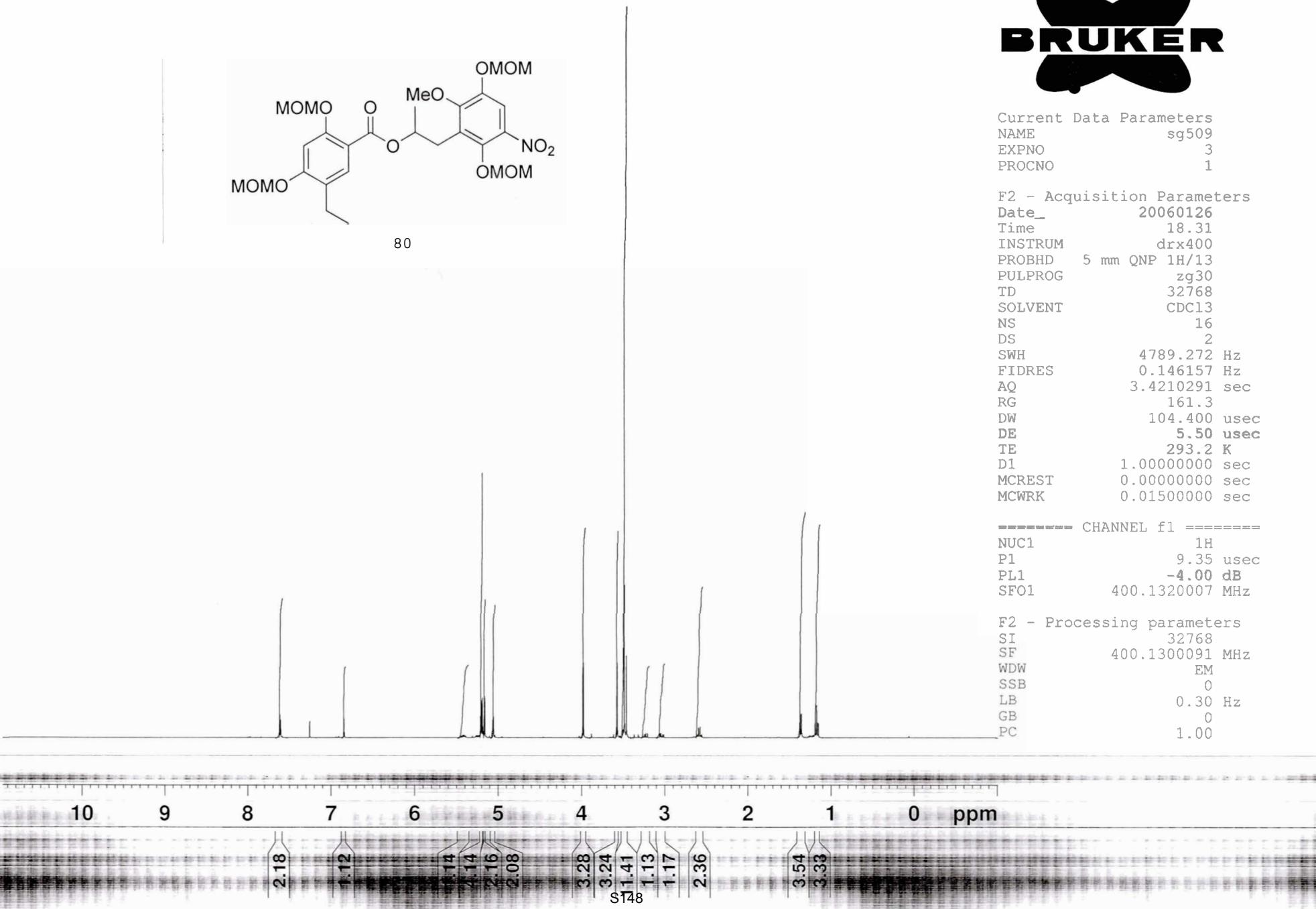
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

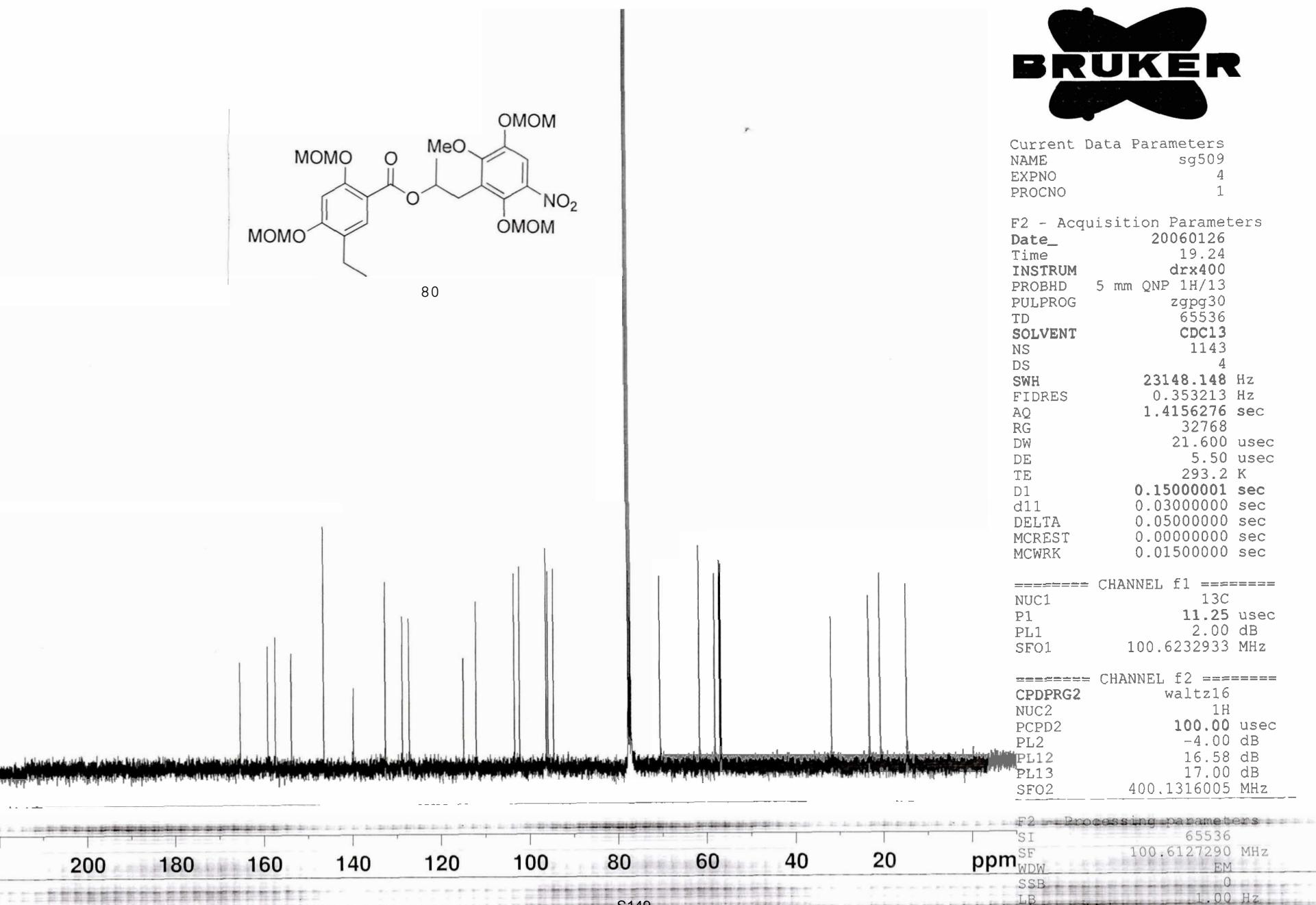
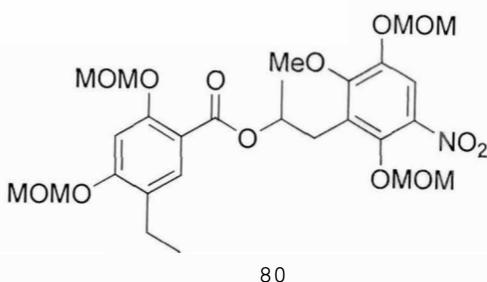
F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

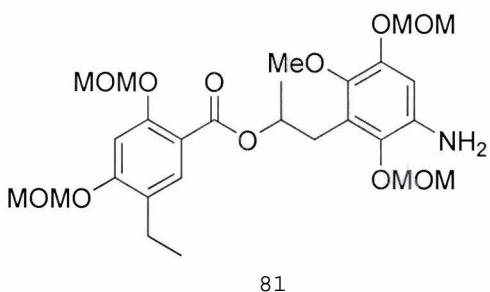
1D NMR plot parameters
 CX 20.00 cm
 CY 2.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PHWCM 11.00000 ppm/cm
 WPHCM 11.00000 Hz/cm



80





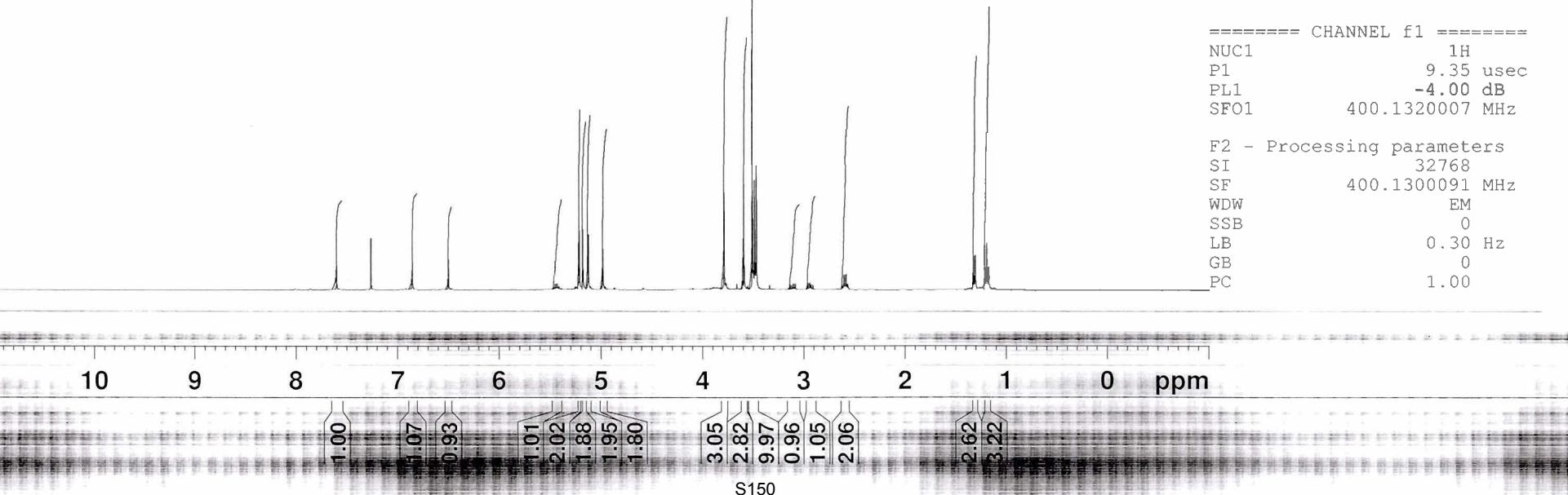


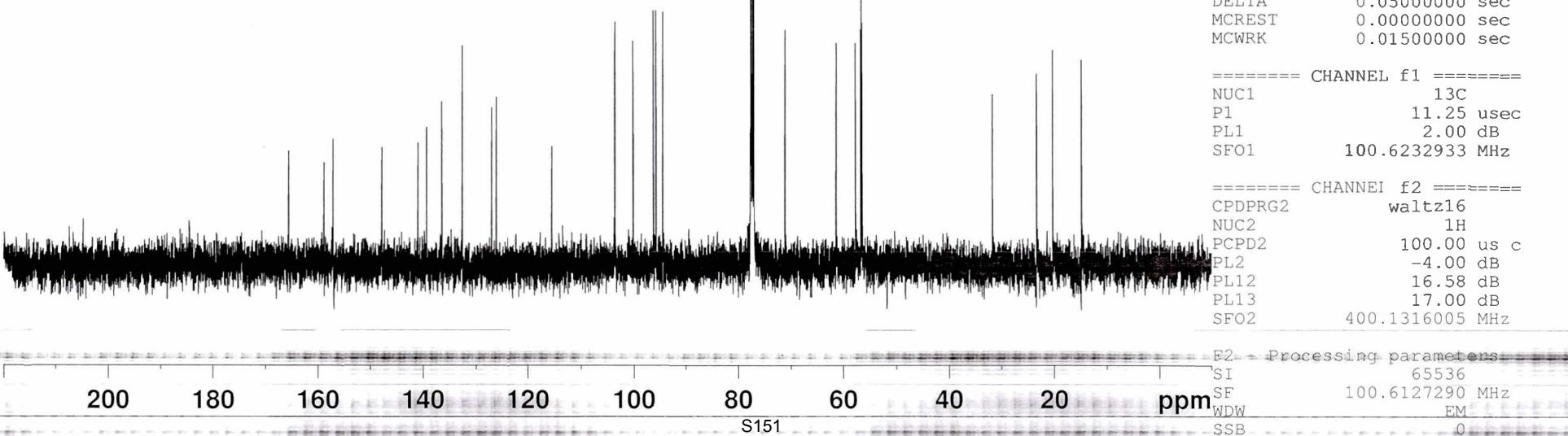
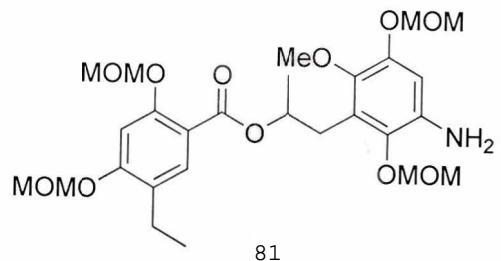
Current Data Parameters
NAME sg509
EXPNO 5
PROCNO 1

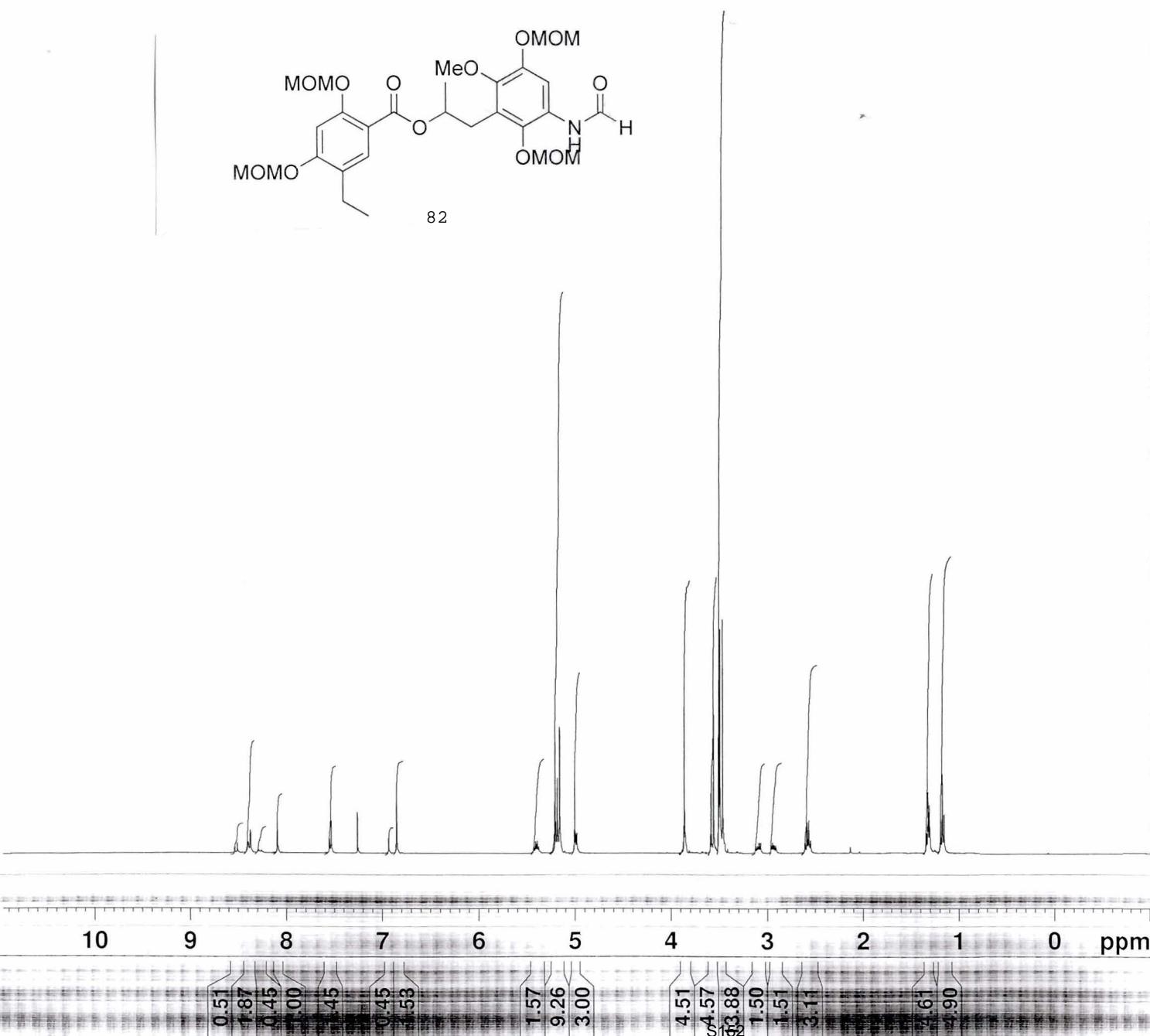
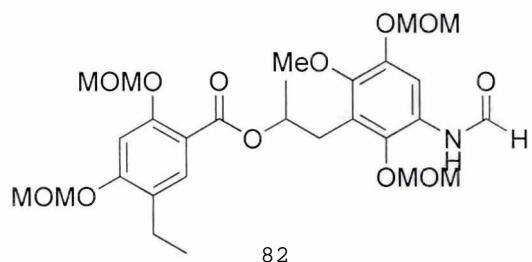
F2 - Acquisition Parameters
Date_ 20060131
Time 19.43
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 287.4
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





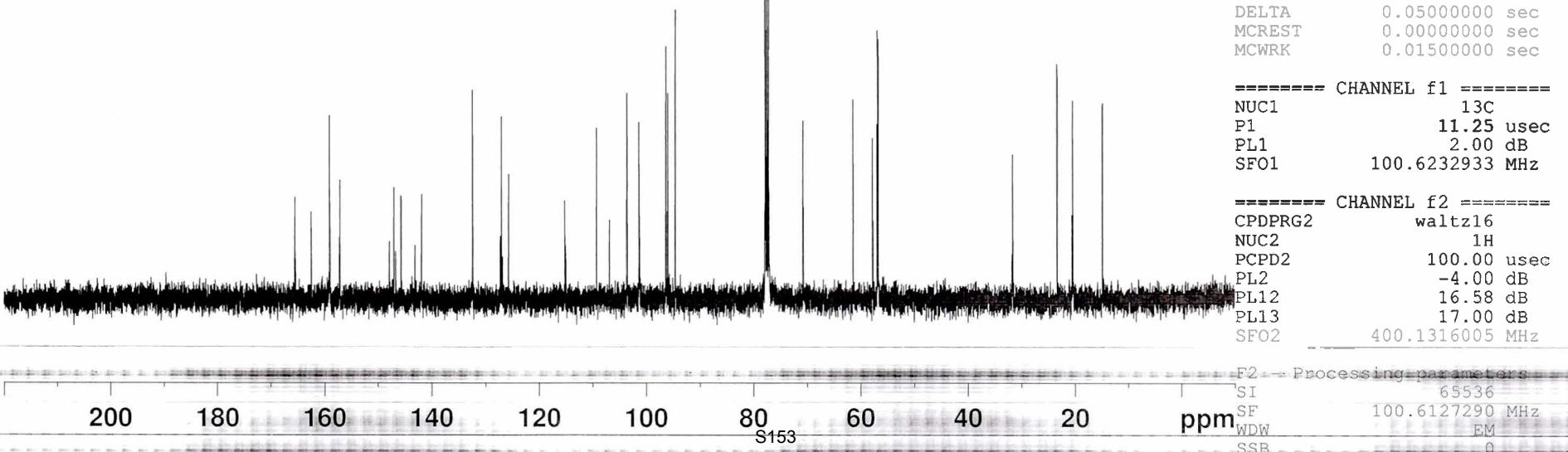
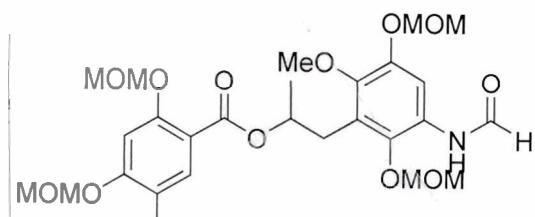


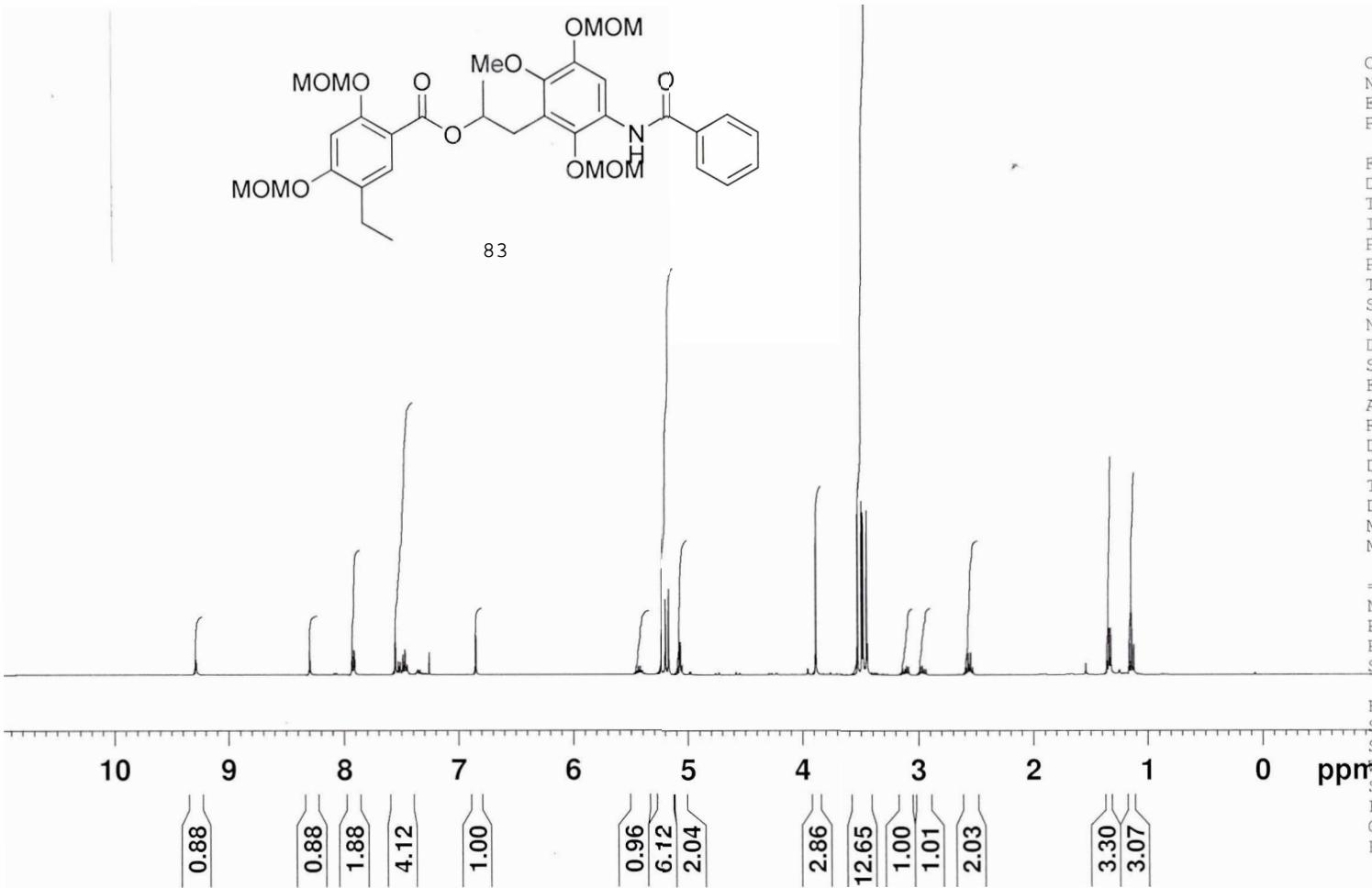
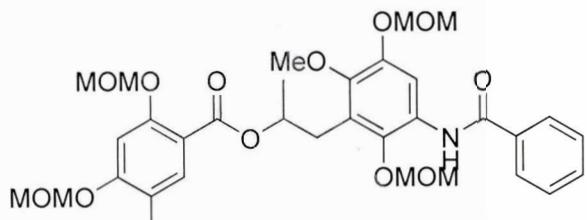
Current Data Parameters
 NAME sg511
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060203
 Time 2.10
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 724.1
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



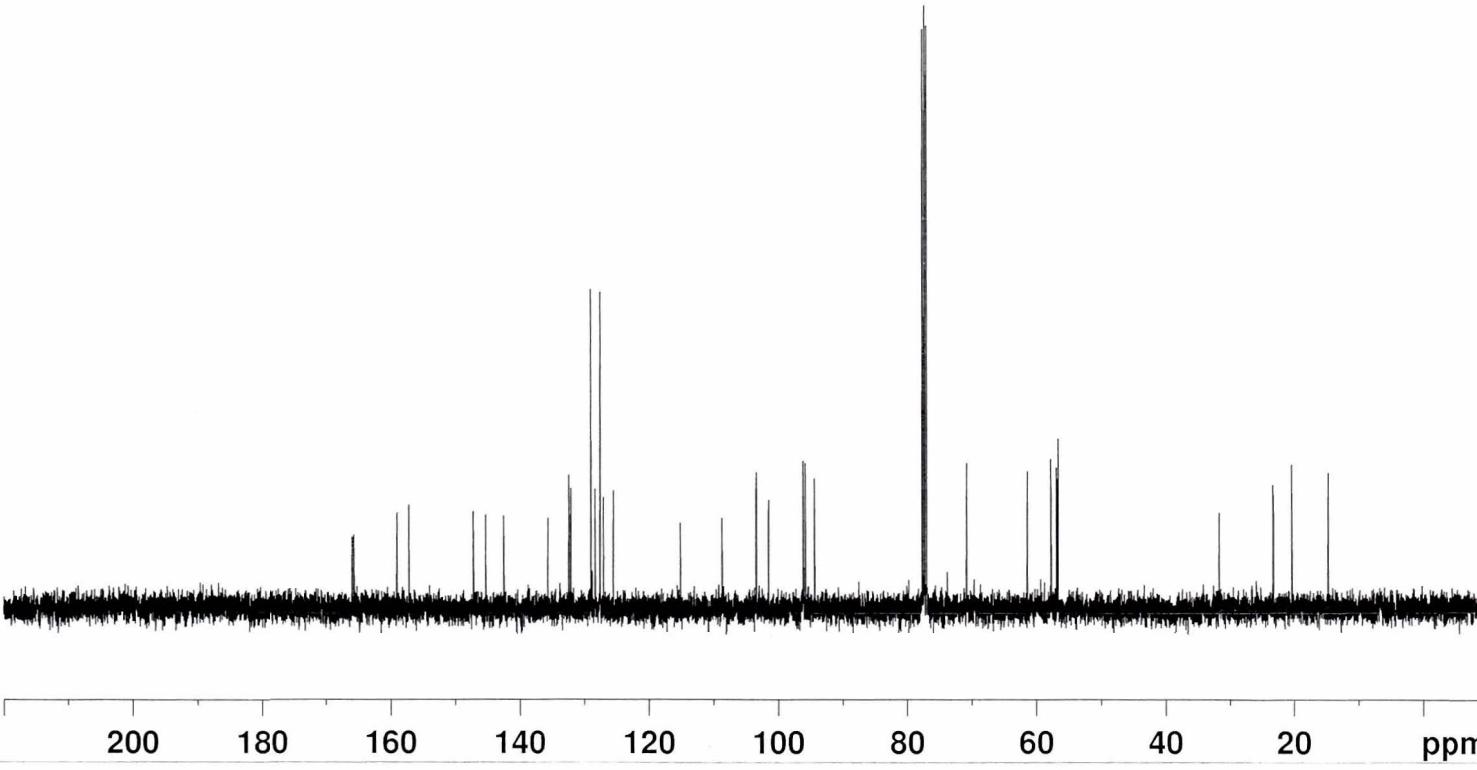
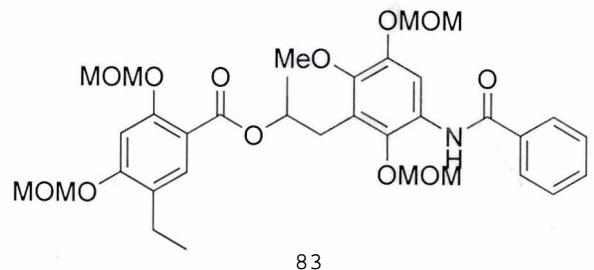


Current Data Parameters
 NAME sg511
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060203
 Time 23.27
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 101.6
 DW 104.400 usec
 DE 5.50 usec
 TE 292.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 SWD EM 0
 SSB 0.30 Hz
 LB 0
 GB 1.00
 PC



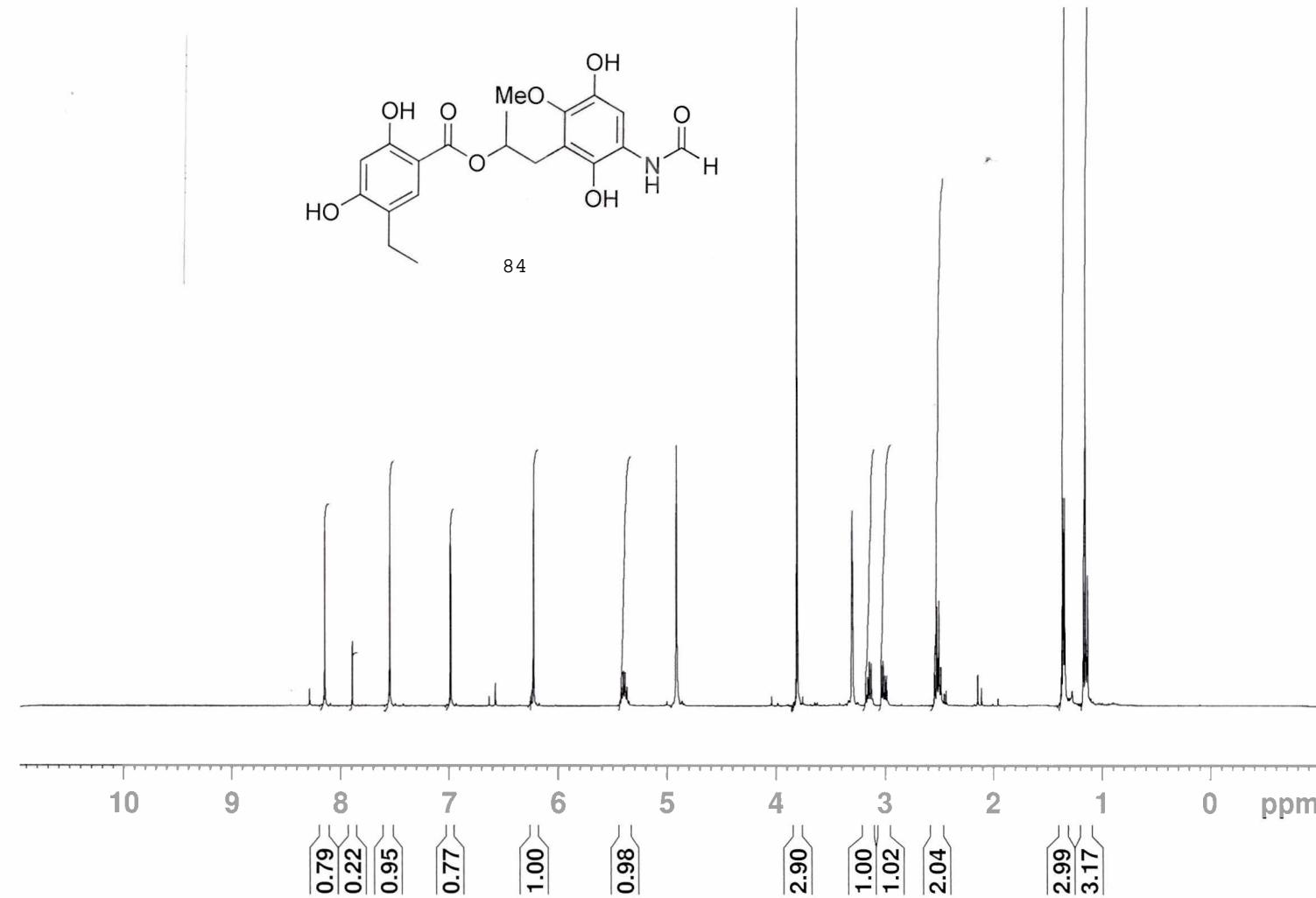
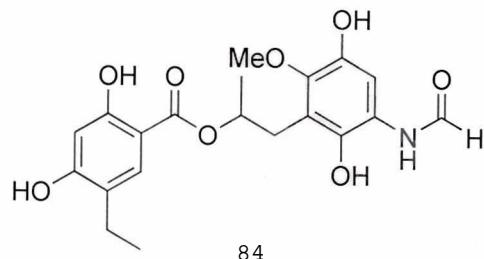
Current Data Parameters
 NAME sg511
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060203
 Time 23.44
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 86
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 292.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100 6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 altz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400 1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



```

=====
EXPNO          2
PROCNO        1

F2 - Acquisition Parameters
Date_   20060205
Time    5.11
INSTRUM  drx400
PROBHD  5 mm QNP 1H/13
PULPROG zg30
TD      32768
SOLVENT  MeOH
NS       16
DS        2
SWH     4789.272 Hz
FIDRES  0.146157 Hz
AQ      3.4210291 sec
RG      256
DW      104.400 usec
DE      5.50 usec
TE      291.2 K
D1      1.0000000 sec
MCREST  0.0000000 sec
MCWRK   0.0150000 sec

```

```

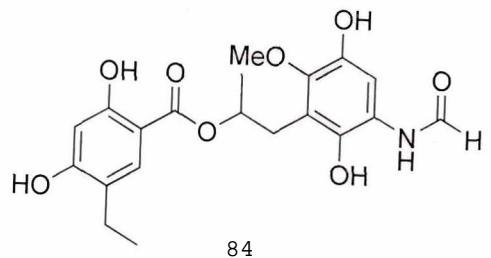
===== CHANNEL f1 =====
NUC1           1H
P1            9.35 usec
PL1          -4.00 dB
SFO1        400.1320007 MHz

```

```

F2 - Processing parameters
SI            32768
SF        400.1300091 MHz
WDW           EM
SSB            0
LB          0.30 Hz
GB            0
PC          1.00

```

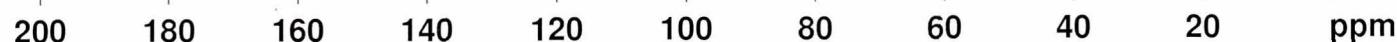


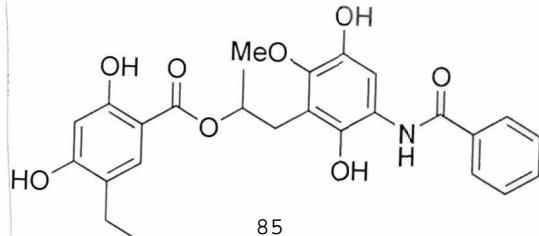
F2 - Acquisition Parameters
 Date_ 20060205
 Time 14.28
 INSTRUM dix400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 20480
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 291.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

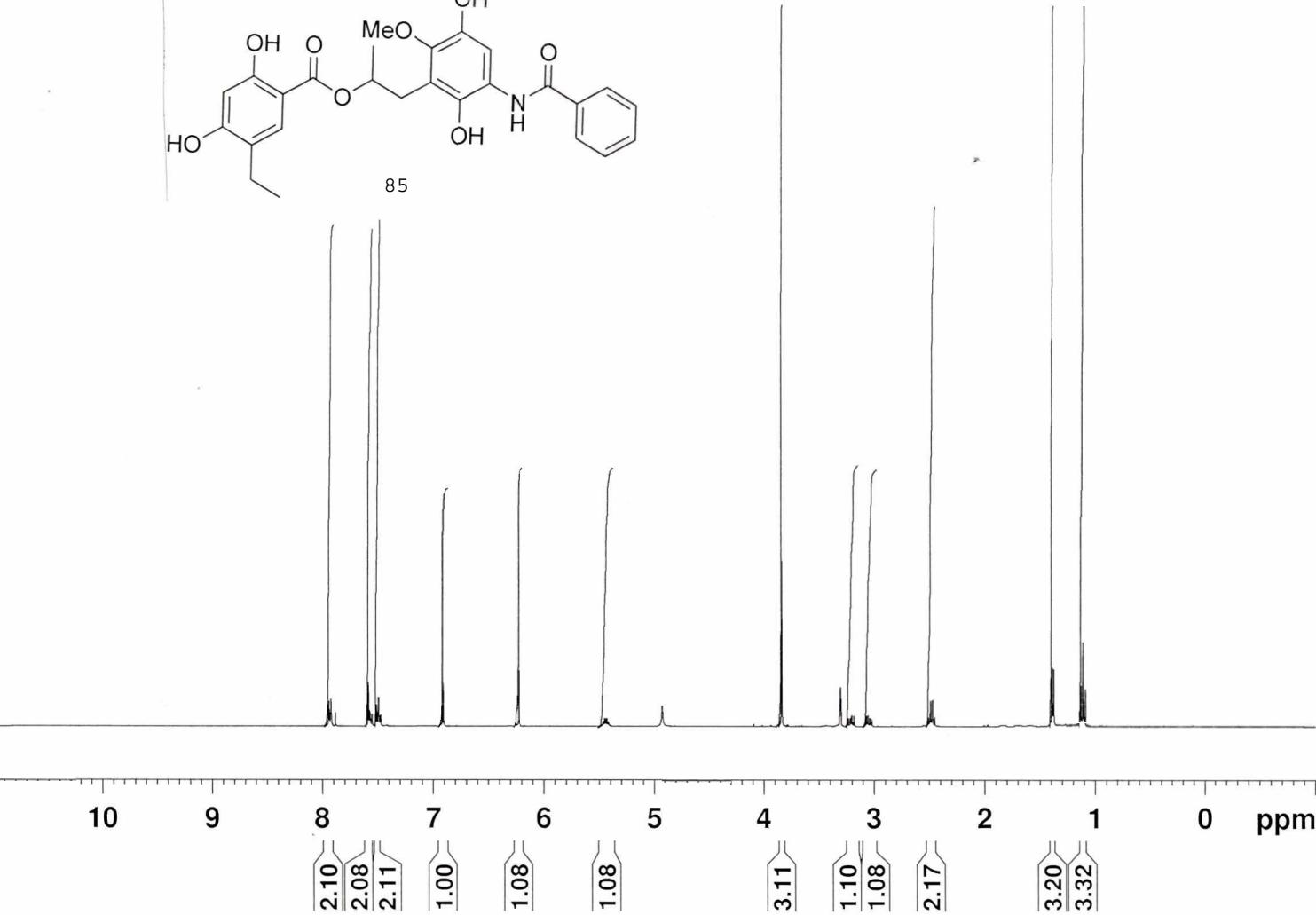
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





85



Current Data Parameters
 NAME sg512phenyl
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060205
 Time 18.03
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT MeOH
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 161.3
 DW 104.400 usec
 DE 5.50 usec
 TE 291.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

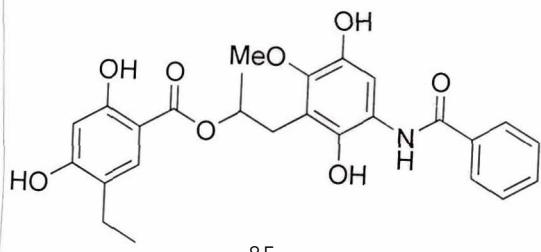
Current Data Parameters
NAME sg512phenyl
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060205
Time 18.53
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT MeOH
NS 1052
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 5.50 usec
TE 291.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

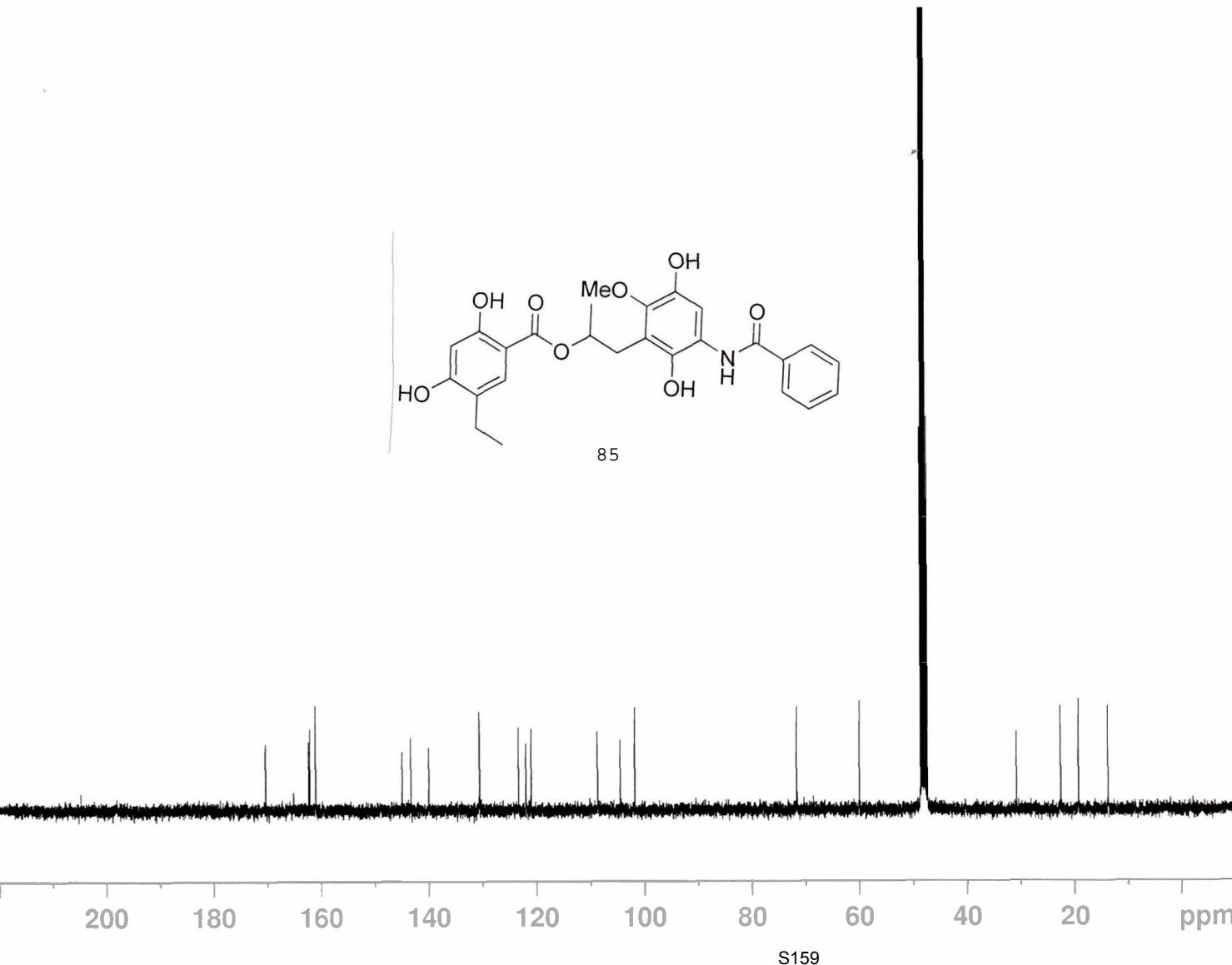
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



85



200

180

160

140

120

100

80

60

40

20

ppm

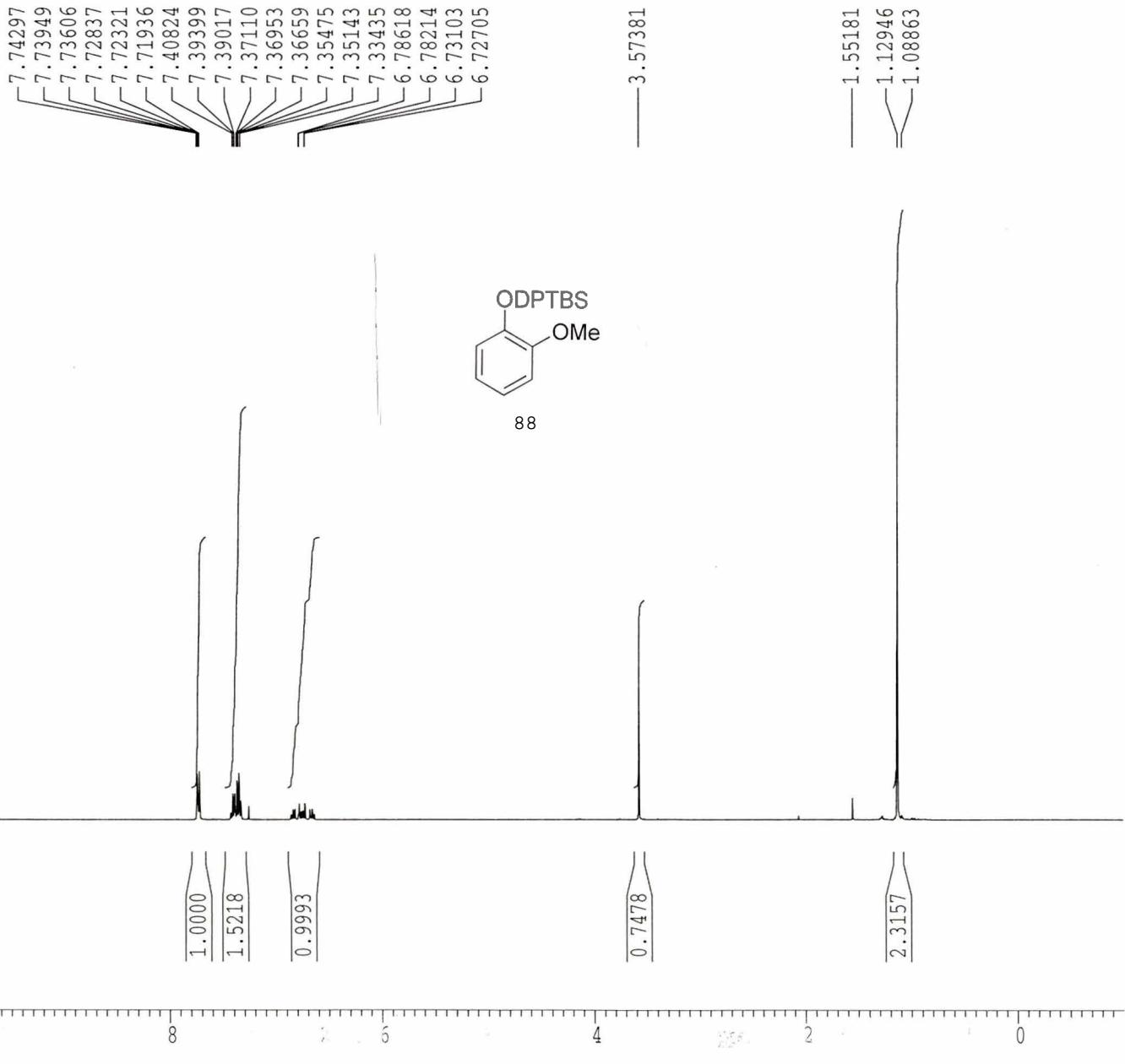
S159

ppm

Integral

ppm

10 8 6 4 2 0



3.57381

1.55181
1.12946
1.08863

Current Data Parameters
 NAME sg493
 EXPNO 1
 PROCN0 1

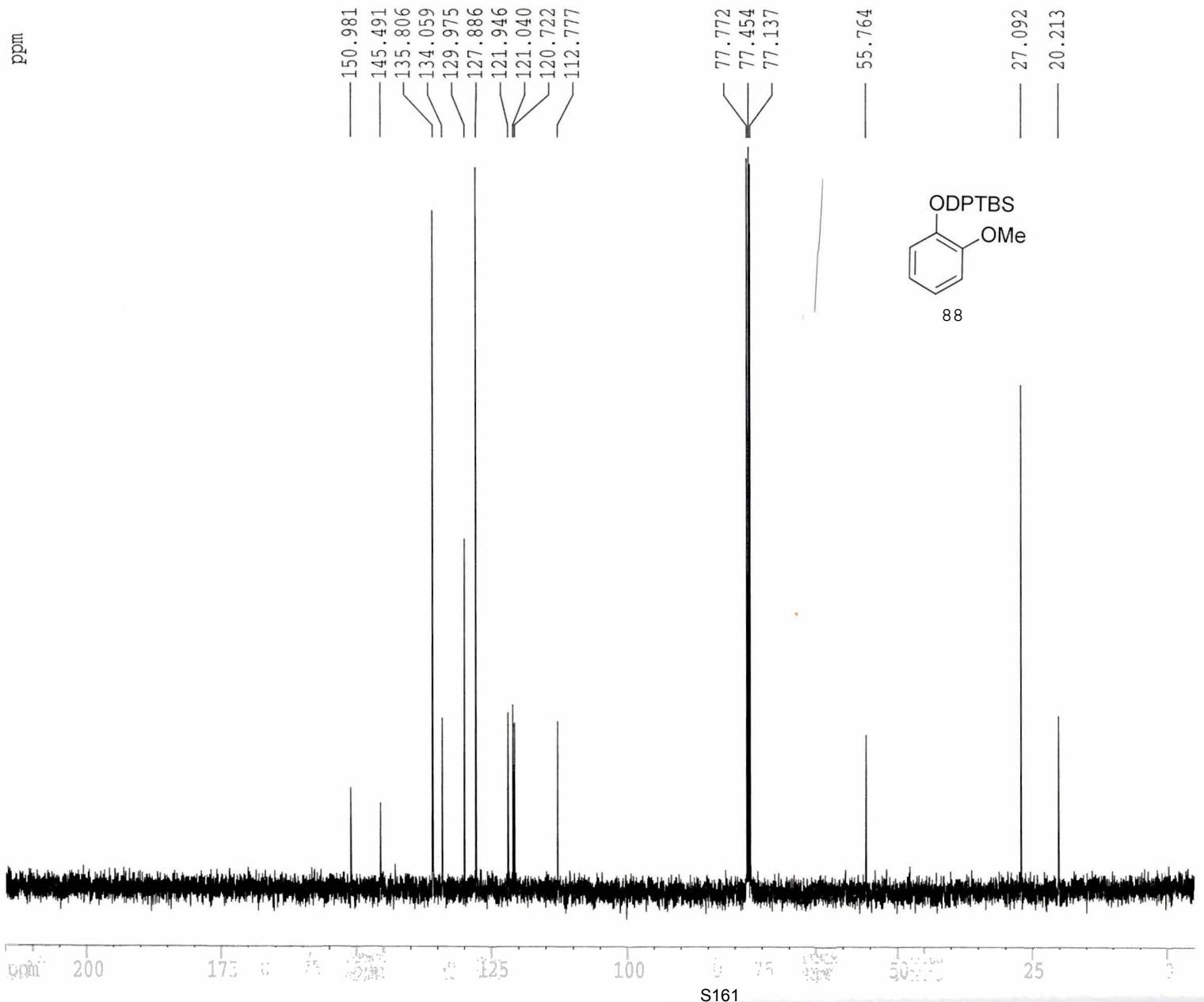
F2 - Acquisition Parameters
 Date_ 20051107
 Time 18.21
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 128
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

ppm



Current Data Parameters
 NAME sg493
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051107
 Time 18.25
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 196
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SPO2 400.1316005 MHz

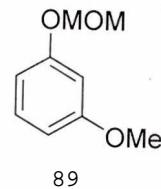
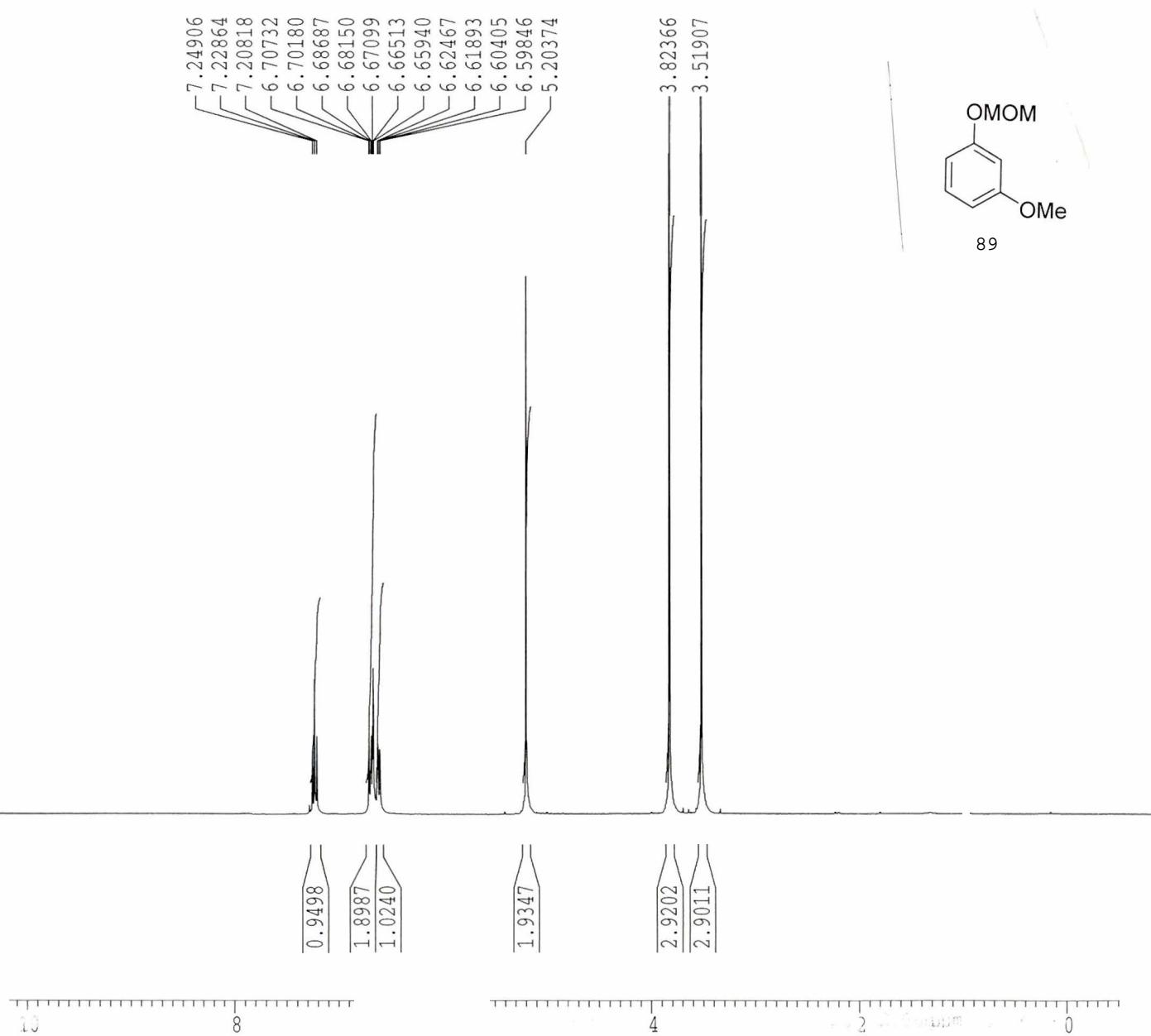
F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 F3P 11.20000 ppm/cm
 F3 1106.73999 Hz/cm

S161

ppm

Integral



Current Data Parameters
 NAME sg478
 EXPNO 1
 PROCNO 1

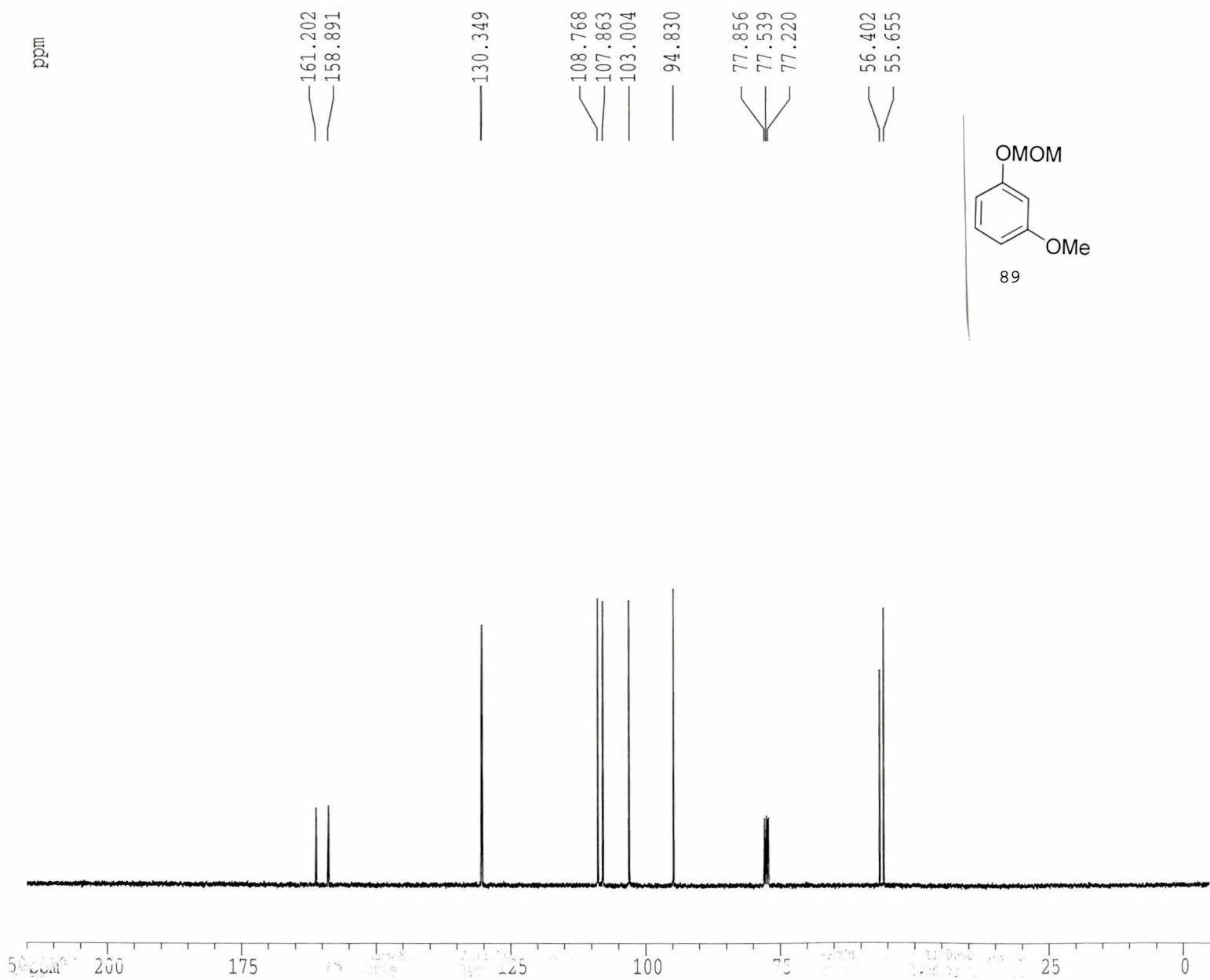
F2 - Acquisition Parameters
 Date_ 20050916
 Time 20.50
 INSTRUM dnx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 32
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

ppm



Current Data Parameters
 NAME sg478
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050916
 Time 20.54
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 135
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.1500001 sec
 d11 0.0300000 sec
 DELTA 0.0500000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PREWV 12.0000 pps/cm
 DM 3399 Hz/cm

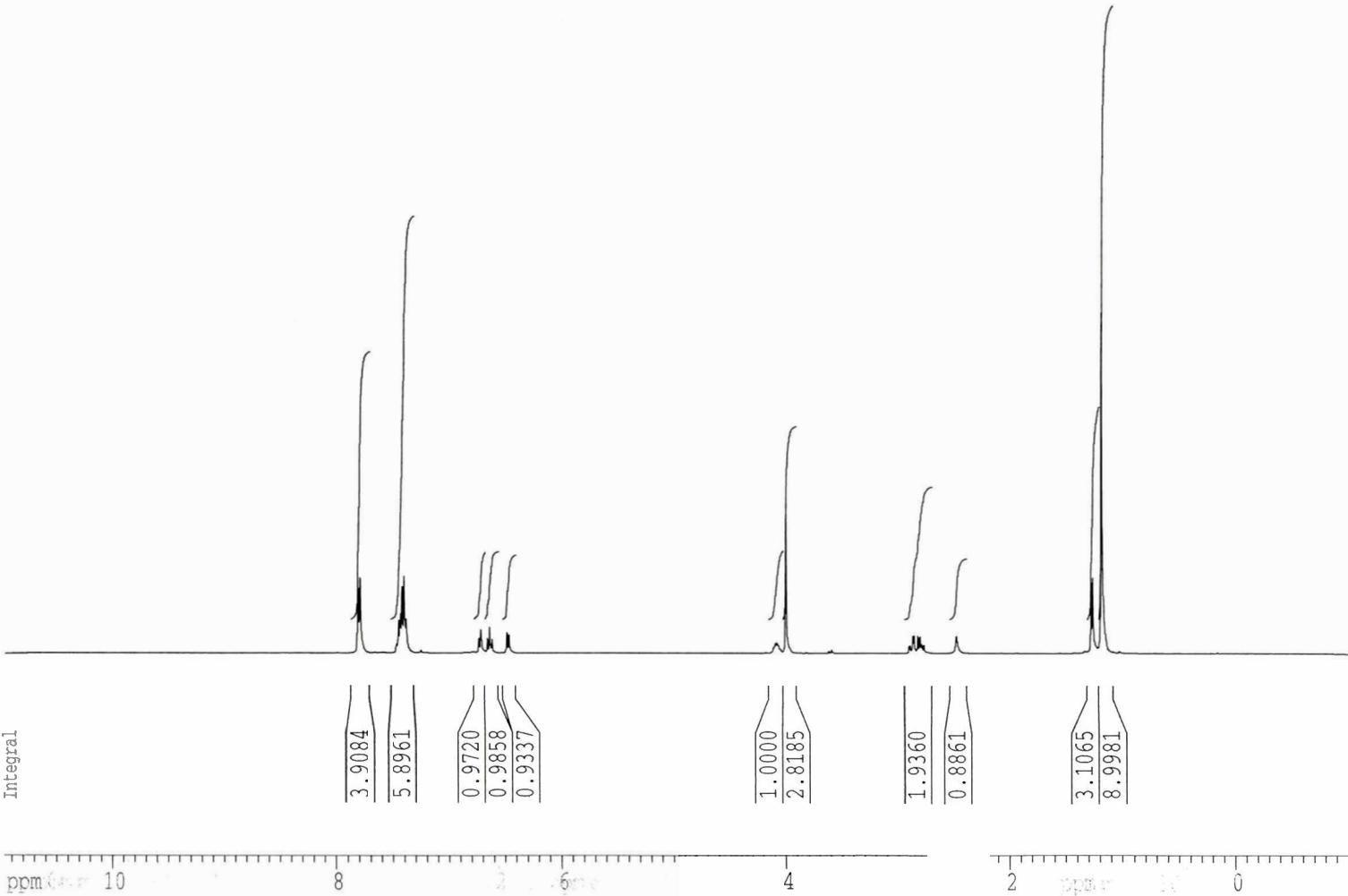
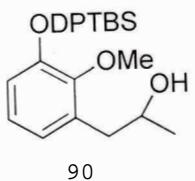
Current Data Parameters
NAME sg496
EXPNO 1
PROCNO 1

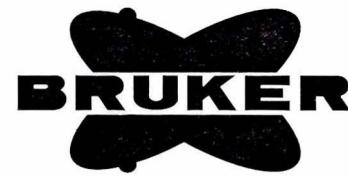
F2 - Acquisition Parameters
Date_ 20051116
Time 16.58
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 25.4
DW 104.400 usec
DE 5.50 usec
TE 294.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SF01 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 11.000 ppm
F1 4401.43 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPMCM 0.60000 ppm/cm
HZCM 240.07800 Hz/cm





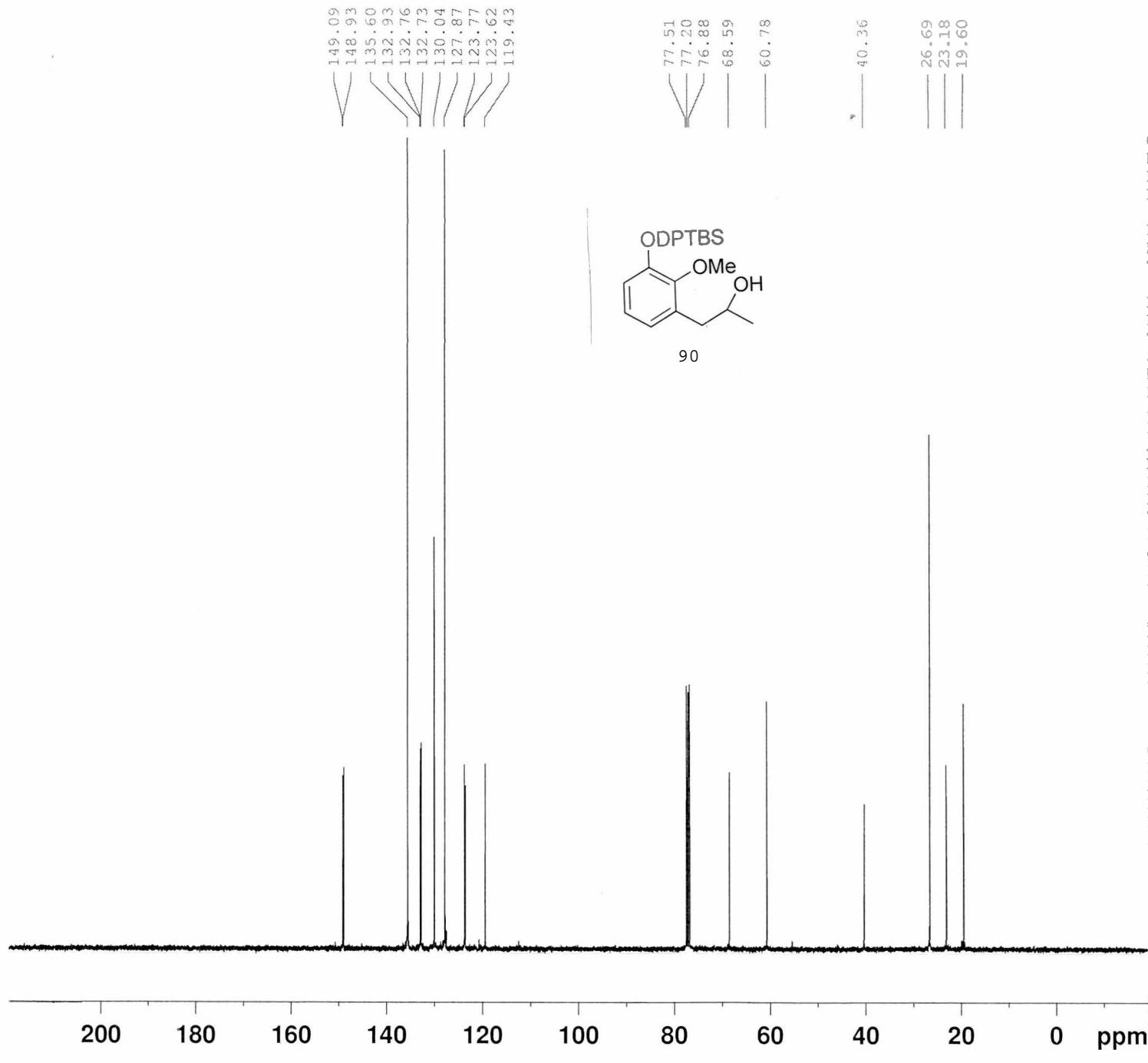
Current Data Parameters
 NAME gang06
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060415
 Time 16.32
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 332
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 32768
 DW 20.850 usec
 DE 6.00 usec
 TE 296.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.85 usec
 PL1 -2.00 dB
 SFO1 100.6228298 MHz

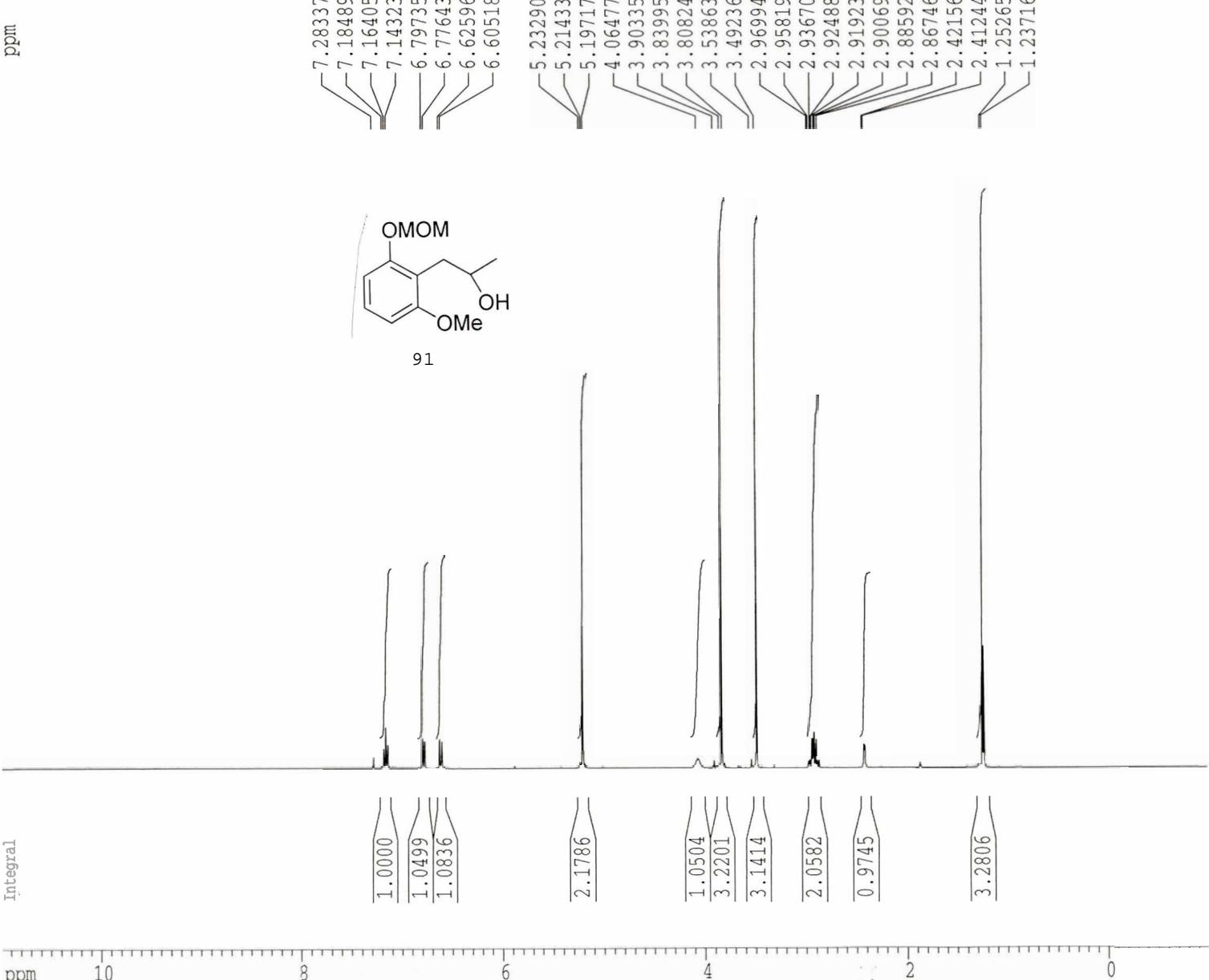
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -5.00 dB
 PL12 14.58 dB
 PL13 120.00 dB
 SFO2 400.1316005 MHz

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



ppm

Integral



Current Data Parameters
 NAME sg481
 EXPNO 1
 PROCN 1

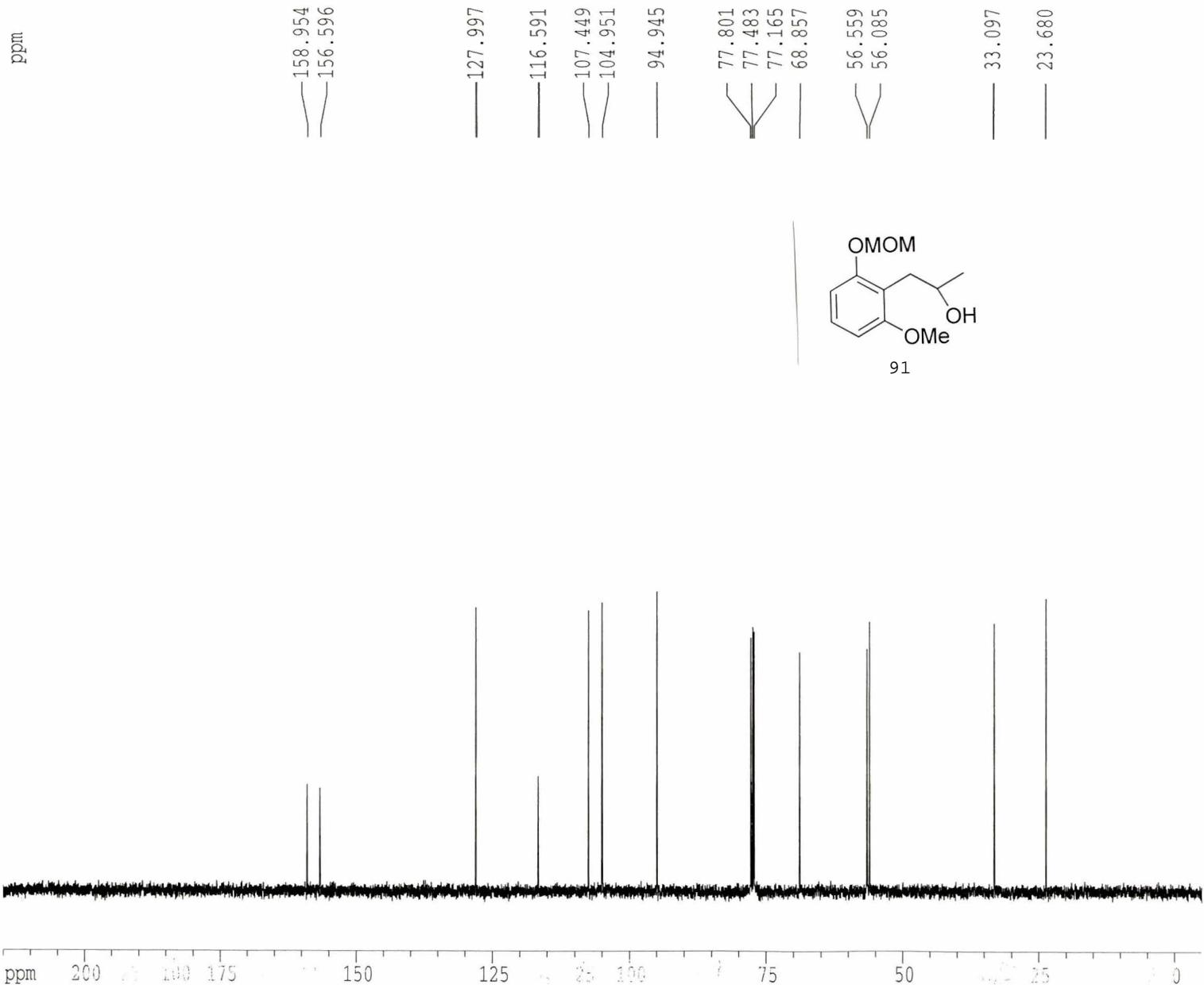
F2 - Acquisition Parameters
 Date_ 20050920
 Time 18.42
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 5.50 usec
 TE 295.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 P11 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

ppm



Current Data Parameters
 NAME sg481
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050920
 Time 18.44
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 92
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 295.2 K
 D1 0.1500001 sec
 d11 0.0300000 sec
 DELTA 0.0500000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

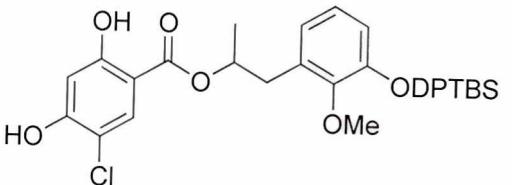
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz, cm

Current Data Parameters
 NAME sg496
 EXPNO 2
 PROCNO 1



F2 - Acquisition Parameters
 Date_ 20051116
 Time 17.03
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 322.5
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

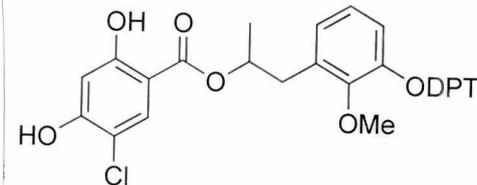
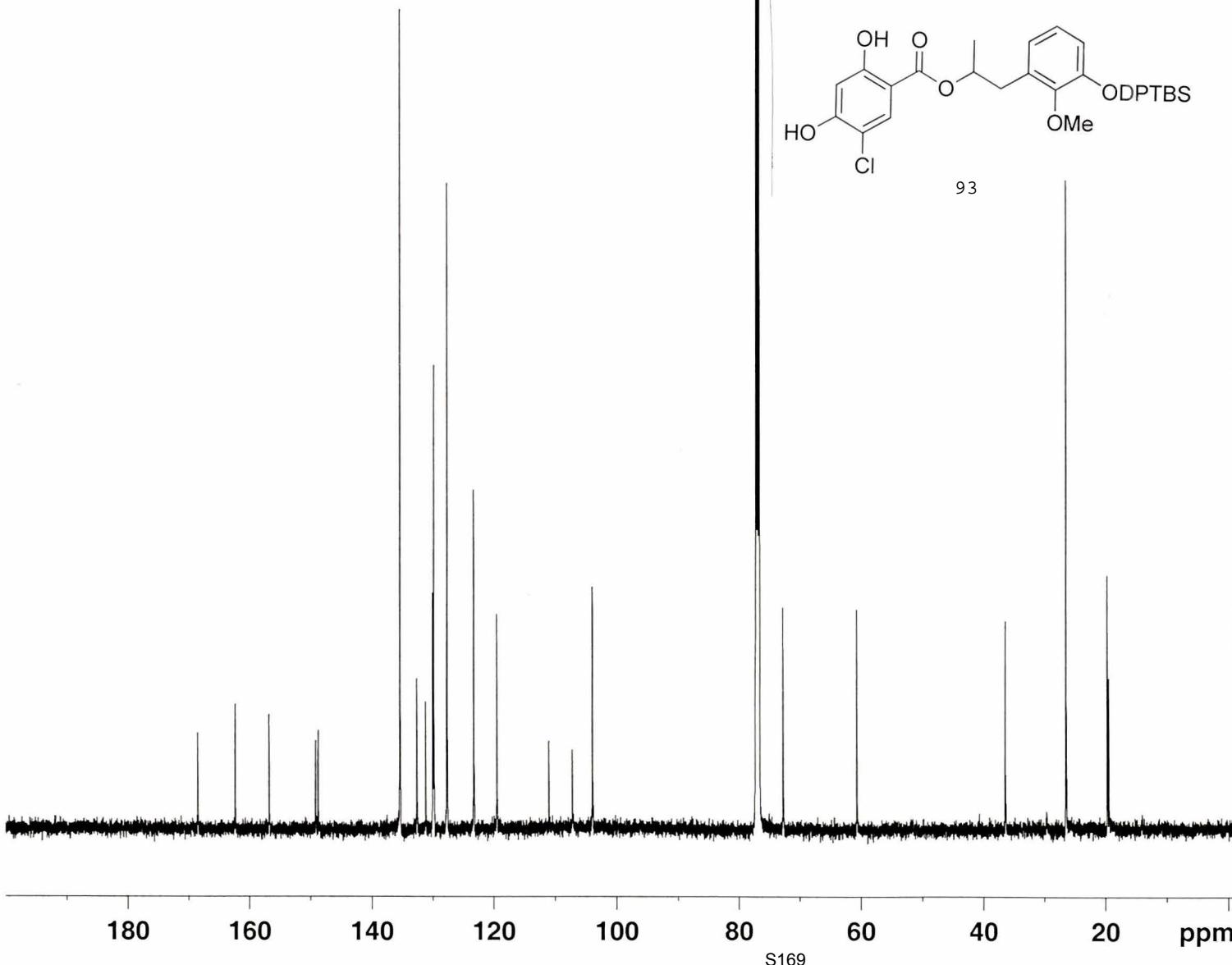
Integral

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0.8810		
1.0756		
3.0169		
1.0352	1.0793	
3.3195	9.3029	

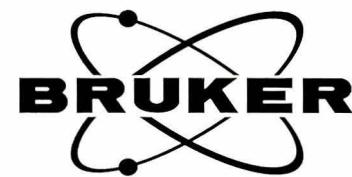
ppm

10 8 6 4 2 0

C13CPD CDC13 opt/topspin gshen 3



93



Current Data Parameters
NAME sg495
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051116
Time 15.36
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 13004
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 13C
P1 9.95 usec
PL1 3.80 dB
SFO1 125.7703640 MHz

===== CHANNEL f2 ======
CPDPG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.20 dB
PL12 16.80 dB
PL13 10.00 dB
SFO2 500.1320000 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

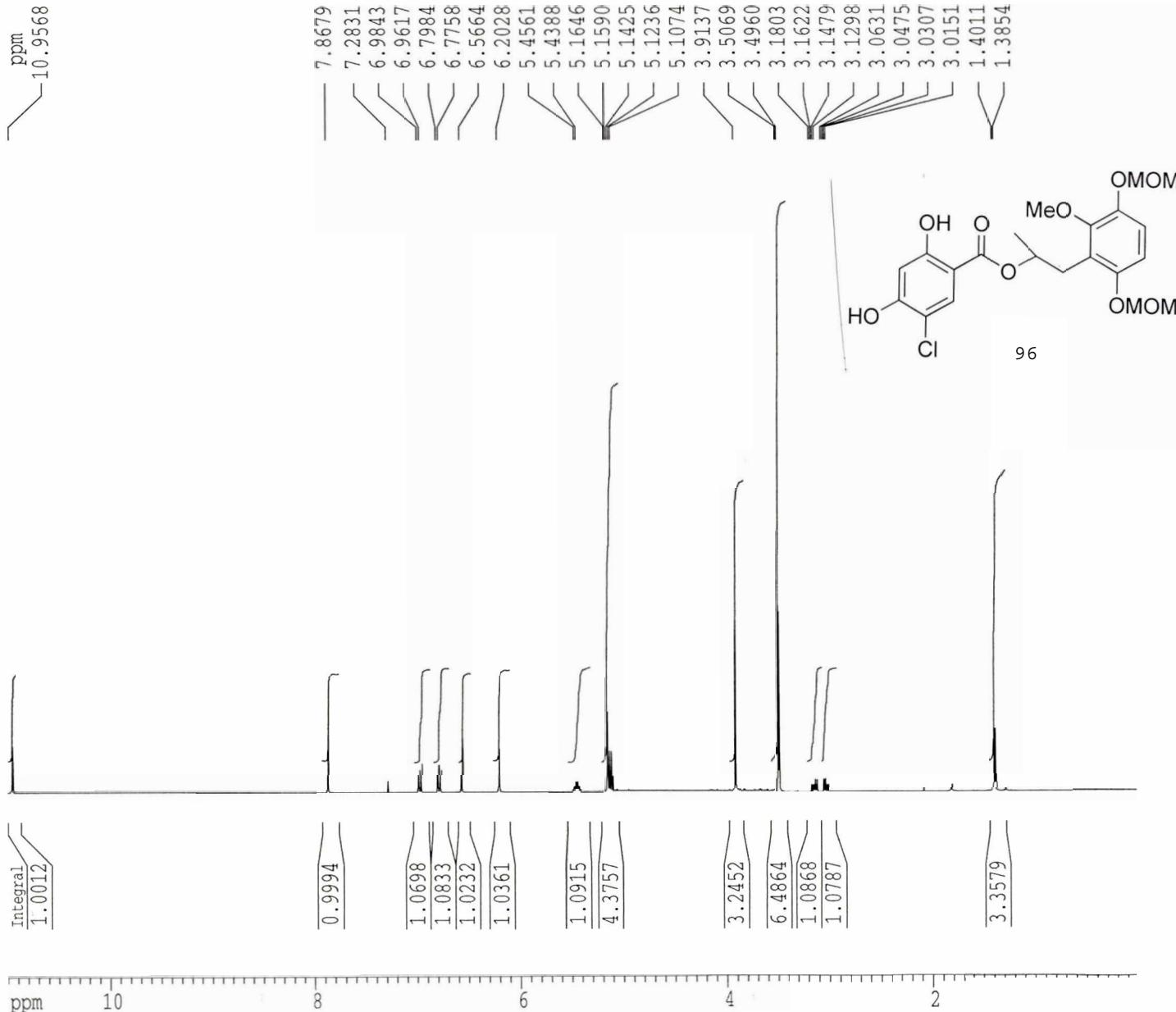
Current Data Parameters
 NAME sg476
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050913
 Time 17.46
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5592.841 Hz
 FIDRES 0.170680 Hz
 AQ 2.9295092 sec
 RG 101.6
 DW 89.400 usec
 DE 5.50 usec
 TE 296.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

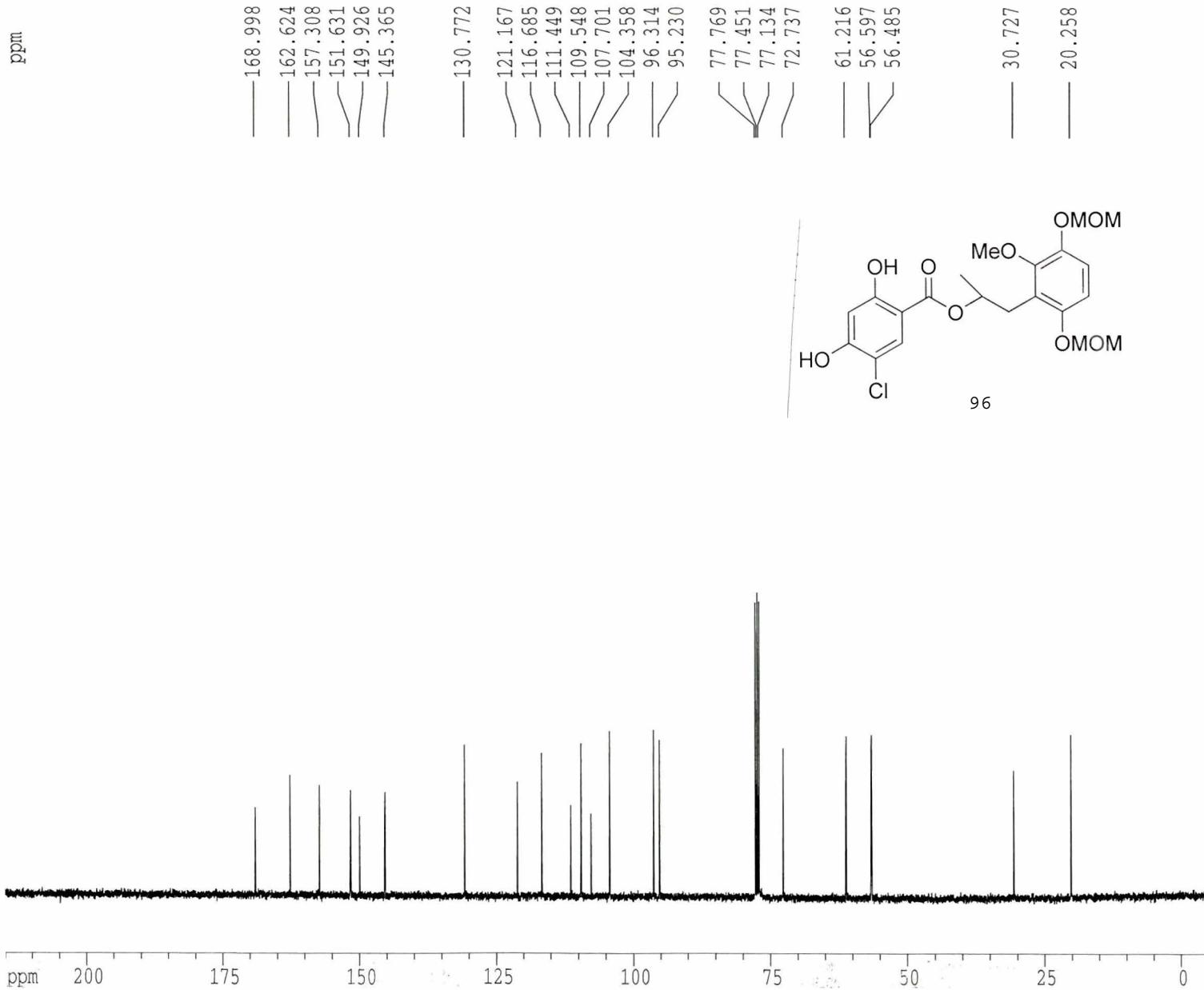
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1328009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 3.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm



ppm



Current Data Parameters
 NAME sg476
 EXPNO 3
 PROCNO 1

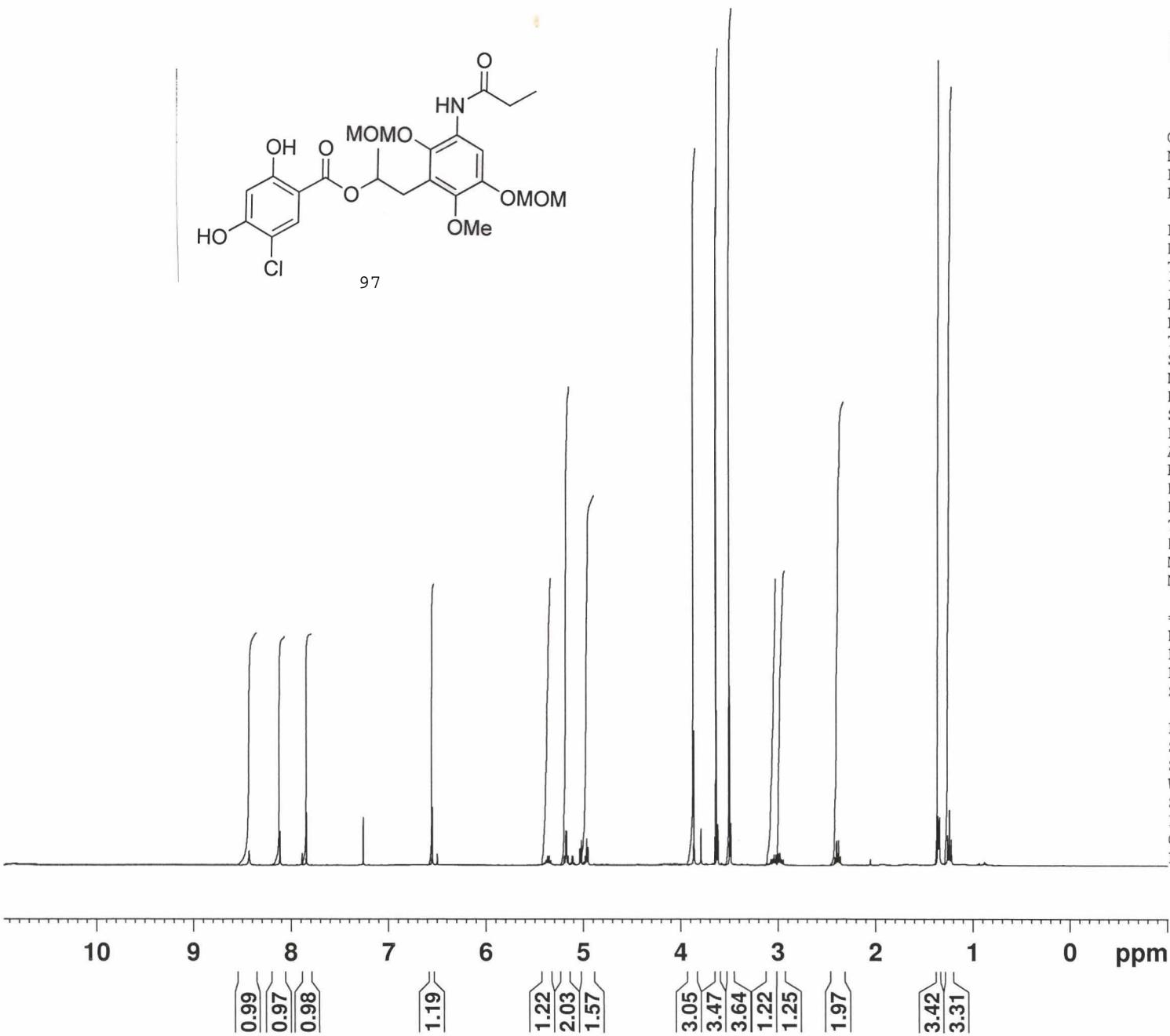
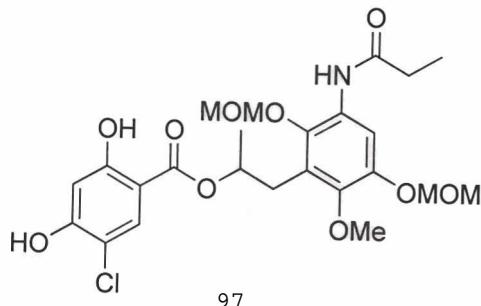
F2 - Acquisition Parameters
 Date_ 20050913
 Time 17.48
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zpgpg30
 TD 65536
 SOLVENT CDCl3
 NS 400
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 296.2 K
 D1 0.1500001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



Current Data Parameters
 NAME sg499
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051122
 Time 6.21
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 228.1
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

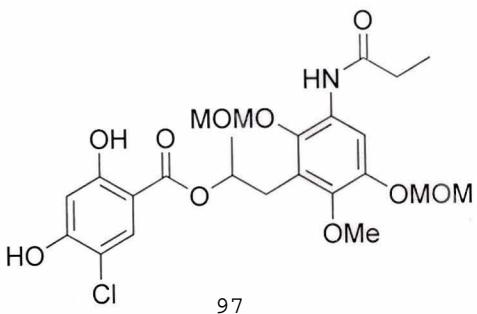
Current Data Parameters
NAME sg499
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051122
Time 13.47
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 16384
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

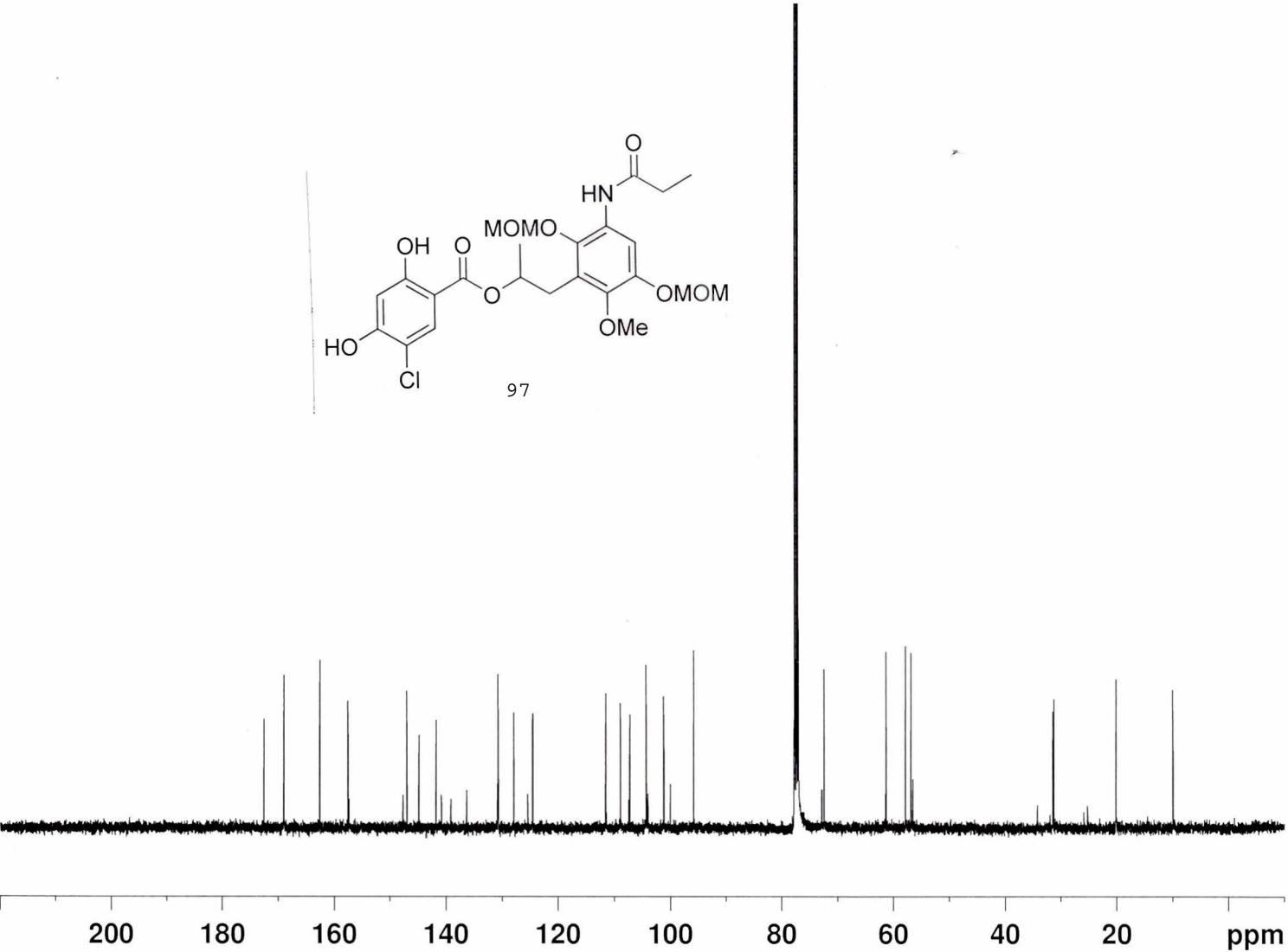
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

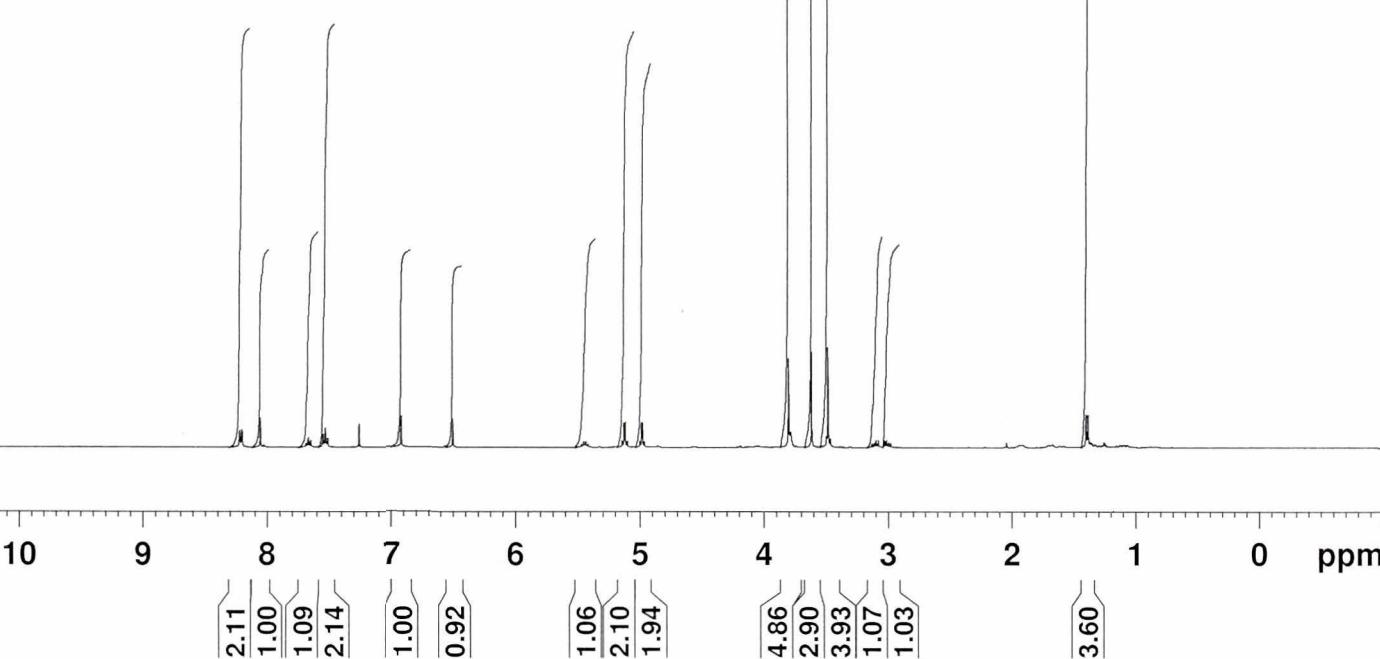
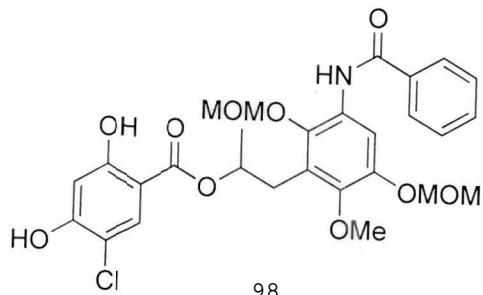
F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



97



BRUKER

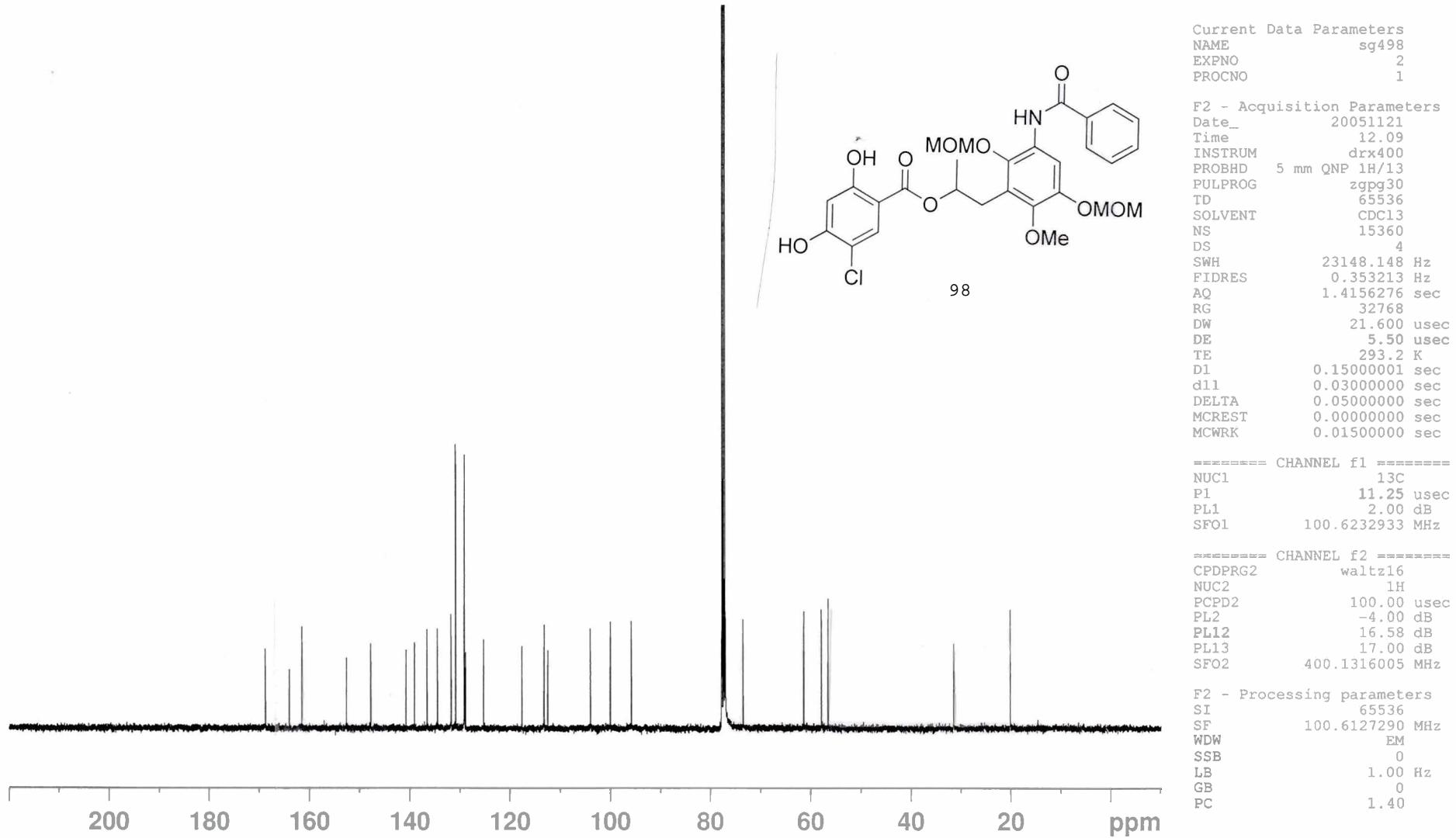


Current Data Parameters
NAME sg498
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051121
Time 5.10
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 203.2
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

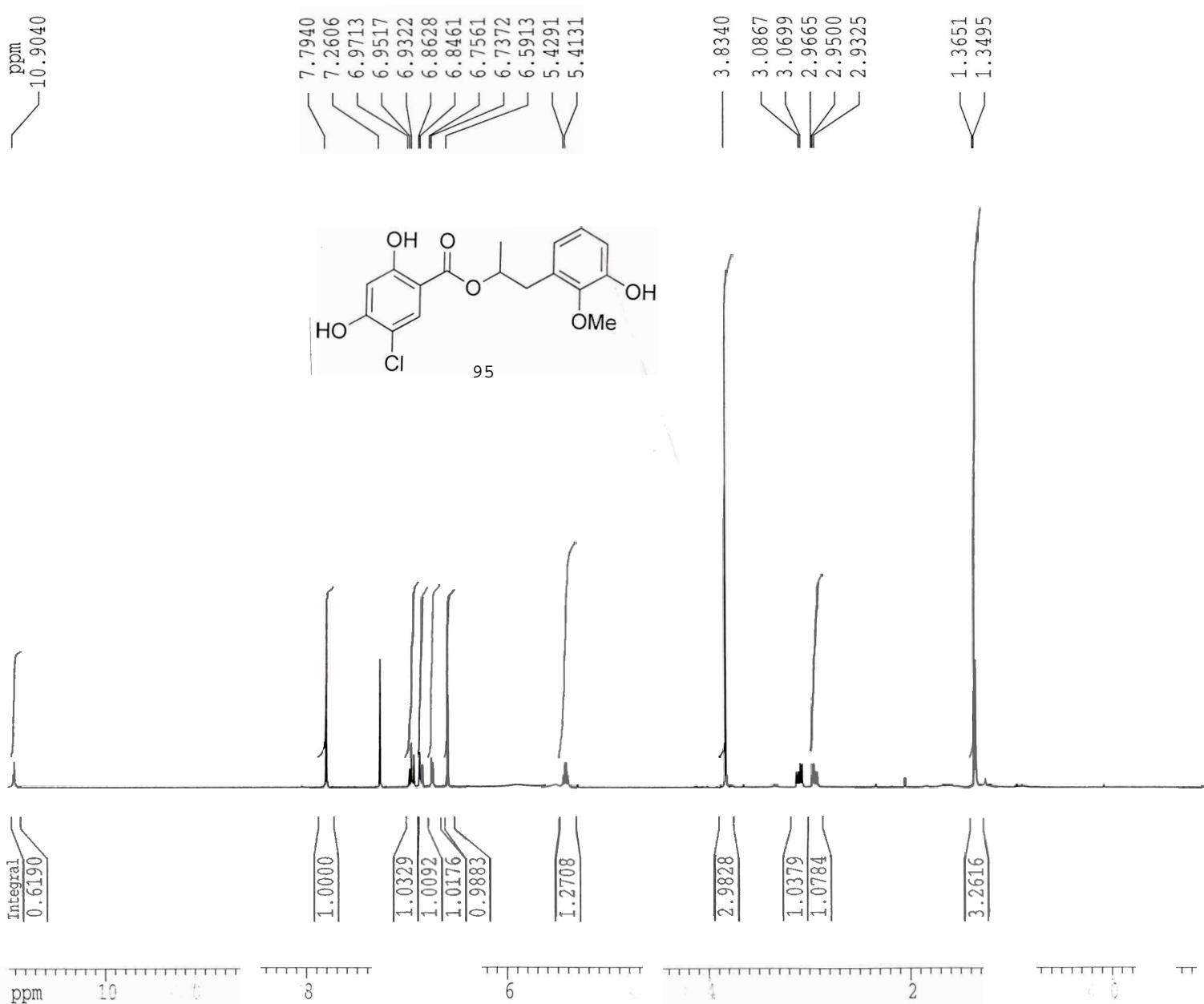
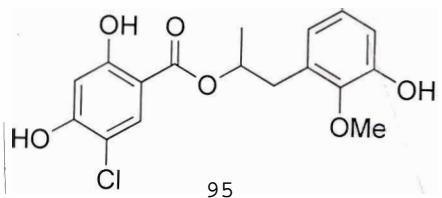
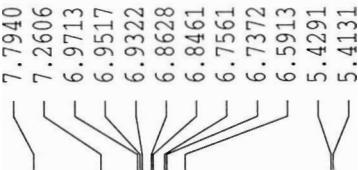
F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



200 180 160 140 120 100 80 60 40 20 ppm

ppm

10.9040



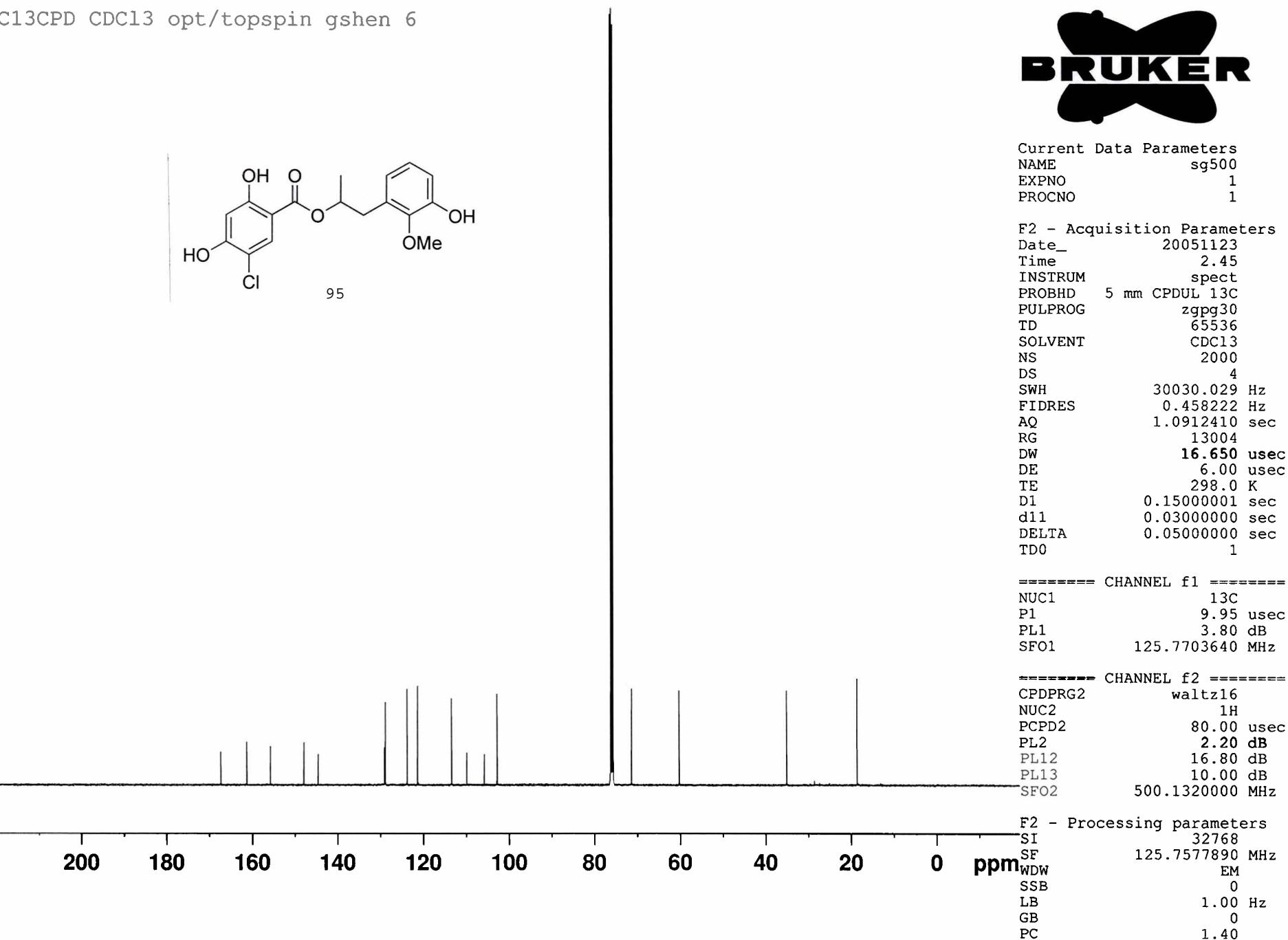
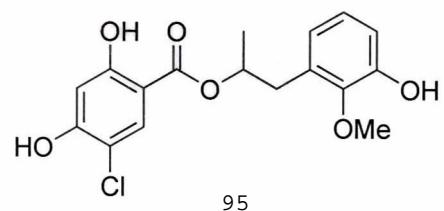
Current Data Parameters
NAME sg500
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051122
Time 13.05
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 406.4
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 ======
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SF01 400.1320007 MHz

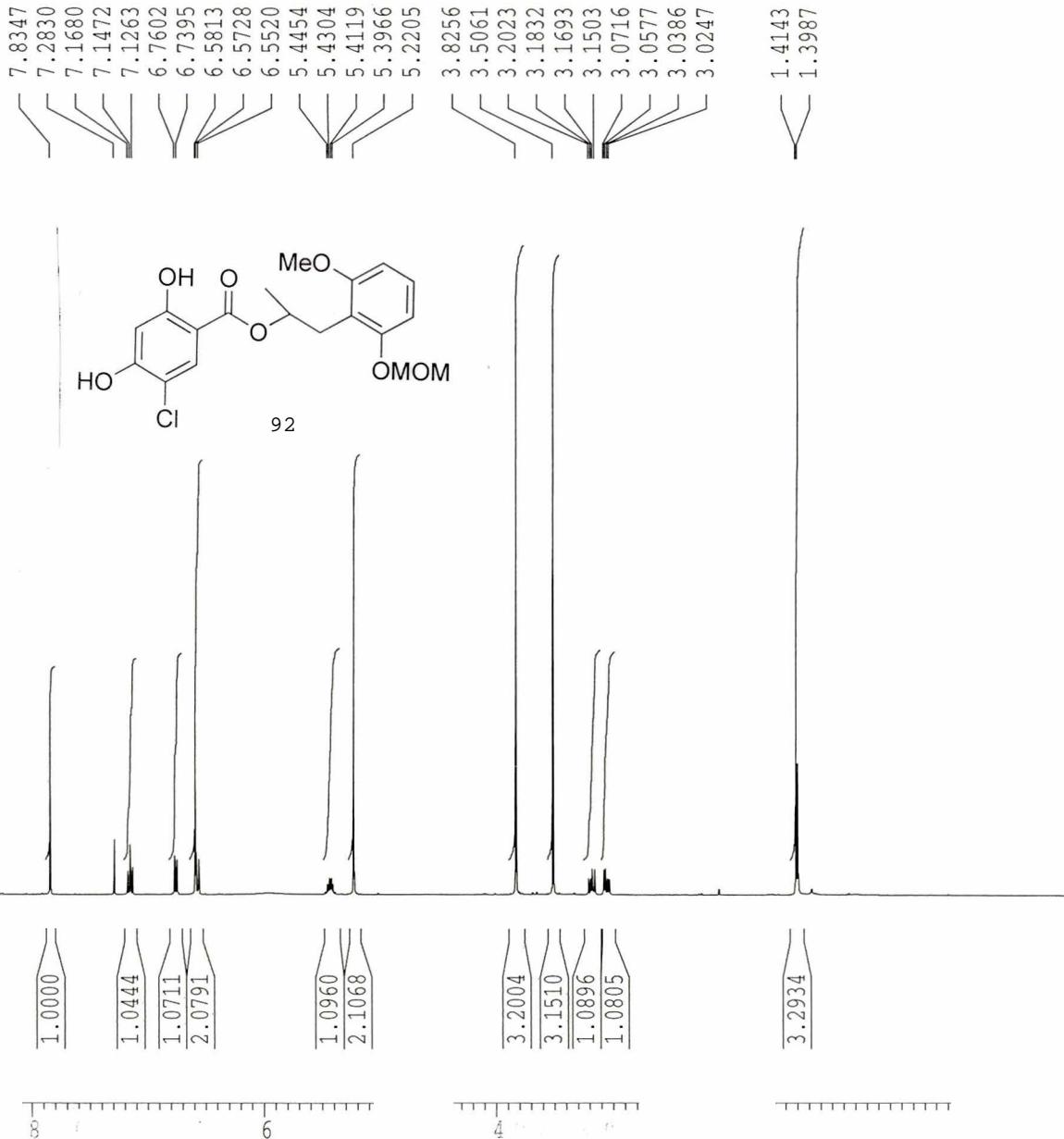
F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 11.000 ppm
F1 4401.43 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPCM 0.60000 ppm/cm
HZCM 240.07800 Hz/cm

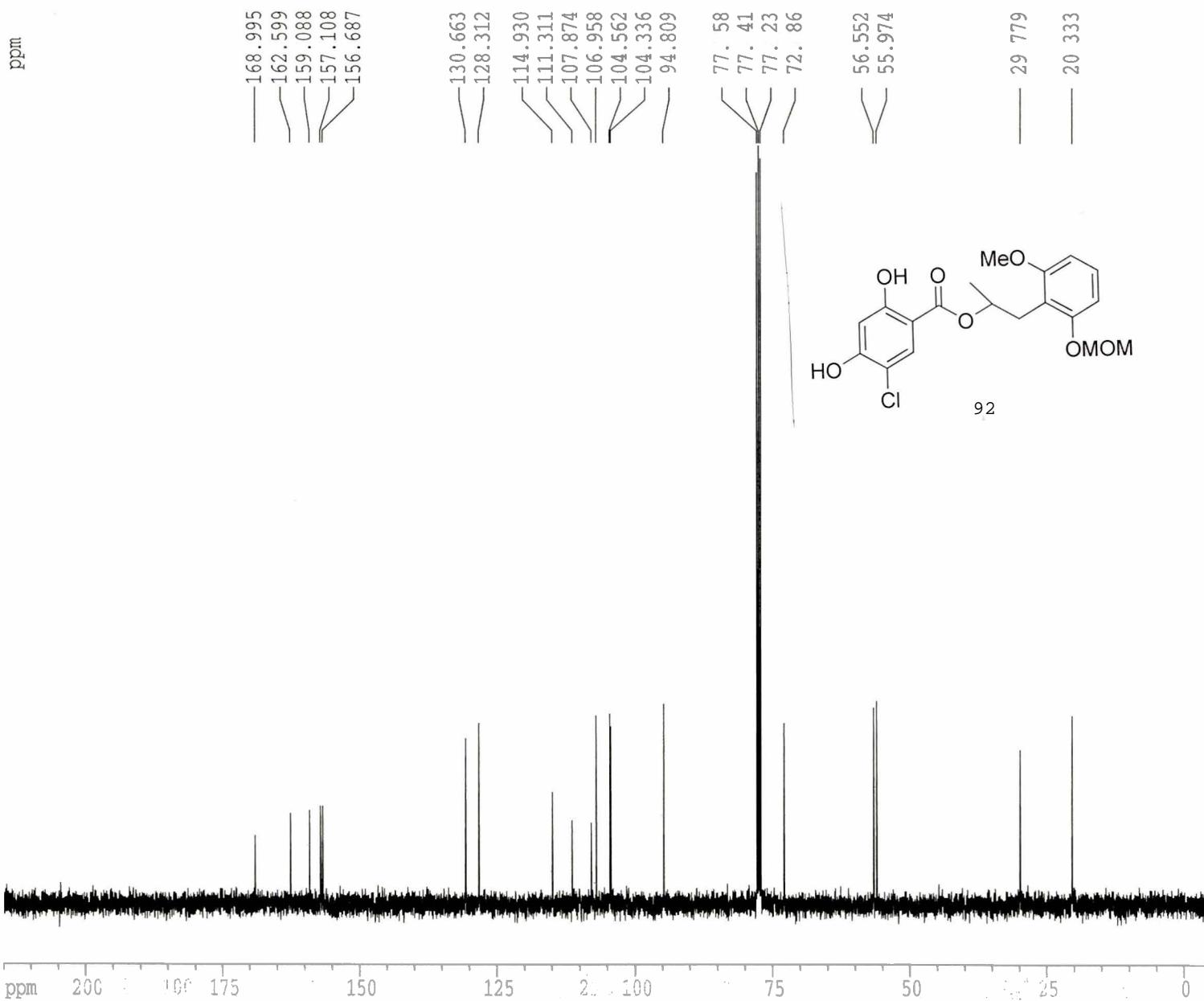


ppm

10.9532



ppm



Current Data Parameters
 NAME sg482
 EXPNO 2
 PROCN 1

F2 - Acquisition Parameters
 Date 20050929
 Time 10.15
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 327
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

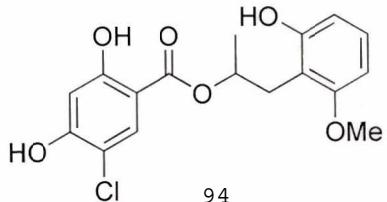
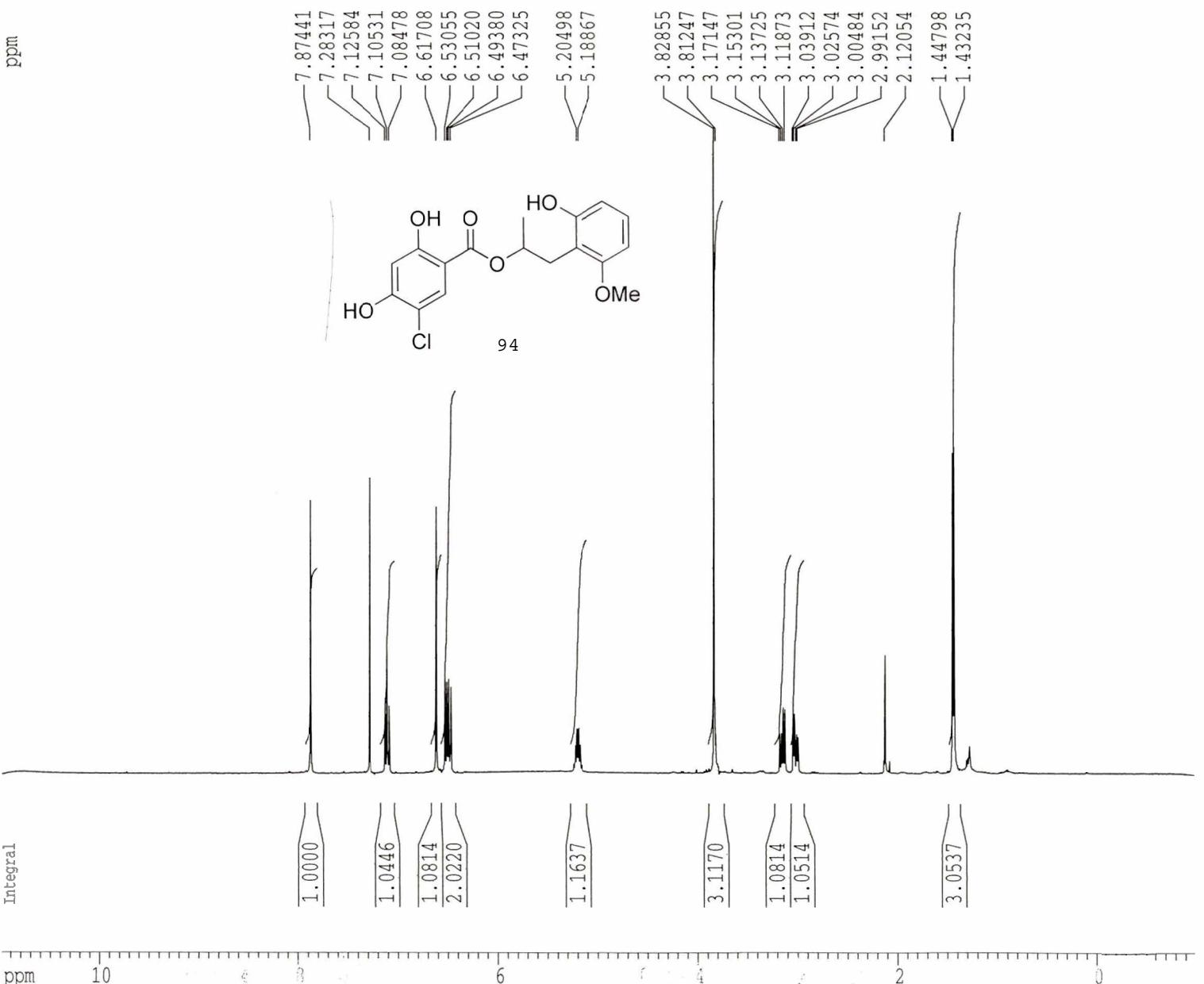
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm

ppm



Current Data Parameters
 NAME sg487
 EXPNO 1
 PROCNO 1

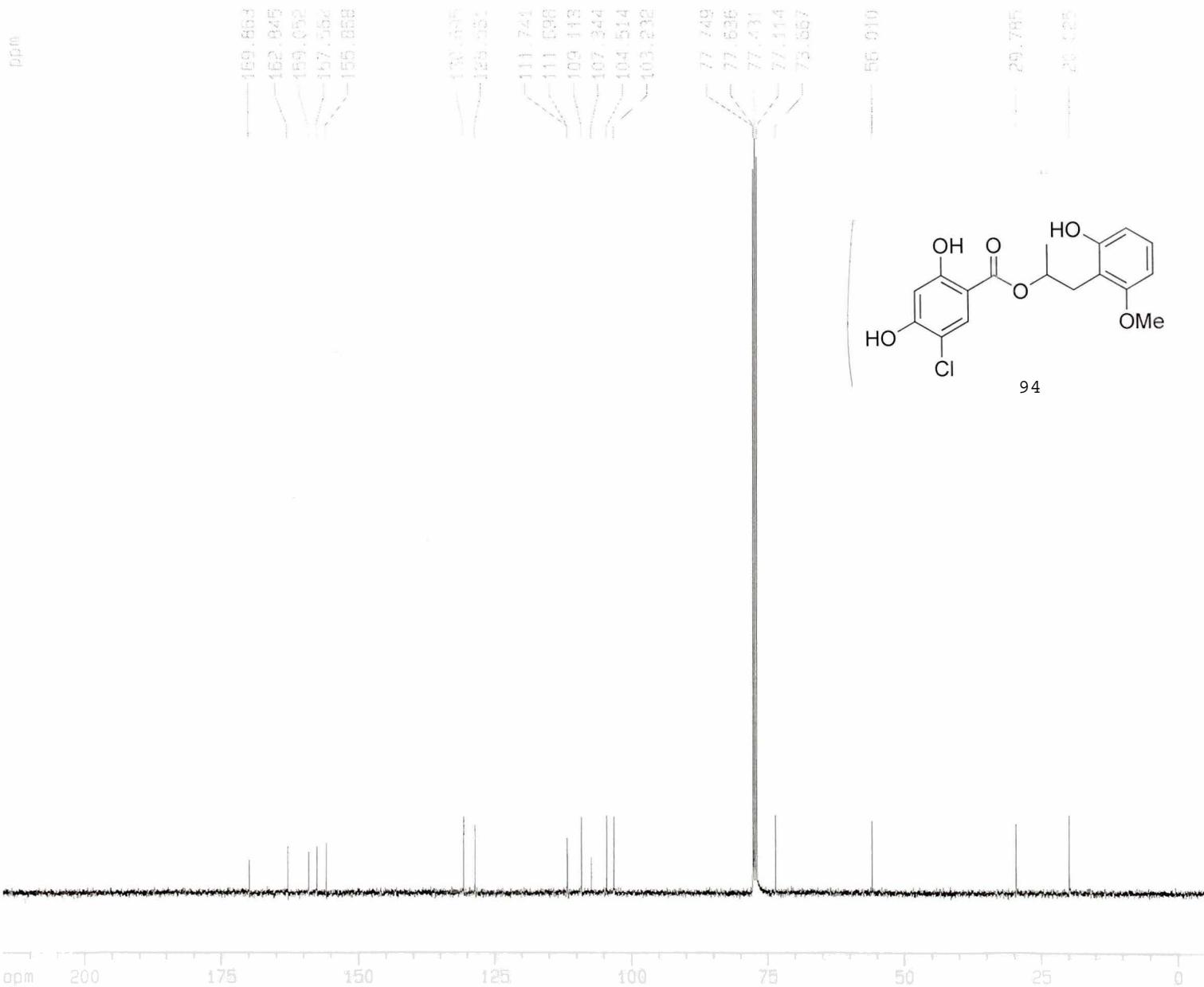
F2 - Acquisition Parameters
 Date_ 20051004
 Time 23.31
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 287.4
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

ppm



Current Data Parameters
 NAME sg487
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051005
 Time 0.55
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 3072
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 HDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 ZC 1.40

ID NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -5.000 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm

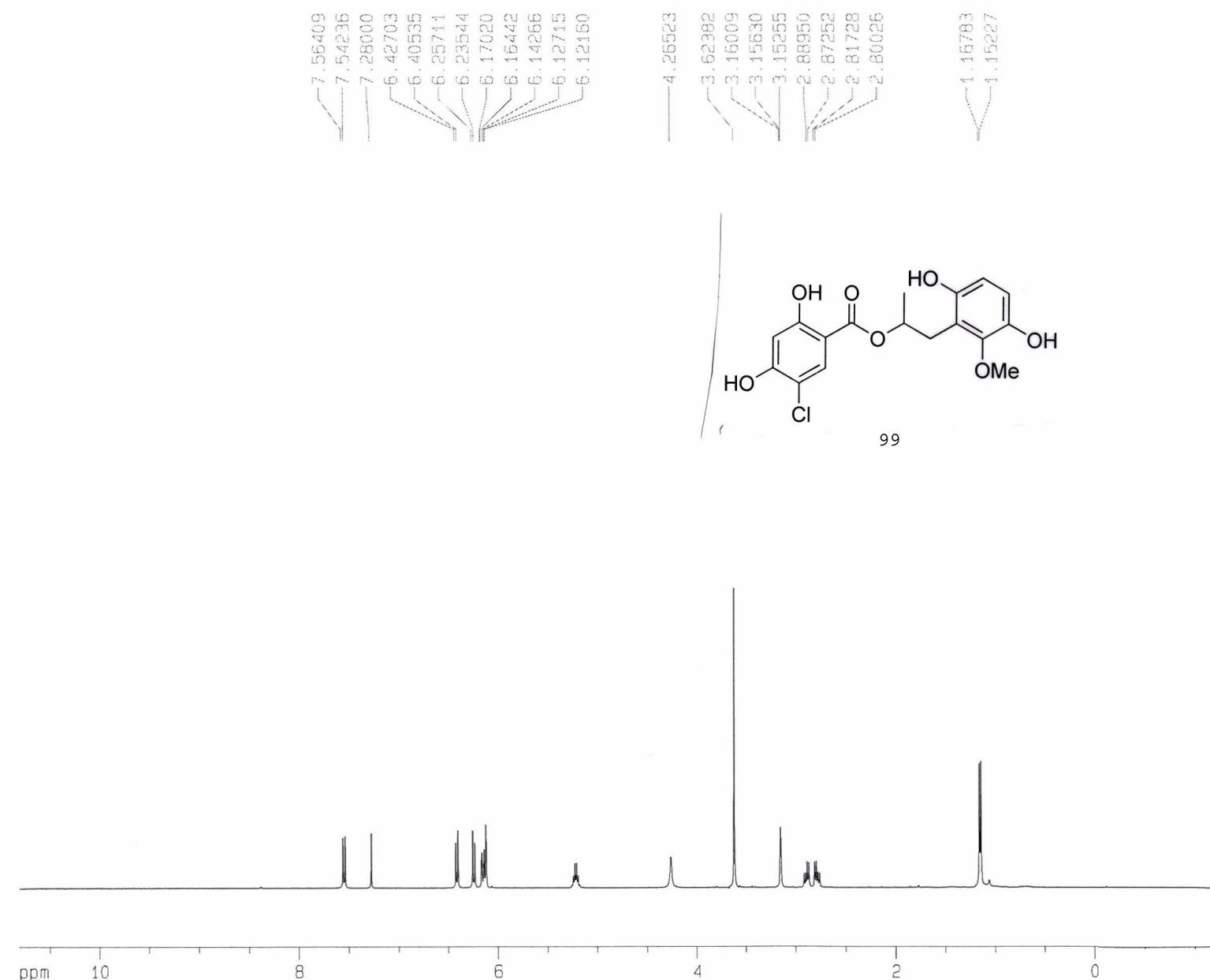
Current Data Parameters
 NAME sg504
 EXPNO 1
 PROCN0 1

F2 - Acquisition Parameters
 Date_ 20051127
 Time 21.46
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT MeOH
 NS 16
 OS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 362
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1301132 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 10.811 ppm
 F1 4325.99 Hz
 F2P -1.158 ppm
 F2 -463.28 Hz
 PPMM 0.59846 ppm/cm
 HZCM 239.46362 Hz/cm



Current Data Parameters
 NAME sg504
 EXPNO 2
 PROCN0 1

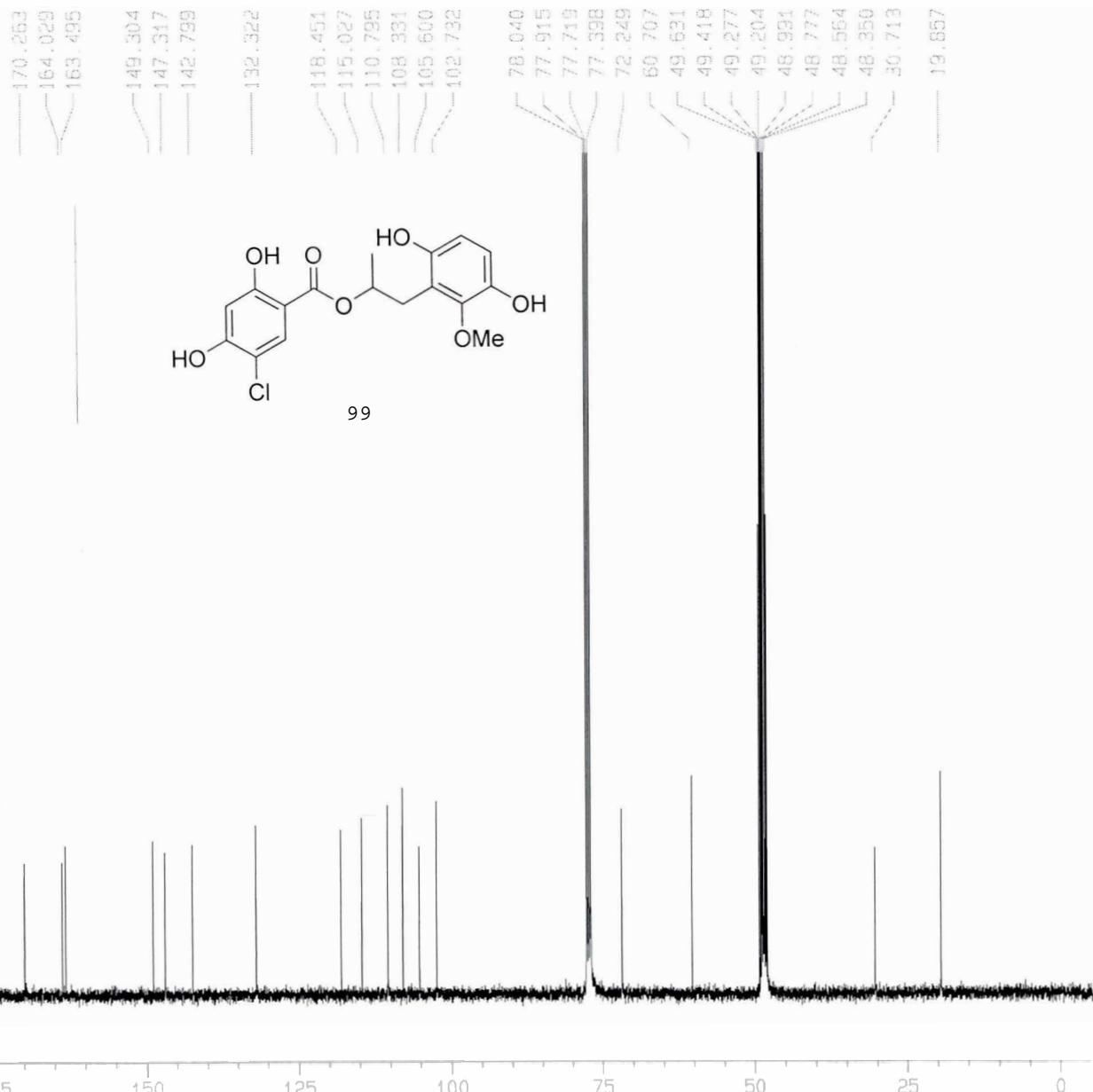
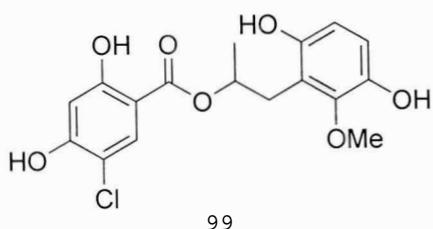
F2 - Acquisition Parameters
 Date_ 20051127
 Time 21.49
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 18432
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

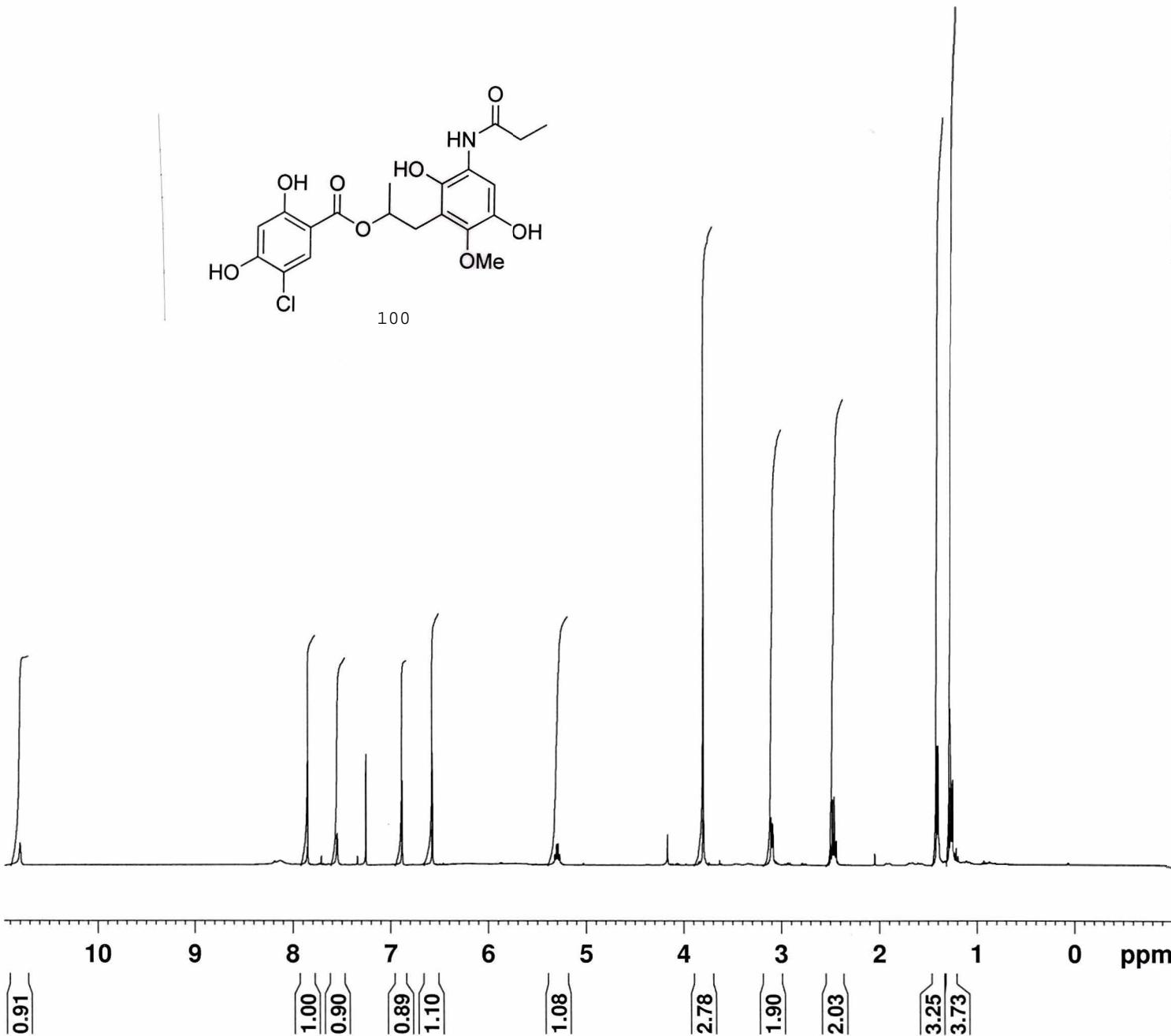
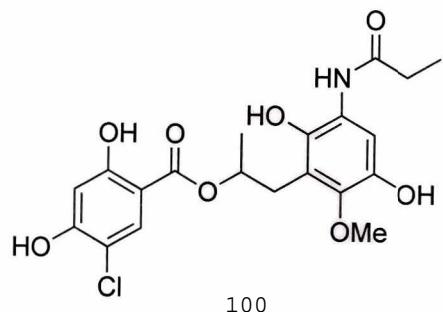
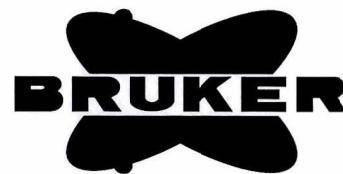
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 50.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm





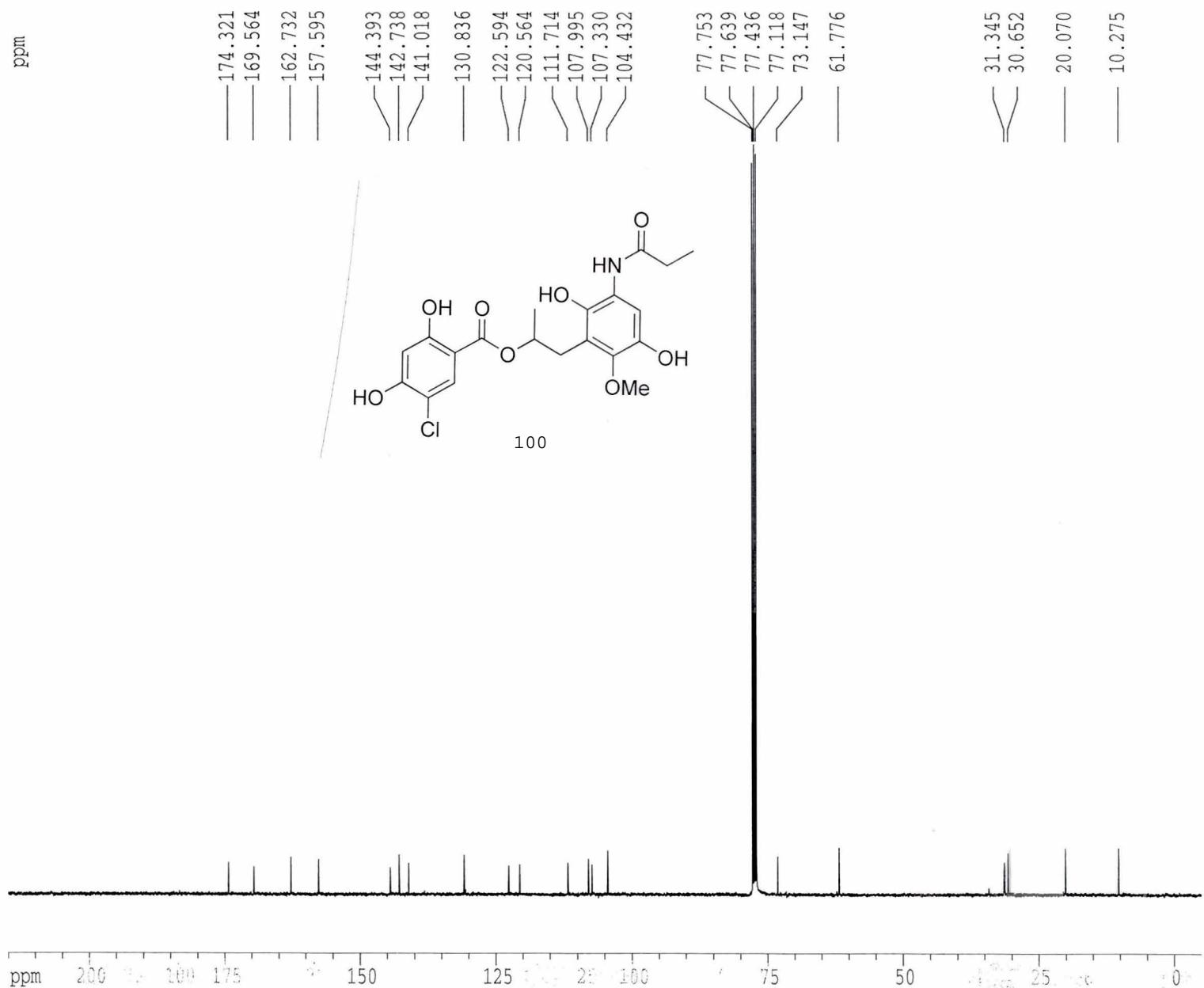
Current Data Parameters
NAME sg501
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051126
Time 7.10
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 4789.272 Hz
FID S 0.146157 Hz
AQ 3.4210291 sec
RG 287.4
DW 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ppm



Current Data Parameters
 NAME sg501
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20051126
 Time 8.33
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 18432
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.1500001 sec
 d11 0.0300000 sec
 DELTA 0.0500000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

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

NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

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

CPDPFG2 waltz16
 NUC2 1H
 PCPDE2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters

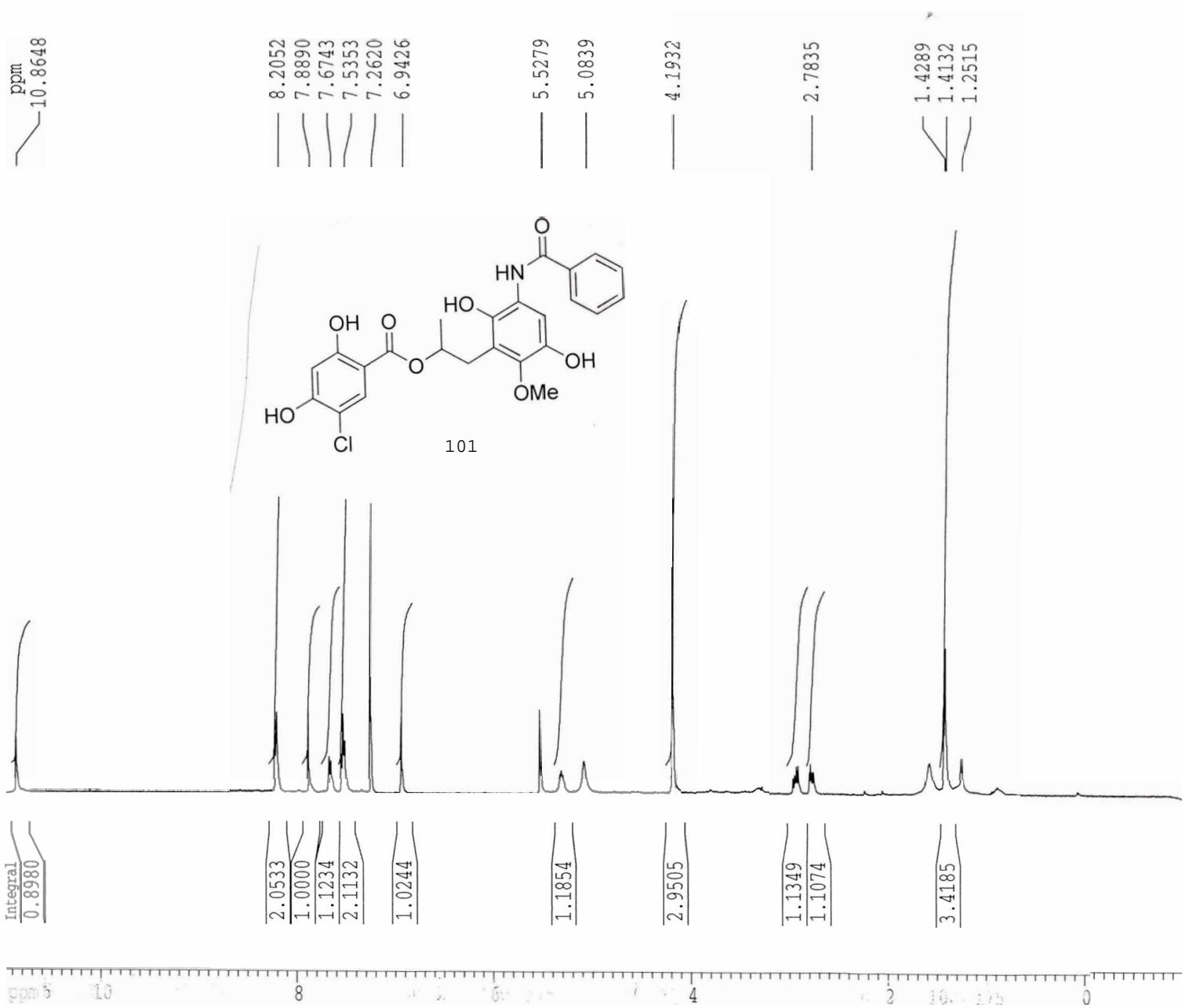
SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 CY 12.50 cm
 F1P 215.00 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm

ppm

10.8648



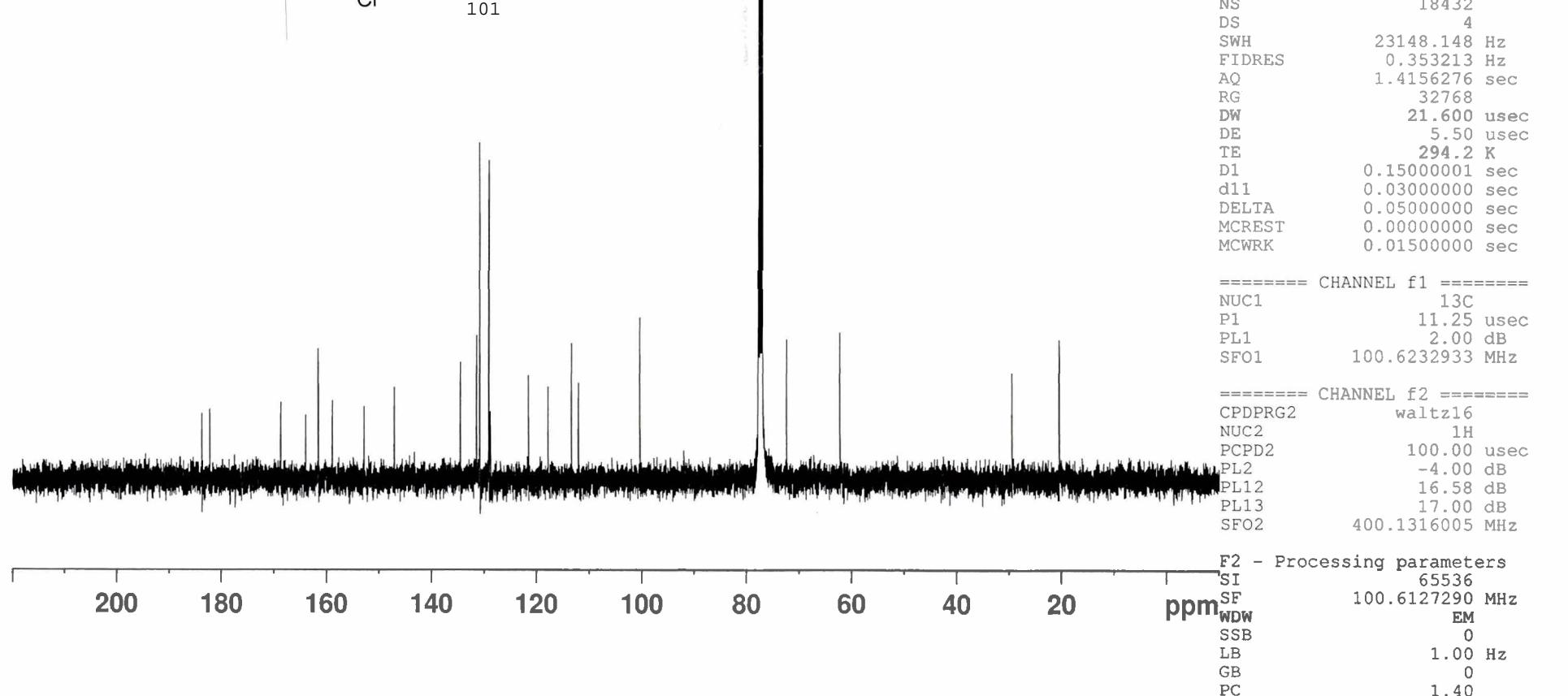
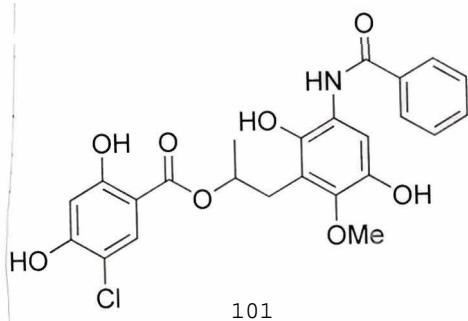
Current Data Parameters
 NAME sg503
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051127
 Time 12.15
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 456.1
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

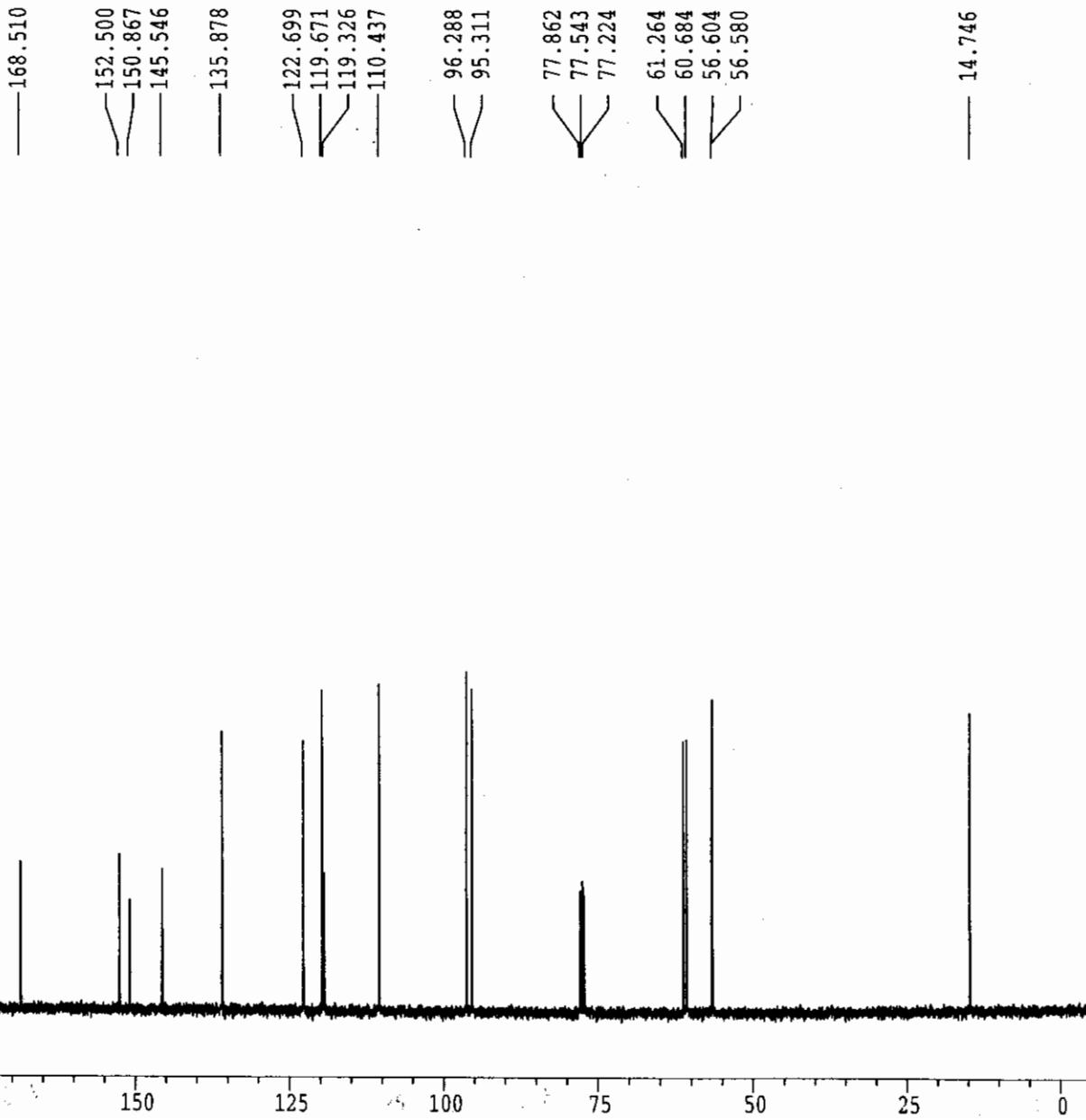
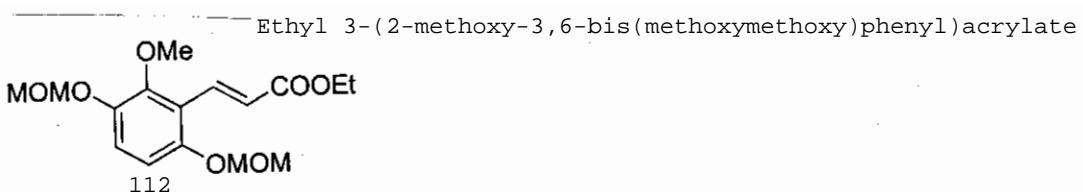
F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm



ppm

ppm 200 100 175 150 125 100 75 50 25 0



Current Data Parameters
 NAME sg434
 EXPNO 2
 PROCNO 1

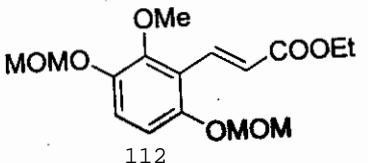
P2 - Acquisition Parameters
 Date_ 20050405
 Time 19.56
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 51
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

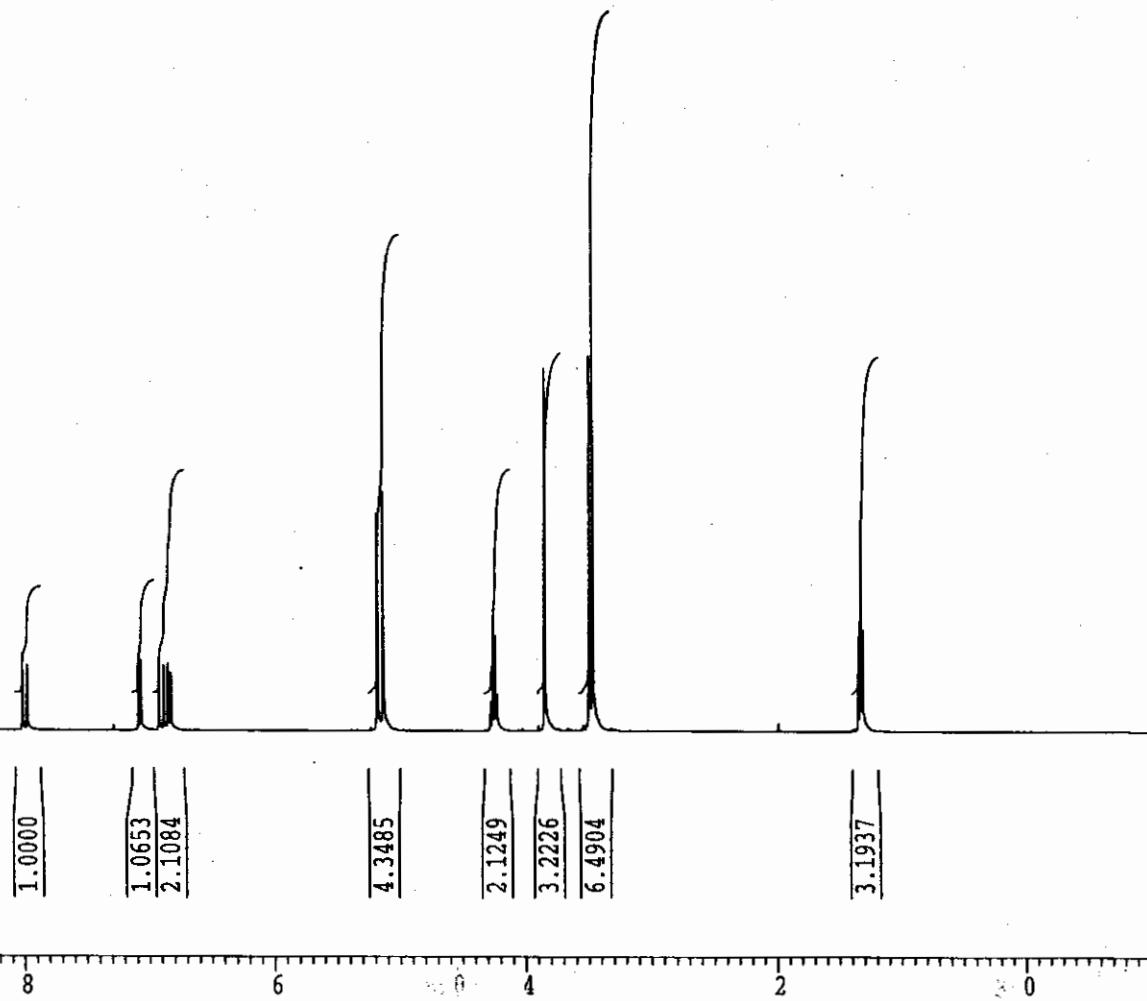
===== CHANNEL f2 =====
 CPDPG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



ppm



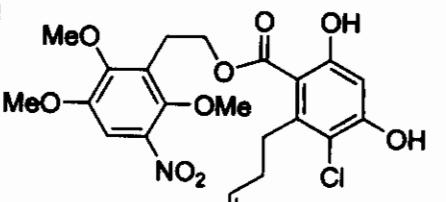
Current Data Parameters
 NAME sg434
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20050405
 Time 19.53
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm



116a

Current Data Parameters
 NAME mww12153
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041215
 Time 22.10
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5175.983 Hz
 FIDRES 0.157958 Hz
 AQ 3.1654389 sec
 RG 90.5
 DW 96.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 9.408 ppm
 F1 3764.45 Hz
 F2P -0.331 ppm
 F2 -132.46 Hz
 PPMCM 0.48696 ppm/cm
 HZCM 194.84593 Hz/cm

Integral

1.0000

0.9750

1.0663

2.0719

2.0019

9.4623

2.0838

2.0677

2.0408

ppm

8

7

6

5

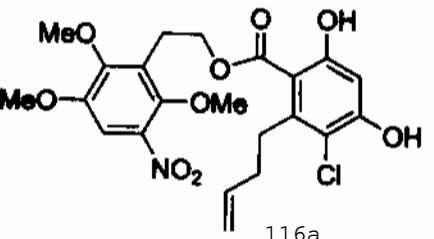
4

3

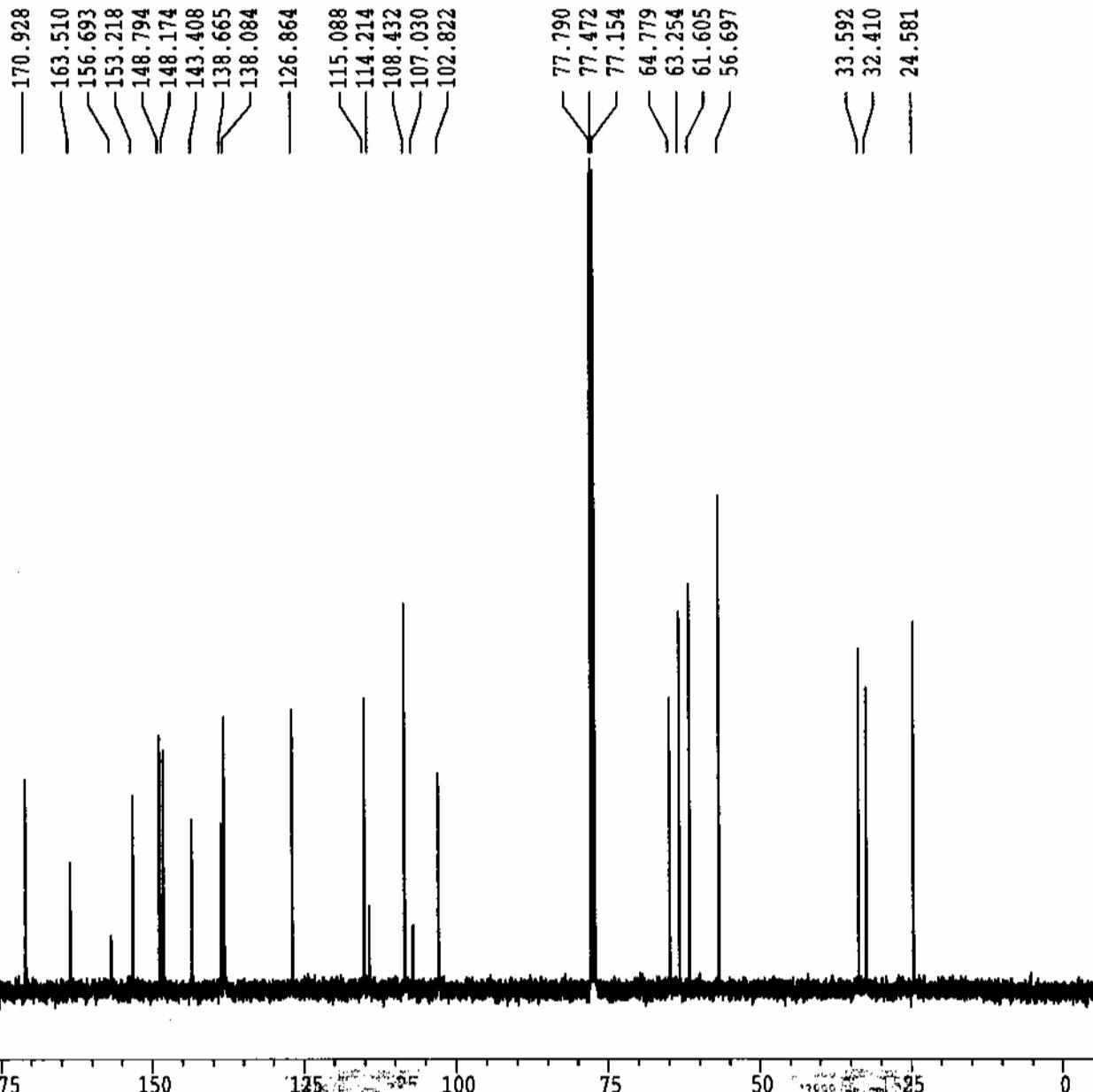
2

1

0



116a



Current Data Parameters
 NAME mmw12154
 EXPNO 1
 PROCN0 1

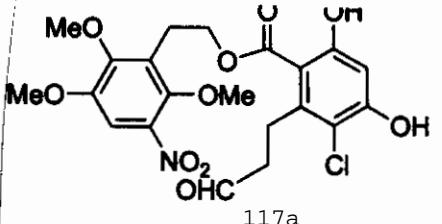
P2 - Acquisition Parameters
 Date 20041215
 Time 22.24
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 439
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 1448.2
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ^{1H}
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SP 100.6127290 MHz
 MDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



117a

Current Data Parameters

NAME wmm12271
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041227
Time 17.14
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 5175.983 Hz
FIDRES 0.157958 Hz
AQ 3.1654389 sec
RG 512
DW 96.600 usec
DE 5.50 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

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

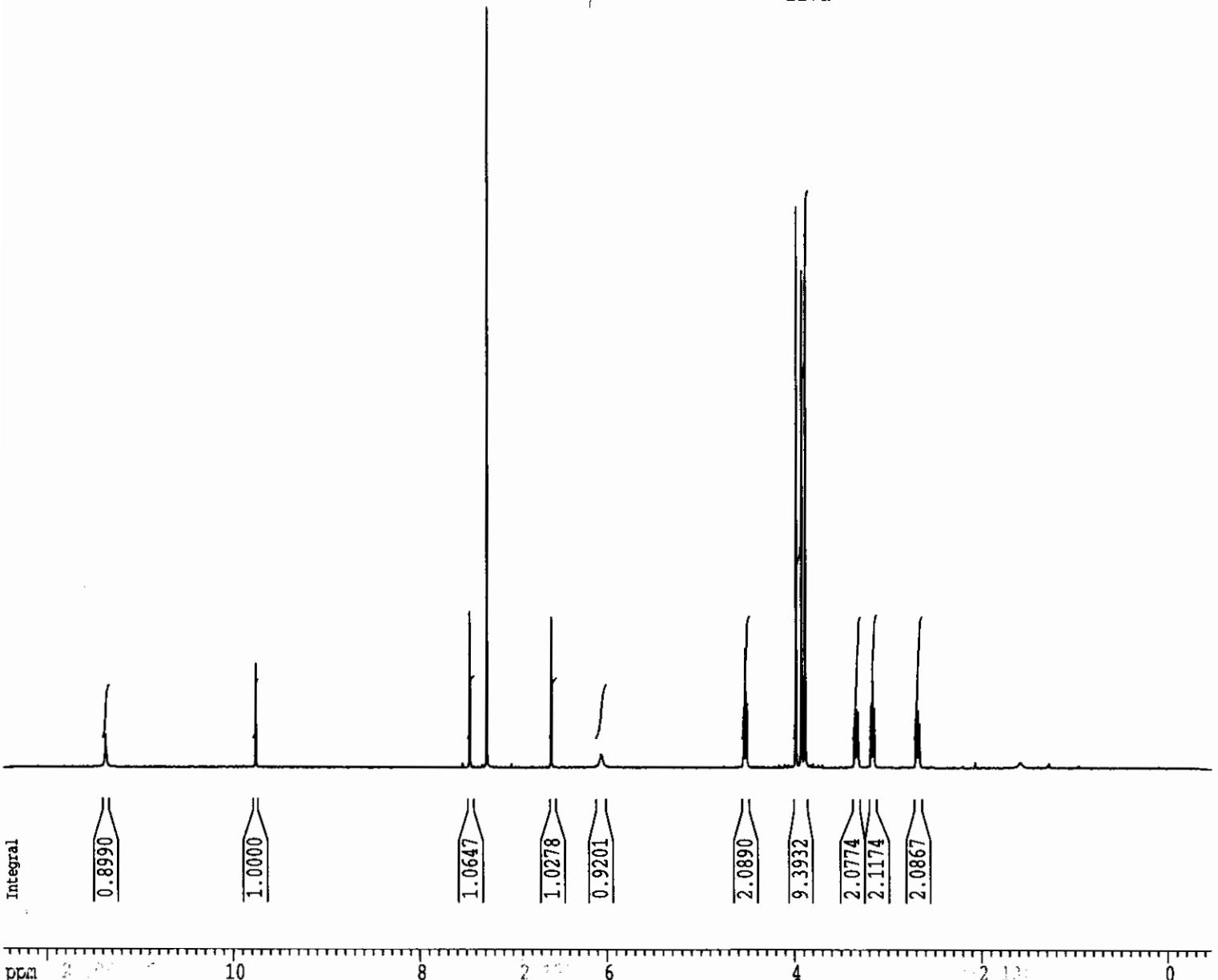
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1324008 MHz

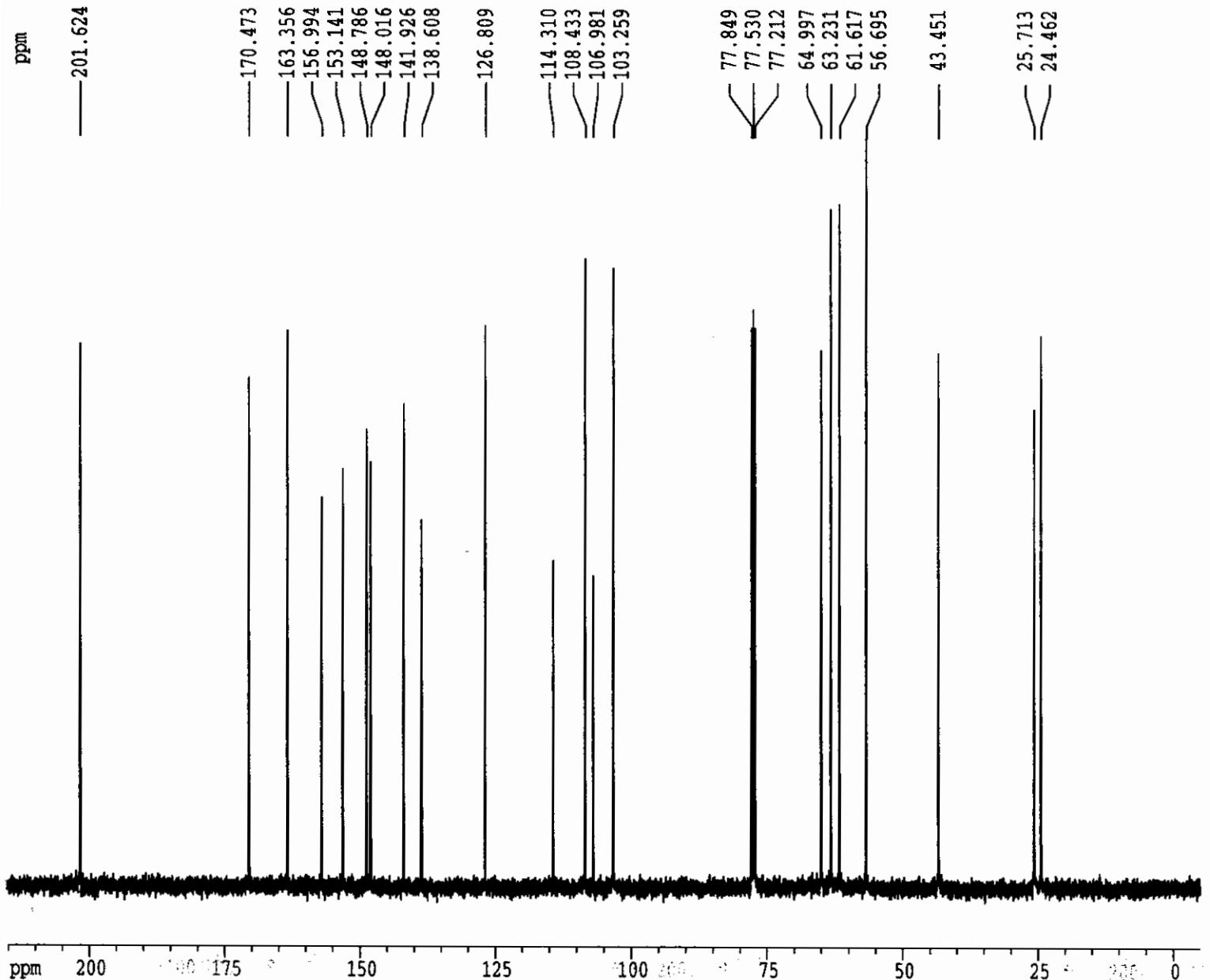
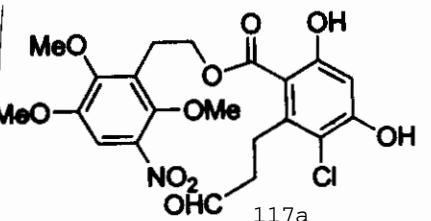
F2 - Processing parameters

SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
CY 12.50 cm
F1P 12.468 ppm
F1 4988.77 Hz
F2P -0.468 ppm
F2 -187.21 Hz
PPMCM 0.64679 ppm/cm
HZCM 258.79919 Hz/cm





Current Data Parameters

NAME wmw12272
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date 20041227
Time 17.42
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 383
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 3649.1
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.1500001 sec
d11 0.0300000 sec
DELTA 0.0500000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

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

NUC1 ¹³C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

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

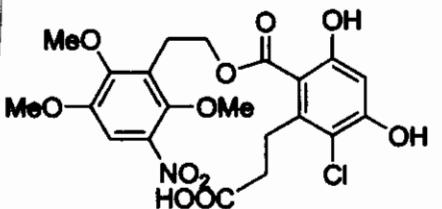
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

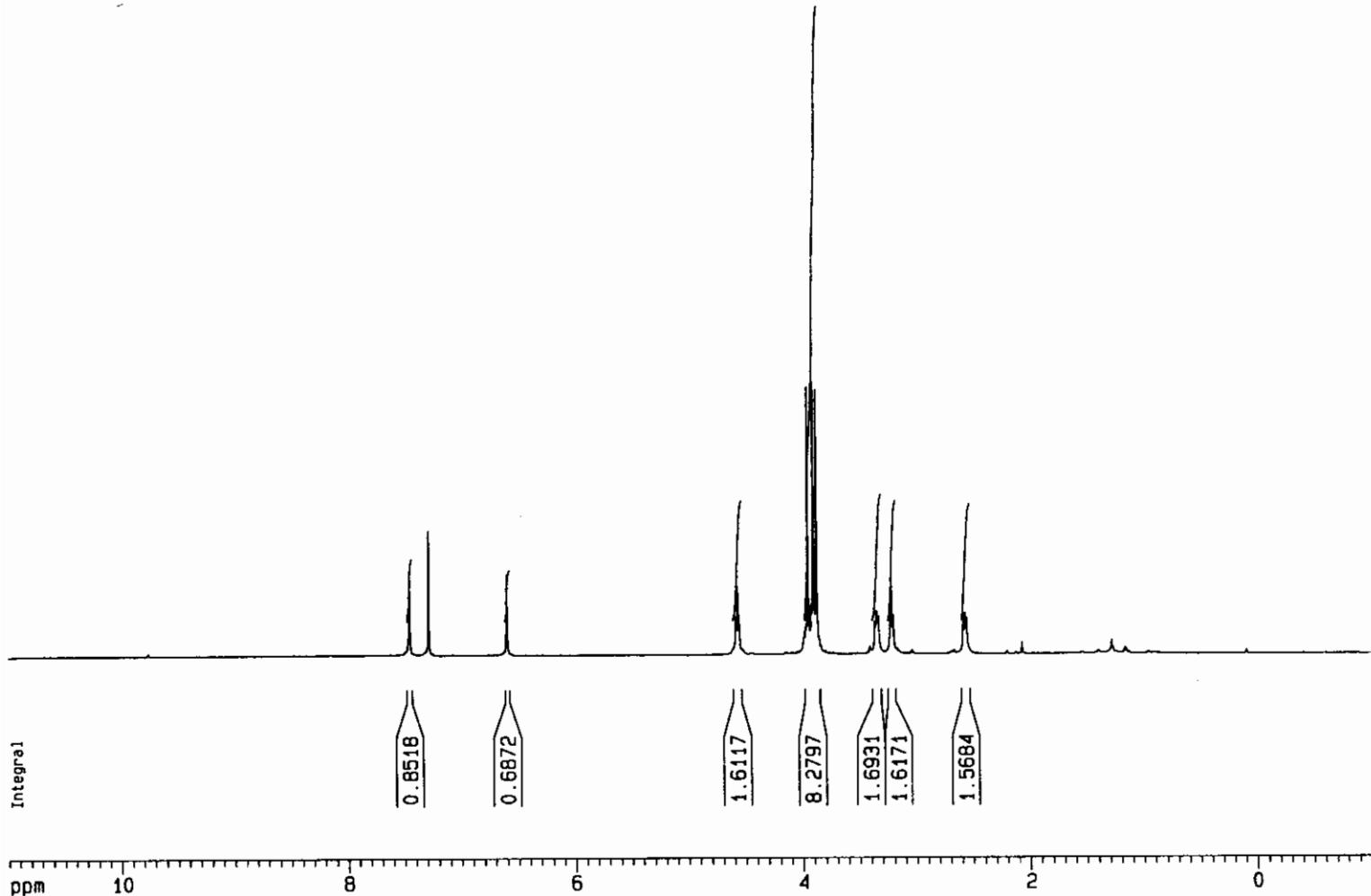
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 0.00 cm
F1P 215.000 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm



118a



Current Data Parameters
 NAME mmw0412281
 EXPNO 1
 PROCN0 1

F2 - Acquisition Parameters
 Date_ 20041229
 Time 9.45
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6009.615 Hz
 F1ORES 0.183399 Hz
 AQ 2.7264309 sec
 RG 362
 DW 83.200 usec
 DE 6.00 usec
 TE 0.0 K
 D1 0.0300000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

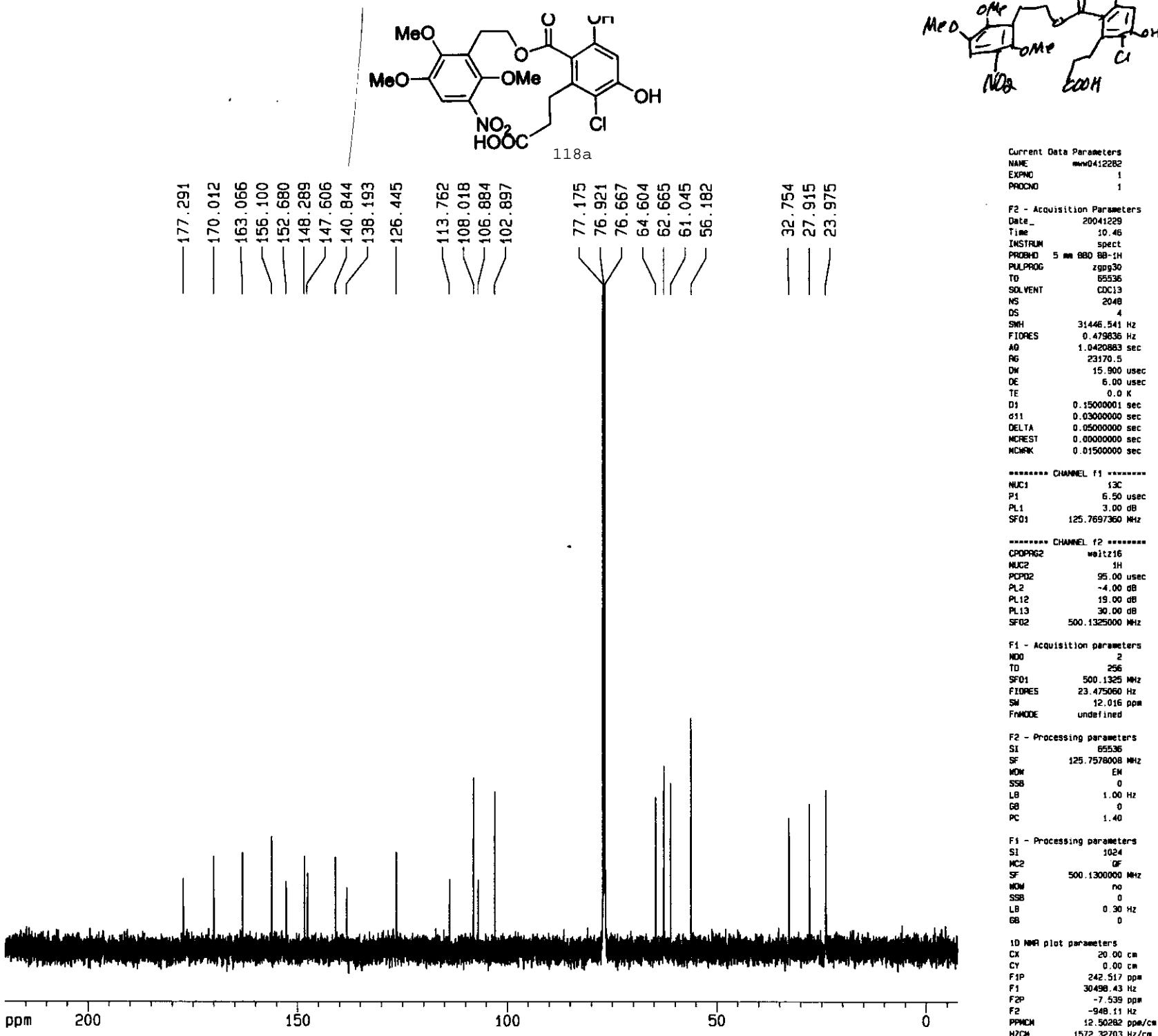
***** CHANNEL f1 *****
 NUC1 1H
 P1 7.70 usec
 PL1 -4.00 dB
 SF01 500.1325006 MHz

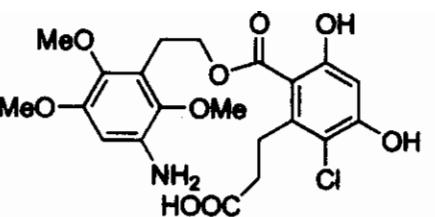
F1 - Acquisition parameters
 NDO 2
 TO 256
 SF01 500.1325 MHz
 F1ORES 23.475060 Hz
 SW 12.016 ppm
 FnMODE undefined

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 0F
 SF 500.1300000 MHz
 MDW no
 SSB 0
 LB 0.30 Hz
 GB 0

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 11.000 ppm
 F1 5501.43 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPWCN 0.50000 ppm/cm
 HZCM 300.07800 Hz/cm





119a

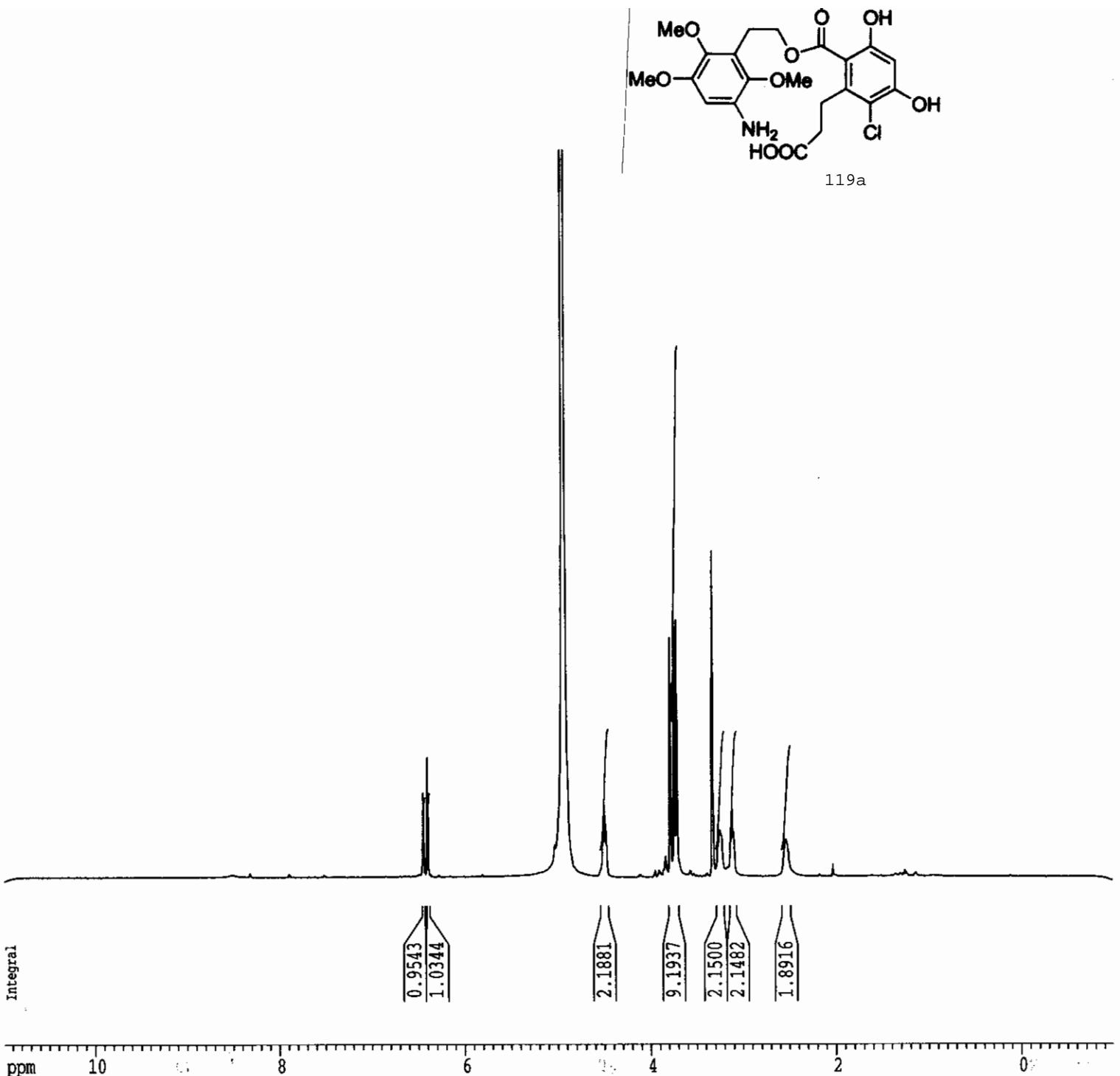
Current Data Parameters
 NAME wnmw41021
 EXPNO 1
 PROCNO 1

P2 - Acquisition Parameters
 Date_ 20050102
 Time 10.10
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT MeOH
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 161.3
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

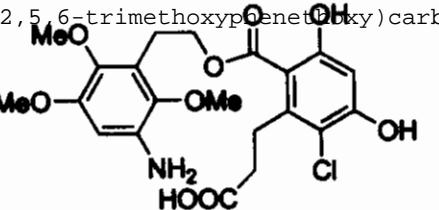
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 80.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

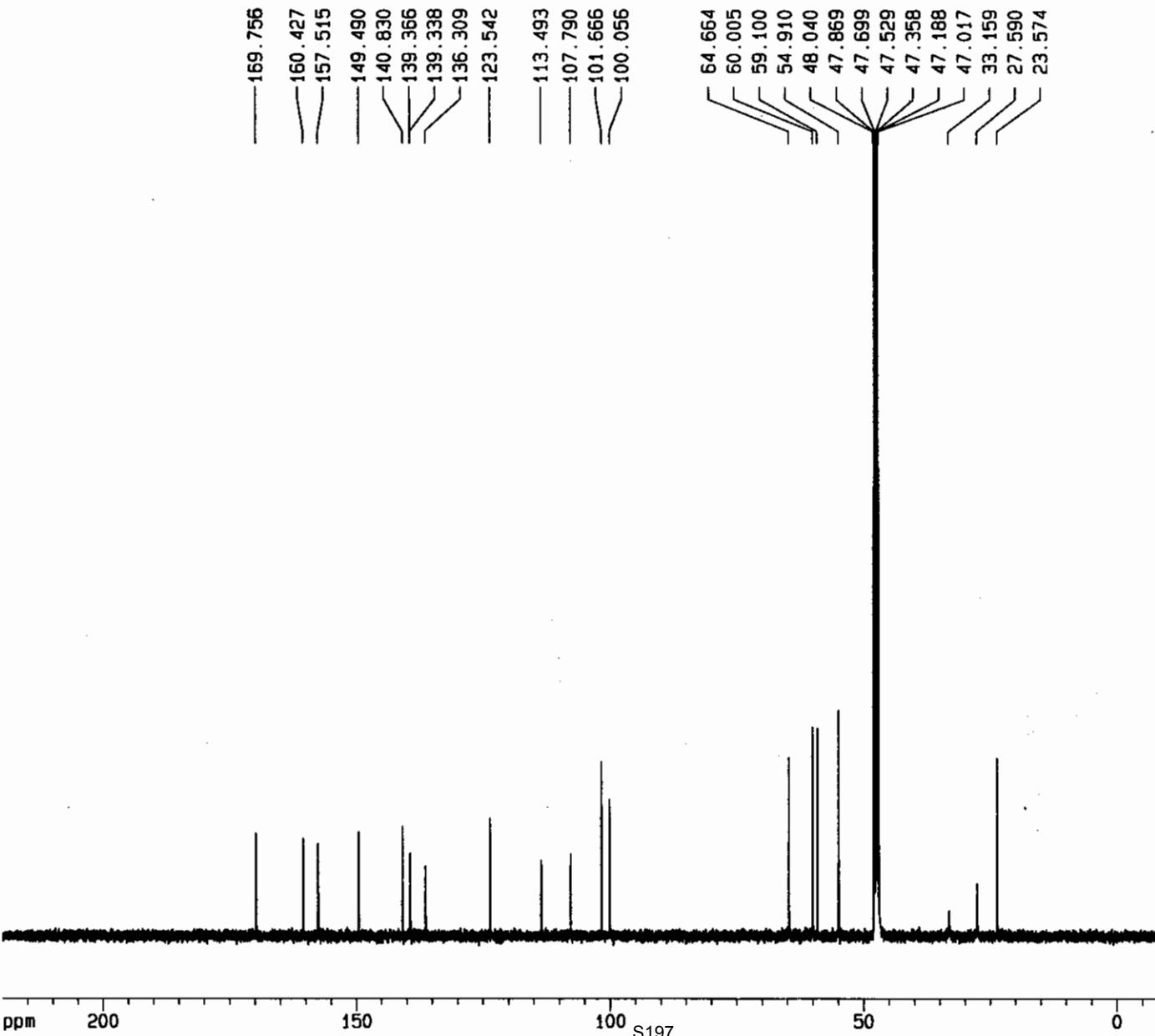


3-((2-((3-amino-2,5,6-trimethoxyphenyl)carbonyl)-6-chloro-3,5-dihydroxyphenyl)propanoic acid



119a

ppm



Current Data Parameters
NAME mm501021
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20050102
Time 11.39
INSTRUM spect
PROBHD 5 mm BBP BE-1H
PULPROG zgpg30
TD 65536
SOLVENT MeOH
NS 2048
DS 4
SWH 31446.541 Hz
FIDRES 0.47936 Hz
AQ 1.0420983 sec
RG 23170.5
DM 15.900 usec
DE 6.00 usec
TE 0.0 K
D1 0.1500001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
NCWECK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 6.50 usec
PL1 3.00 dB
SF01 125.7697360 MHz

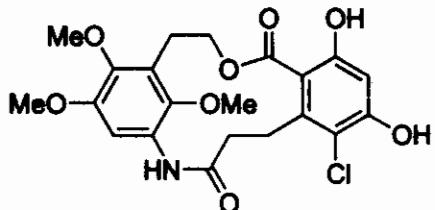
***** CHANNEL f2 *****
CPDPK02 waltz16
NUC2 1H
PCP02 95.00 usec
PL2 -4.00 dB
PL12 19.00 dB
PL13 30.00 dB
SF02 500.1325000 MHz

F1 - Acquisition parameters
NOD 2
TD 256
SF01 500.1325 MHz
FIDRES 23.475000 Hz
SW 12.016 ppm
F1MODE undefined

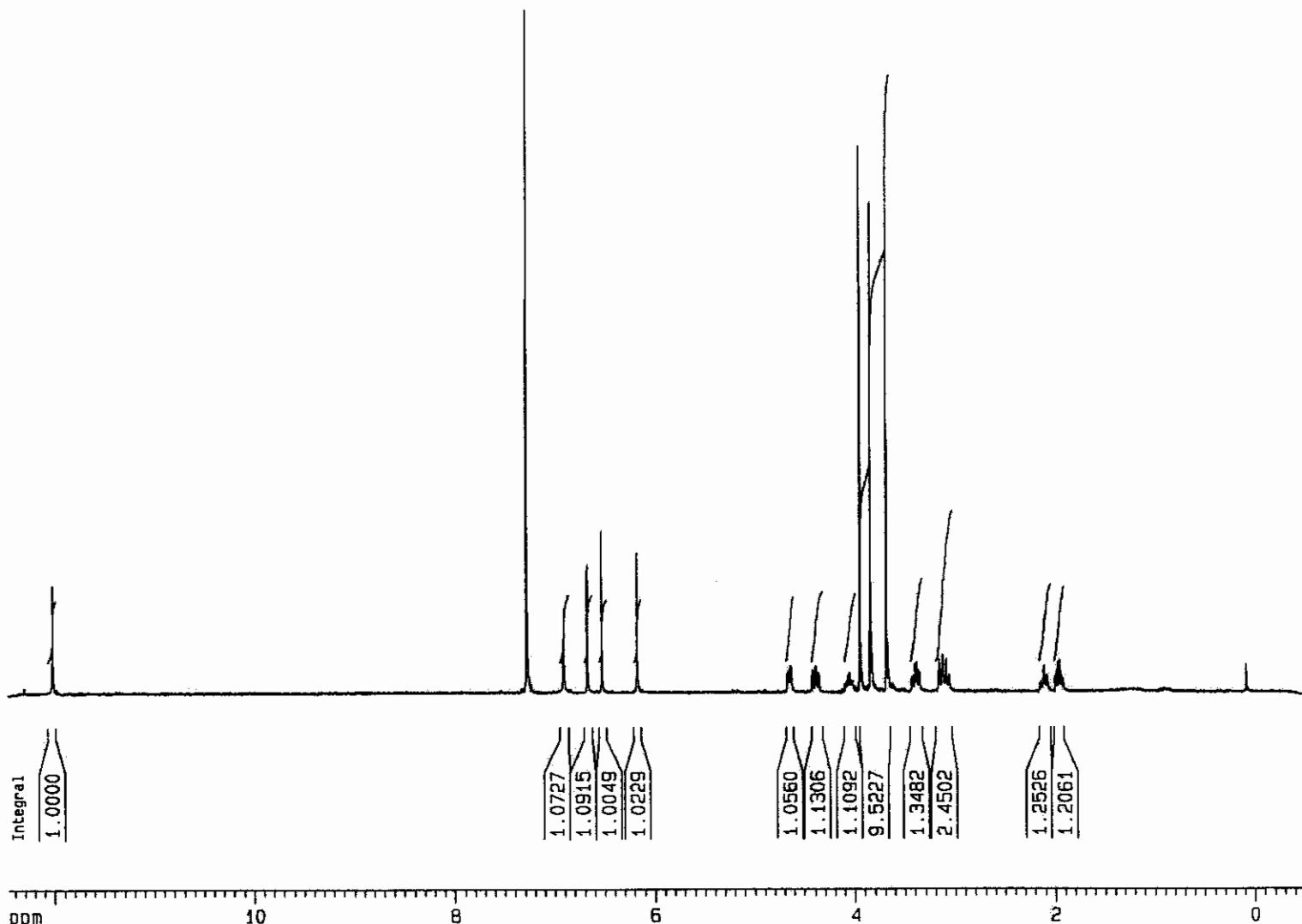
F2 - Processing parameters
SI 65536
SF 125.7578008 MHz
MW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
NC2 0F
SF 500.1300000 MHz
MW no
SSB 0
LB 0.30 Hz
GB 0

1D NMR plot parameters
CX 20.00 cm
CY 50.00 cm
F1P 242.517 ppm
F1 30498.43 Hz
F2P -7.539 ppm
F2 -948.11 Hz
PPM01 12.5028 ppm/cm
HZCM 1572.32703 Hz/cm



120a



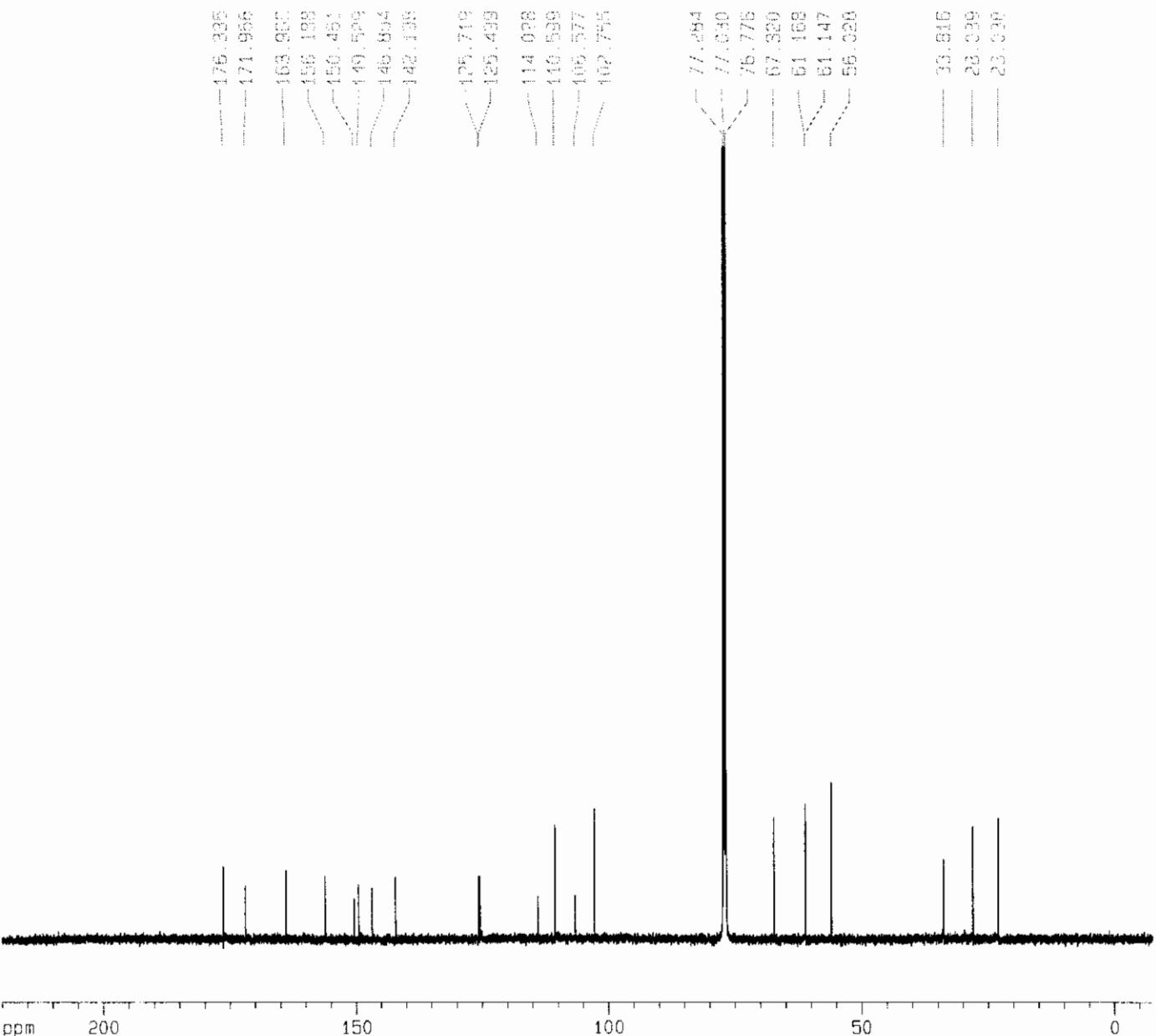
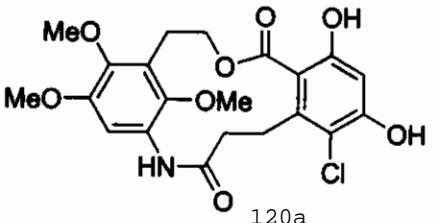
Current Data Parameters
 NAME wmm52091
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050209
 Time 14.11
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 5175.983 Hz
 FIDRES 0.157958 Hz
 AQ 3.1654389 sec
 RG 512
 DW 96.600 usec
 DE 5.50 usec
 TE 292.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWAK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1324008 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WMW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 15.00 cm
 F1P 12.468 ppm
 F1 4988.77 Hz
 F2P -0.468 ppm
 F2 -187.21 Hz
 PPMCM 0.64679 ppm/c
 HZCM 258.79919 Hz/cm



Current Data Parameters
 NAME WMW_MeO_2
 EXPNO 2
 PROCNO 1

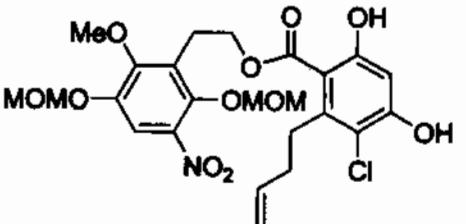
F2 - Acquisition Parameters
 Date 20050210
 Time 21.38
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 3072
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420724 sec
 RG 8192
 DW 15.900 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -4.90 dB
 SF01 125.7697360 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 9.54 dB
 PL13 10.00 dB
 SF02 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 100.00 cm
 F1P 242.517 ppm
 F1 30498.43 Hz
 F2P -7.539 ppm
 F2 -948.11 Hz
 PPMCM 12.50282 ppm/cm
 HZCM 1572.32690 Hz/cm



116c

Current Data Parameters
 NAME www501291
 EXPNO 2
 PROCNO 1

P2 - Acquisition Parameters
 Date_ 20050129
 Time 15.03
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5175.983 Hz
 FIDRES 0.157958 Hz
 AQ 3.1654389 sec
 RG 256
 DW 96.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SPO1 400.1324008 MHz

P2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 7.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral

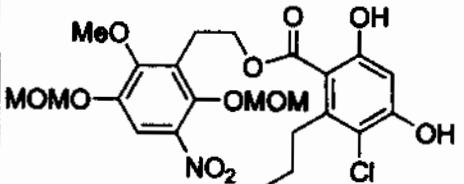
ppm

10

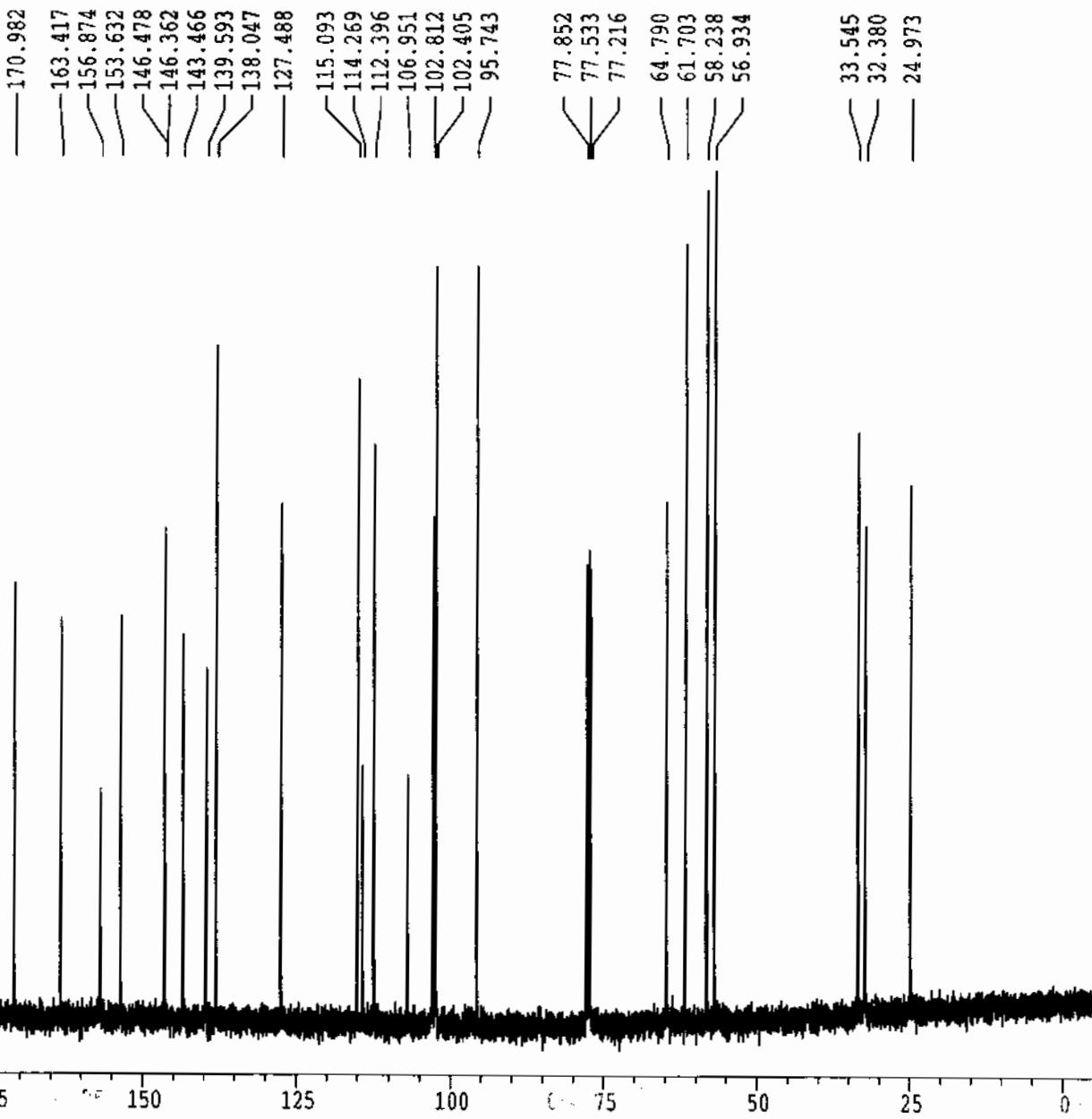


ppm

ppm 200 175 150 125 100 75 50 25 0



116c



Current Data Parameters

NAME mmw501292
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date 20050129
Time 15.18
INSTRUM drx400
PROBHD 5 mm QNP 1R/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 142
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 6502
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 ¹³C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

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

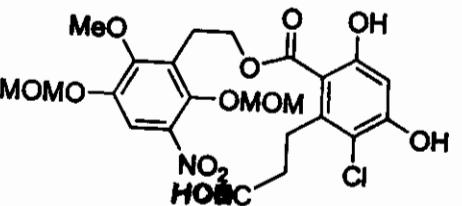
CPDPGR2 waltz16
NUC2 ¹H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm



118c

Current Data Parameters
 NAME www501314
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050131
 Time 20.57
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 322.5
 DW 104.400 usec
 DE 5.50 usec
 TE 292.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

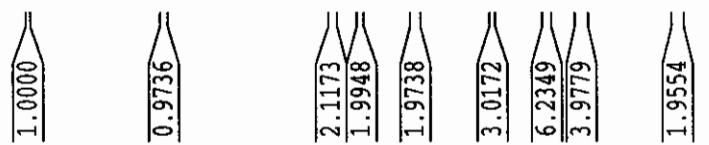
F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

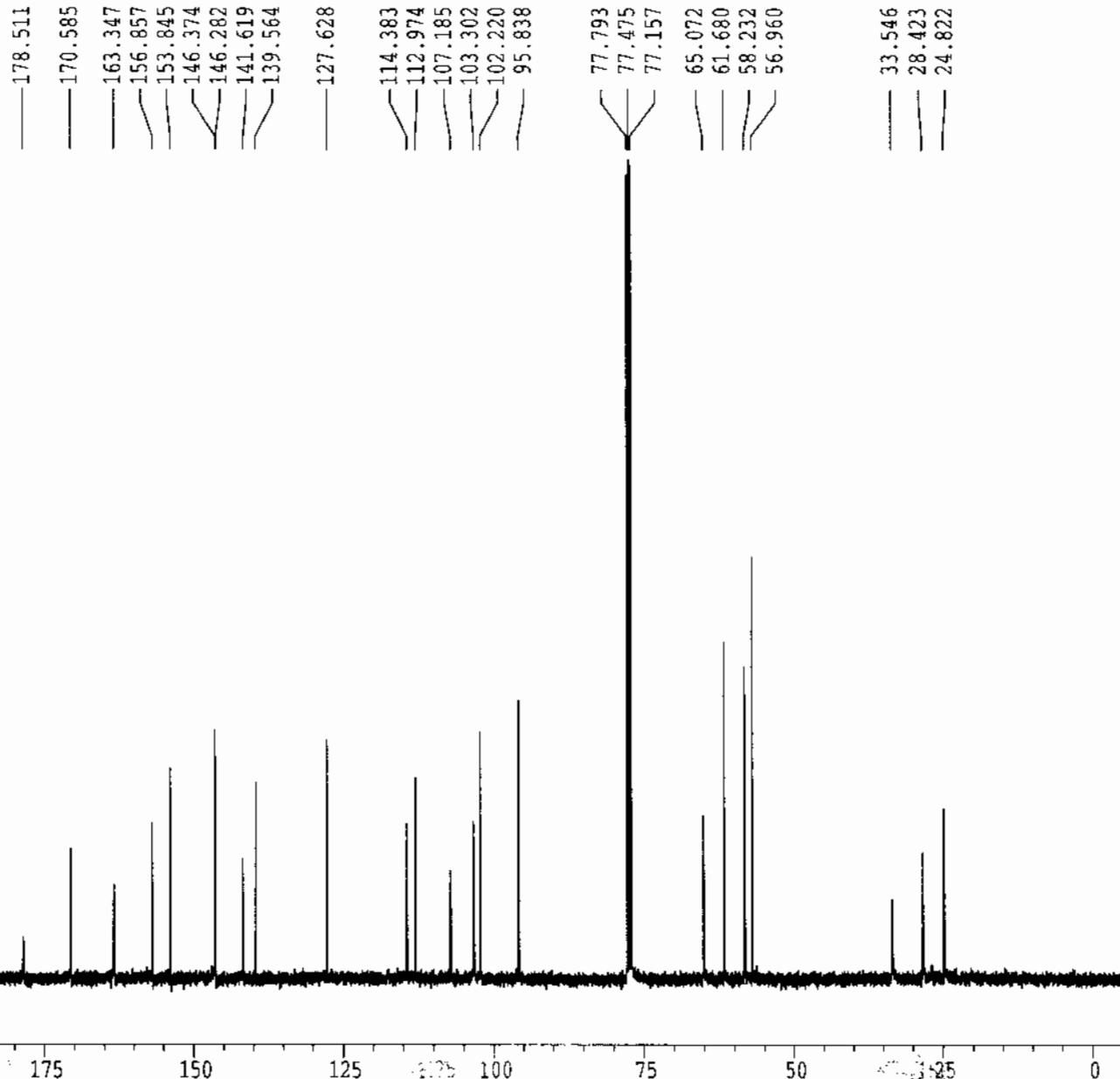
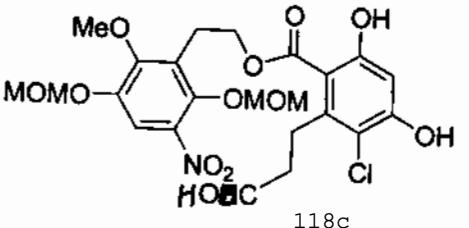
1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral

ppm

10 8 6 4 2 0





Current Data Parameters

NAME wmm501315
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050131
Time 21.26
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpp30
TD 65536
SOLVENT CDCl3
NS 628
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 5160.6
DW 21.600 usec
DE 5.50 usec
TB 292.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SF01 100.6232933 MHz

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

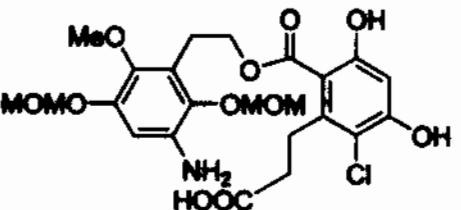
CPDPG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SF02 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 21631.74 Hz
F2P -5.00 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm⁻¹



119c

Current Data Parameters
 NAME wmm502021
 EXPNO 2
 PROCN0 1

F2 - Acquisition Parameters
 Date 20050202
 Time 9.36
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT MeOH
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 128
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

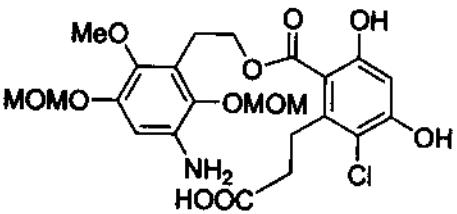
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

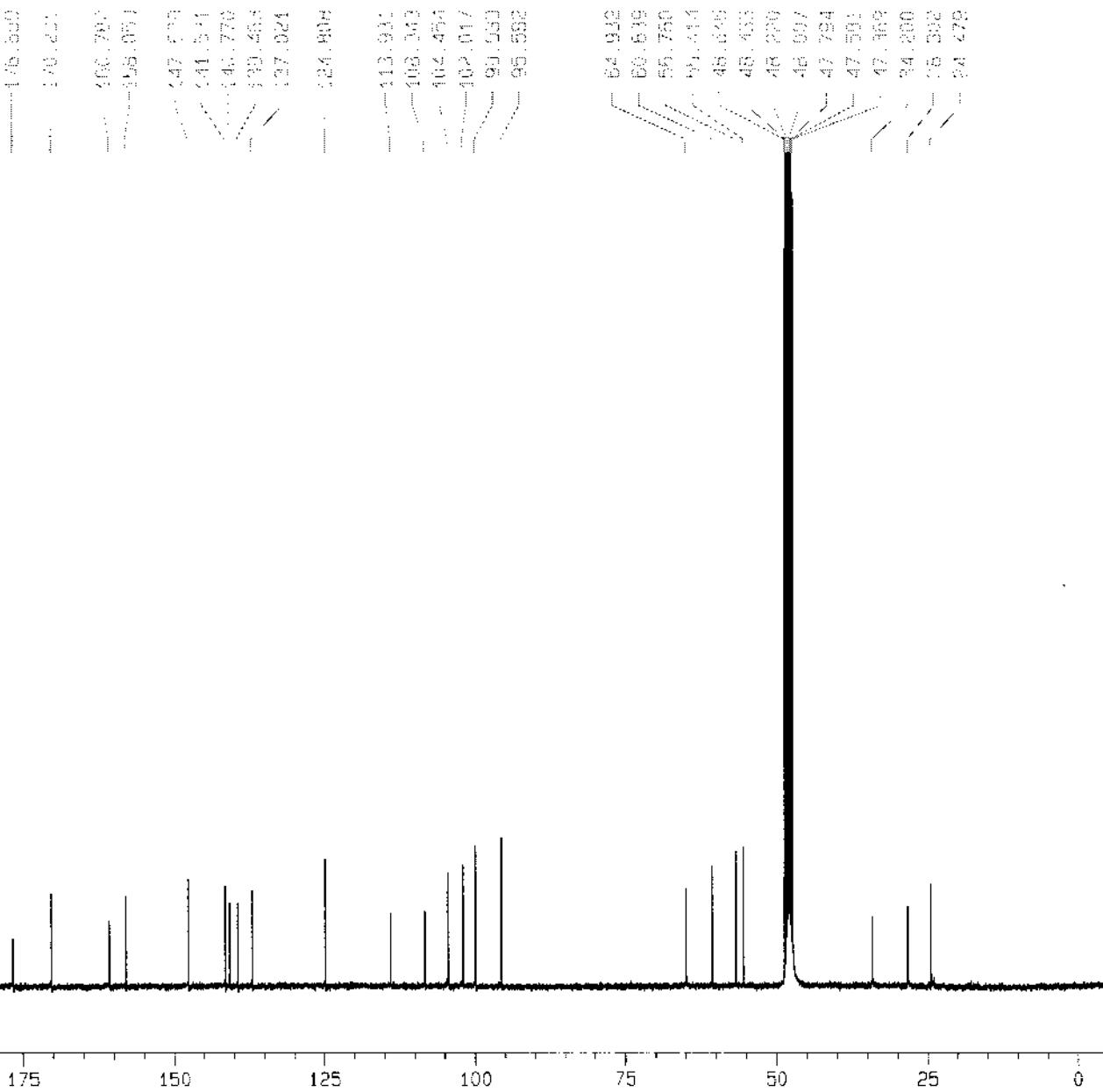
1D NMR plot parameters
 CX 20.00 cm
 CY 50.00 cm
 F1P 8.039 ppm
 F1 3216.67 Hz
 F2P -0.459 ppm
 F2 -183.52 Hz
 PPMCM 0.42489 ppm/cm
 HZCM 170.00981 Hz/cm

Integral

ppm



119c



Current Data Parameters

NAME mmw502021c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050202
Time 22.14
INSTRUM dnx400
PROBHD 5 mm QNP 1H/13
PULPROG zpg30
TD 65536
SOLVENT MeOH
NS 23552
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 2048
DW 21.600 usec
DE 5.50 usec
TE 292.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 ¹³C
P1 11.25 usec
PL1 2.00 dB
SF01 100.6232933 MHz

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

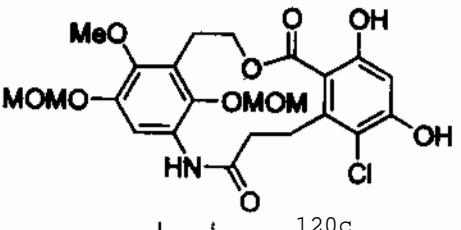
CPDPG2 waltz16
NUC2 ¹H
PCPQ2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SF02 400.1316005 MHz

F2 - Processing parameters

SI 65536
SF 100.6127290 MHz
WOW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 80.00 cm
F1P 215.00 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm



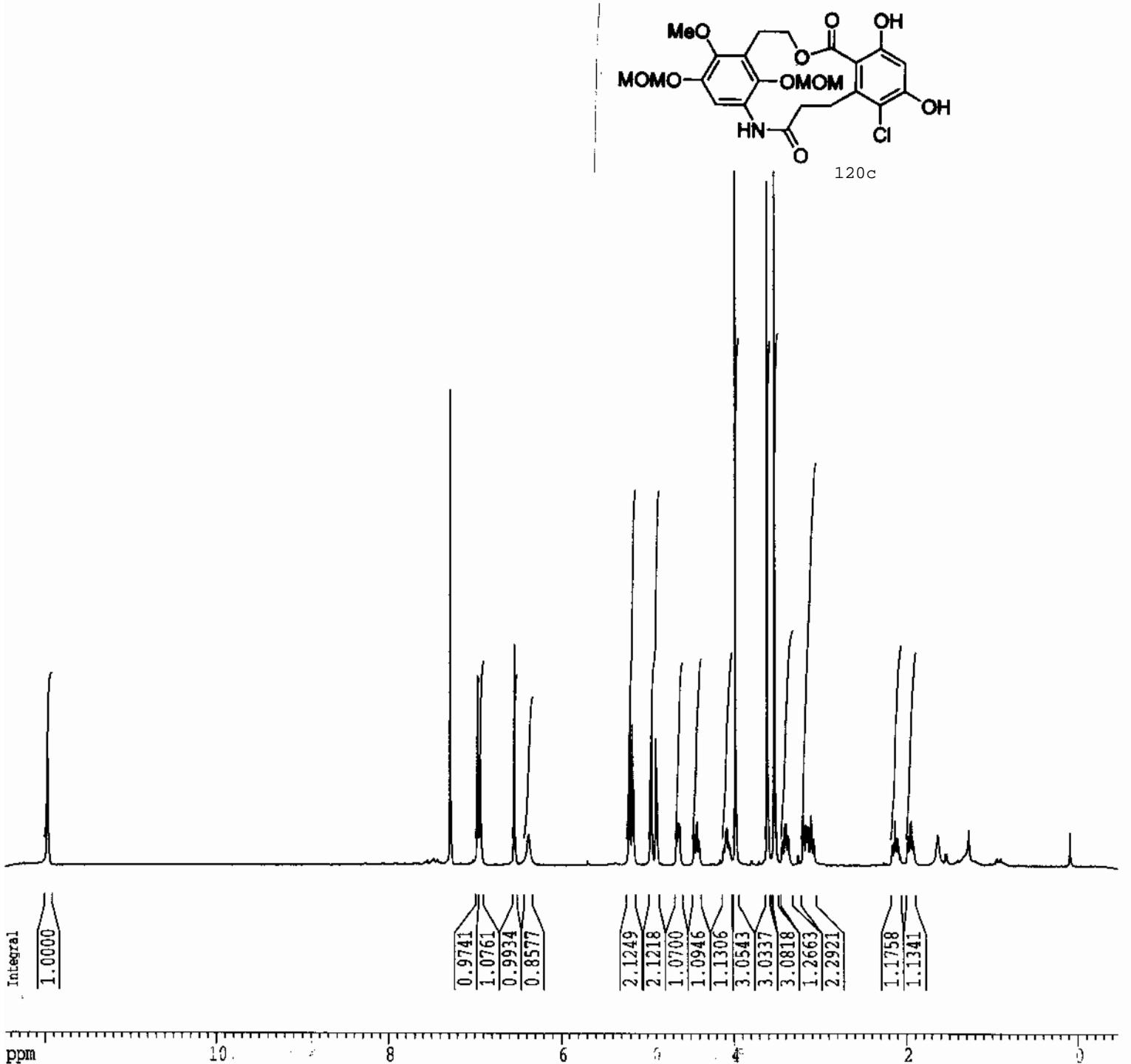
Current Data Parameters
 NAME wnm52141
 EXPNO 1
 PROCNO 1

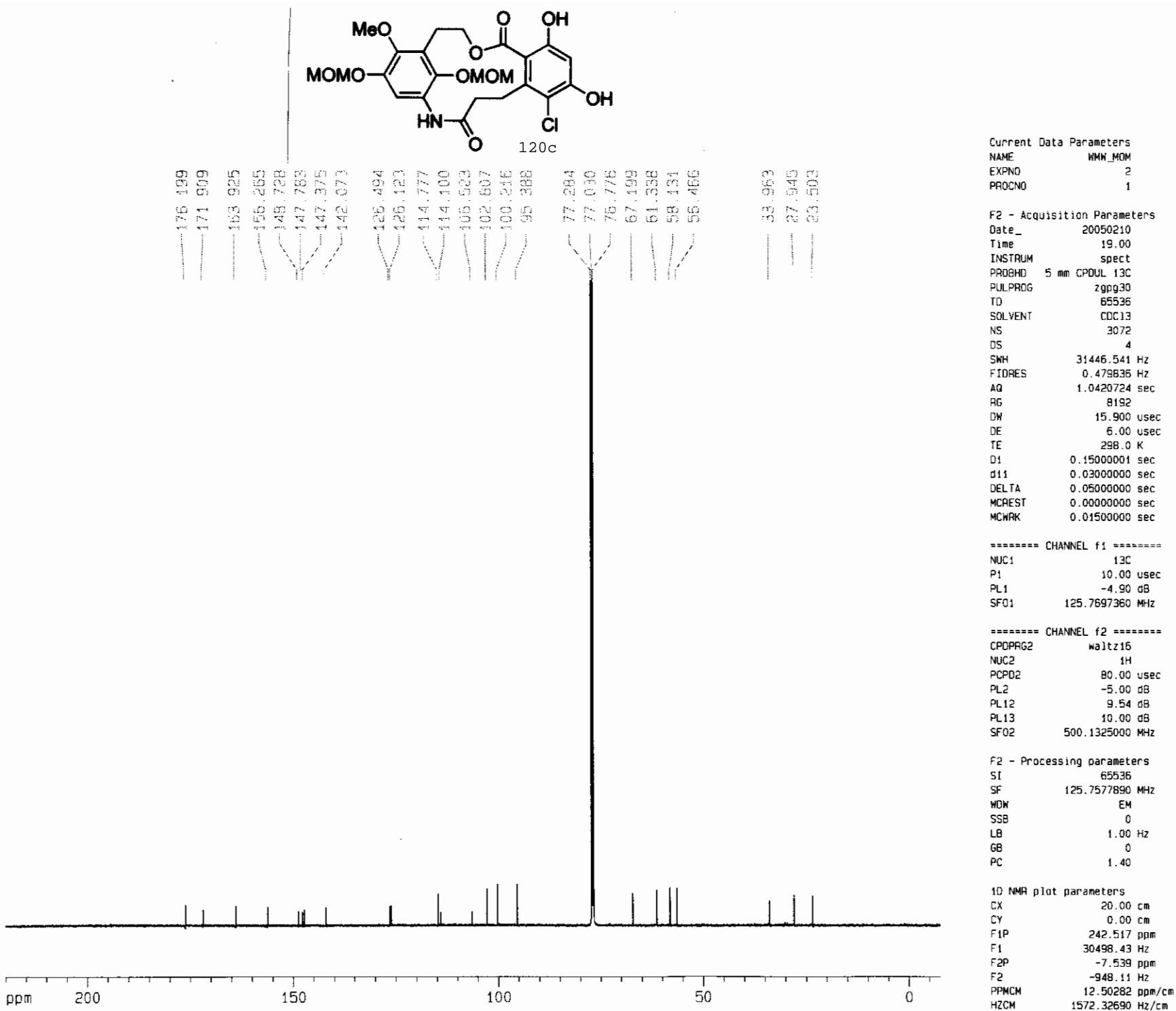
F2 ~ Acquisition Parameters
 Date_ 20050215
 Time 14.36
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5175.983 Hz
 FIDRES 0.157958 Hz
 AQ 3.1654389 sec
 RG 362
 DW 96.600 usec
 DE 5.50 usec
 TE 292.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

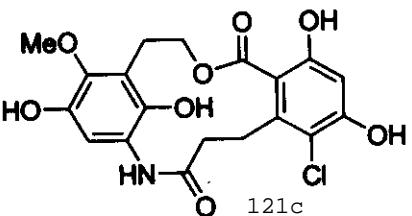
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1324008 MHz

F2 ~ Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 12.468 ppm
 F1 4988.77 Hz
 F2P -0.468 ppm
 F2 -187.21 Hz
 PPMCM 0.64679 ppm/cm
 HZCM 258.79916 Hz/cm







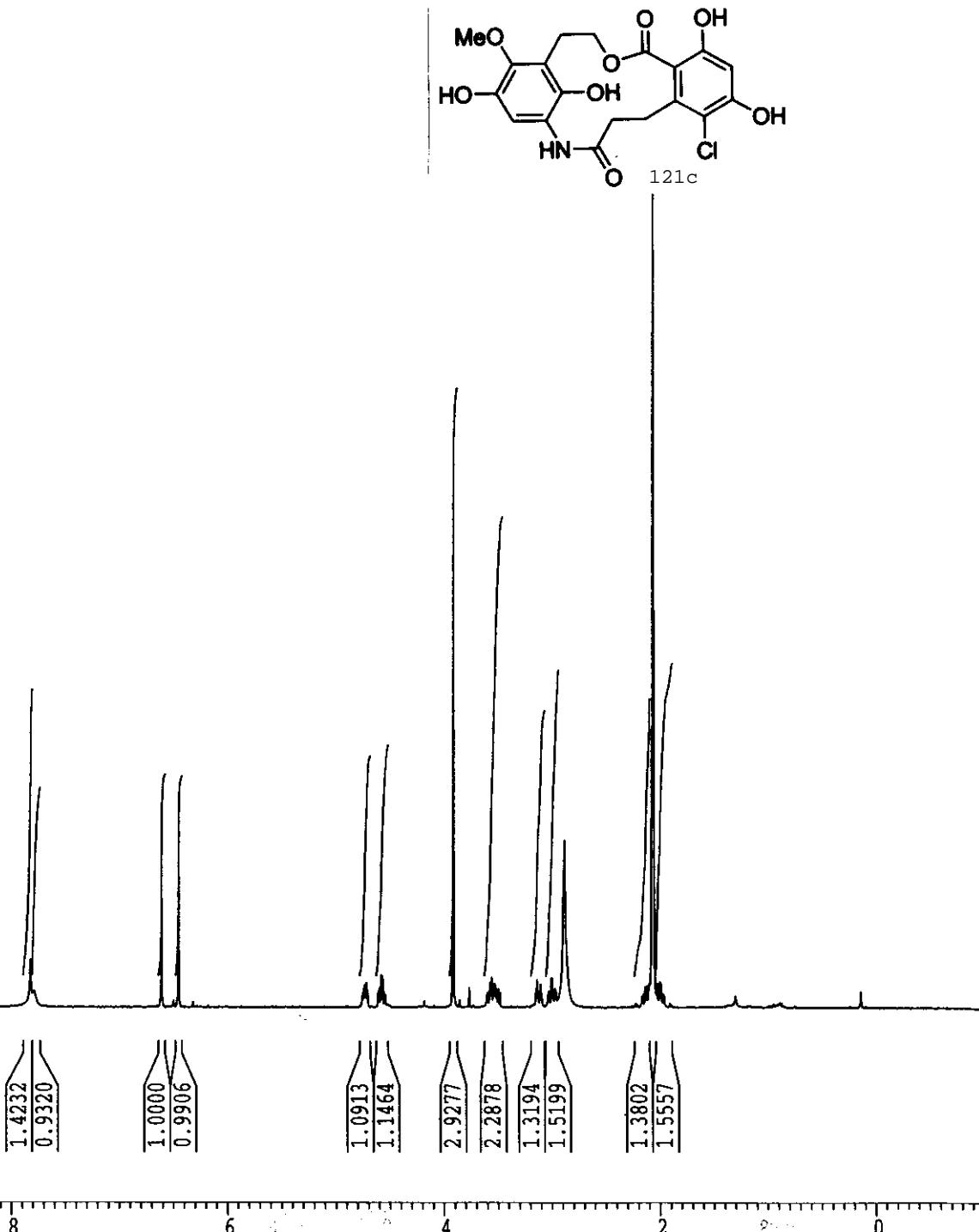
Current Data Parameters
 NAME wmm52233
 EXPNO 2
 PROCNO 1

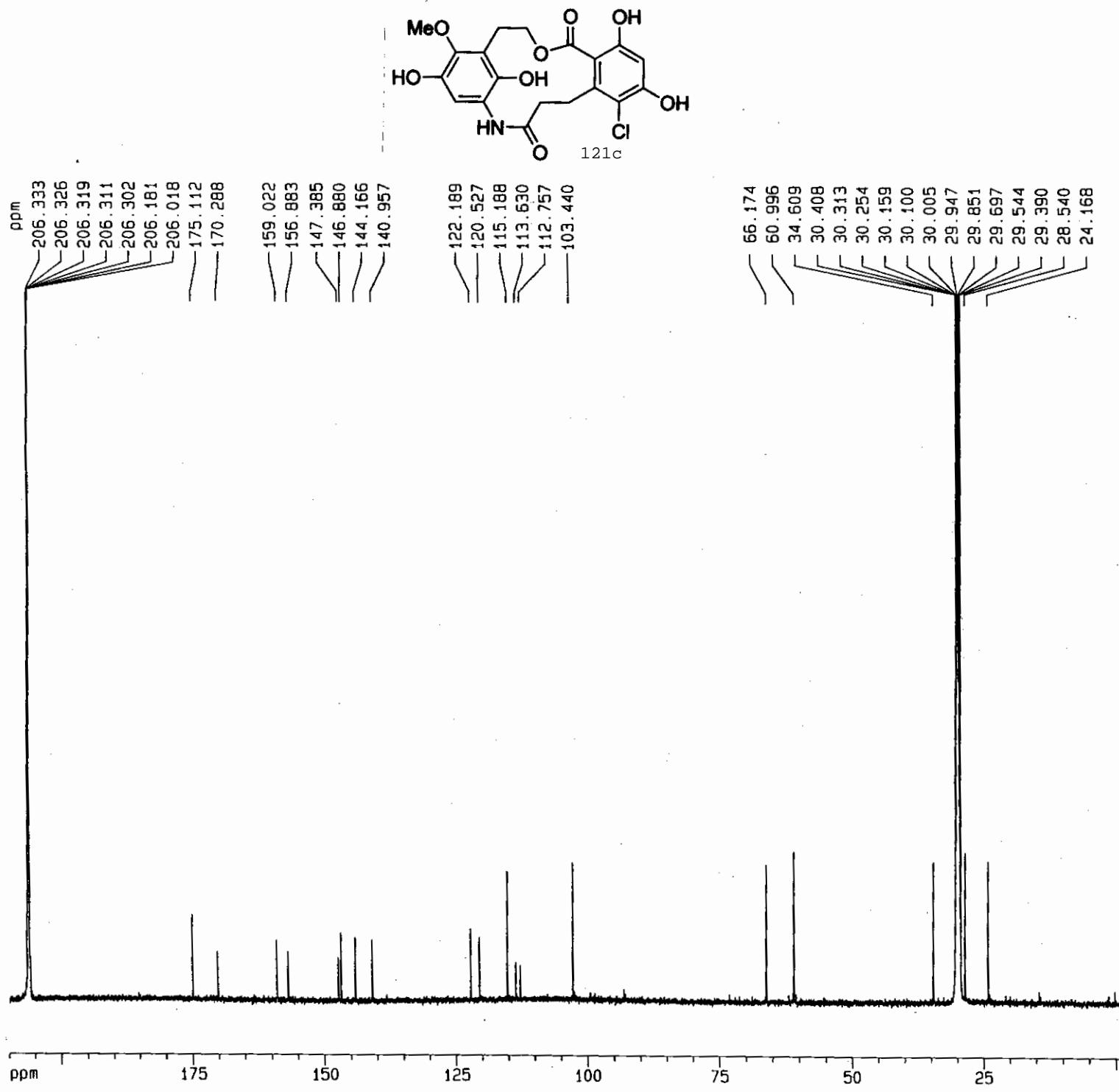
F2 - Acquisition Parameters
 Date_ 20050223
 Time 23.12
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT Aceton
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 512
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm





Current Data Parameters

NAME	^{13}C
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date	20050221
Time	10.34
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	Aceton
NS	3060
DS	4
SWH	31446.541 Hz
FIDRES	0.479836 Hz
AQ	1.0420883 sec
RG	8192
DW	15.900 usec
DE	6.00 usec
TE	298.0 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

----- CHANNEL f1 -----

NUC1	^{13}C
P1	10.00 usec
PL1	-4.90 dB
SFO1	125.7697360 MHz

----- CHANNEL f2 -----

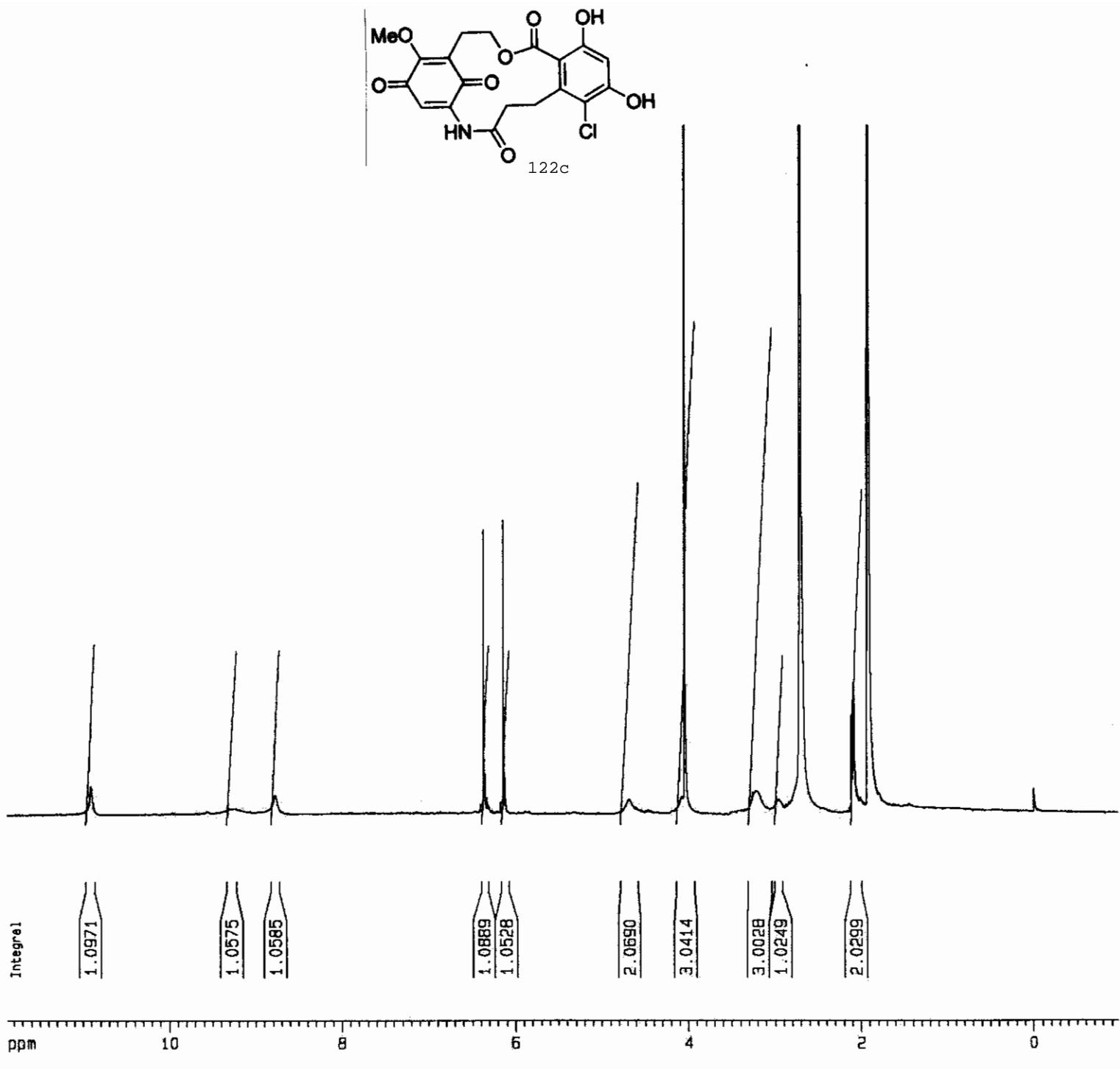
CPDPRG2	waltz16
NUC2	^1H
PCPD2	80.00 usec
PL2	-5.00 dB
PL12	9.54 dB
PL13	10.00 dB
SFO2	500.1325000 MHz

F2 - Processing parameters

SI	65536
SF	125.7576758 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
CY	0.00 cm
F1P	210.000 ppm
F1	26409.11 Hz
F2P	-1.00 ppm
F2	-125.76 Hz
PPMCM	10.55000 ppm/cm
HZCM	1326.74341 Hz/cm

**Current Data Parameters**

NAME 8
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date 20050221
Time 10.40
INSTRUM spect
PROBHD 5 mm CP/MAL 13C
PULPROG zg30
TD 65536
SOLVENT Aceton
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1718923 sec
RG 64
DW 48.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

CHANNEL f1

NUC1 1H
P1 15.00 usec
PL1 -5.00 dB
SF01 500.1330885 MHz

F1 - Acquisition parameters

N00 2
TD 256
SF01 500.1325 MHz
FIDRES 23.475060 Hz
SW 12.016 ppm
Fr1NOE undefined

F2 - Processing parameters

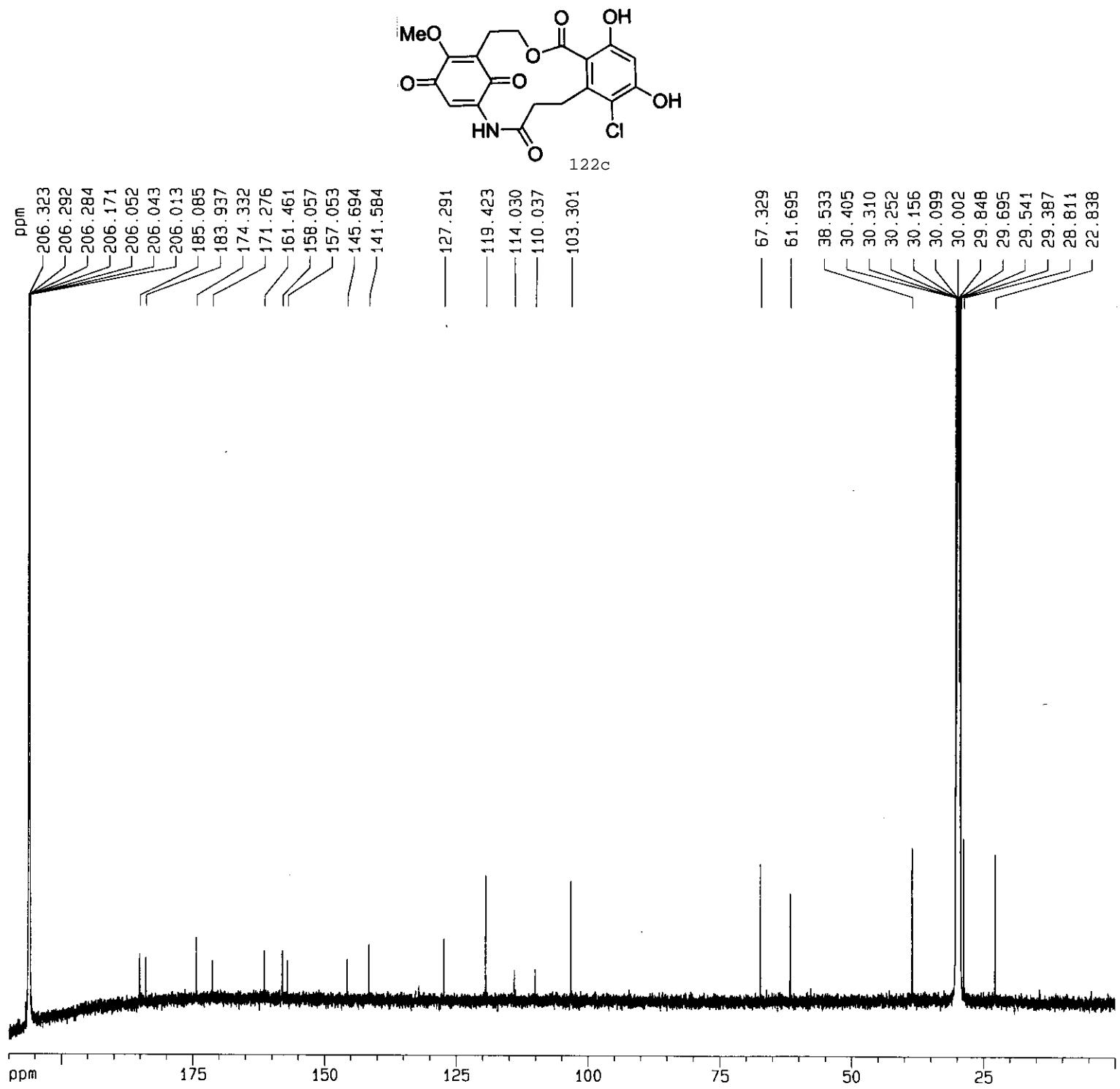
SI 32768
SF 500.1300734 MHz
WN 8F
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters

SI 1024
MC2 8F
SF 500.1300000 MHz
WN GSINE
SSB 0
LB 0.30 Hz
GB 0

1D NMR plot parameters

CX 20.00 cm
CY 30.00 cm
F1P 11.878 ppm
F1 5940.75 Hz
F2P -0.971 ppm
F2 -485.60 Hz
PPMCH 0.64247 ppm/cm
HZCN 321.31729 Hz/cm



Current Data Parameters

NAME 2_0
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

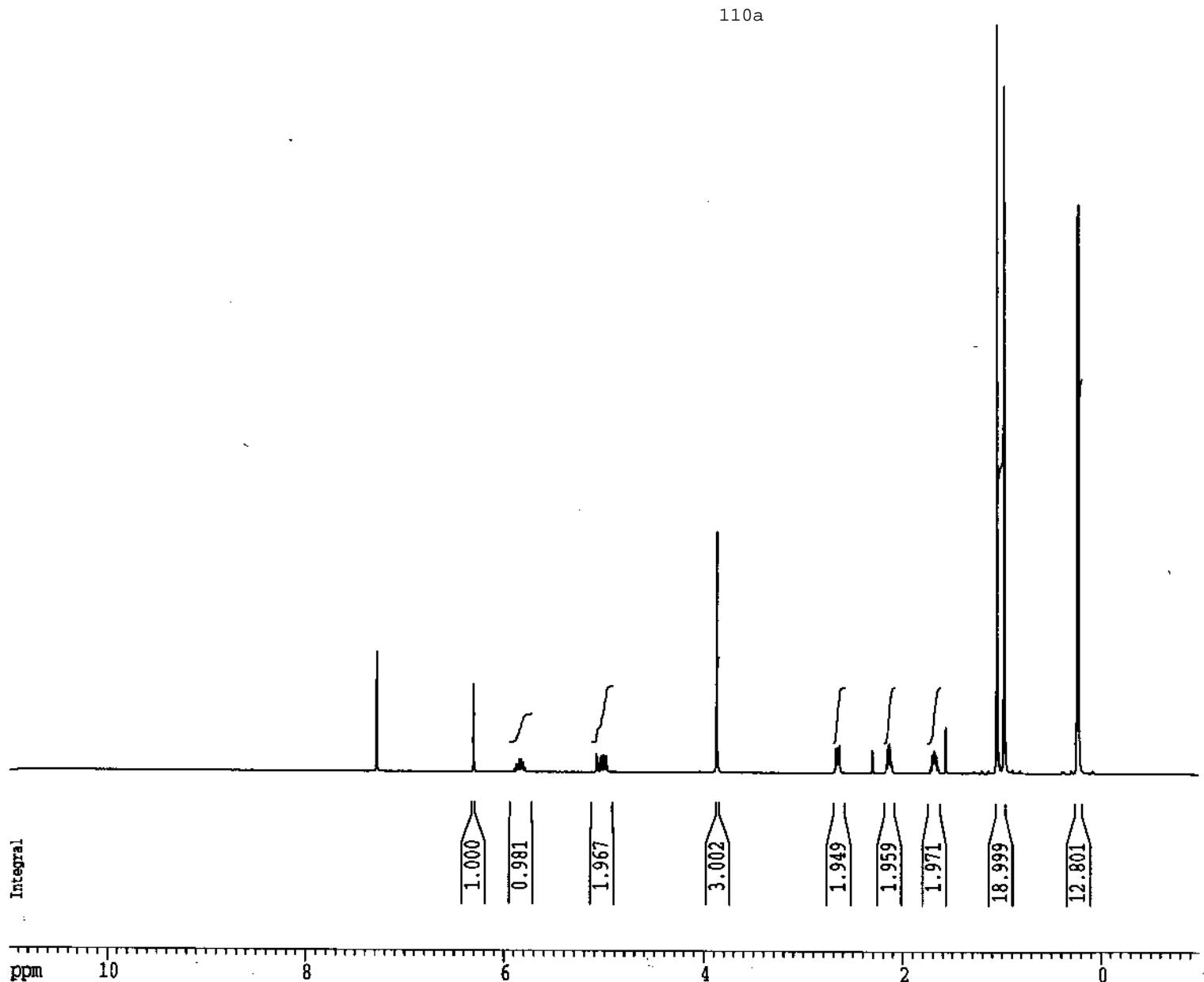
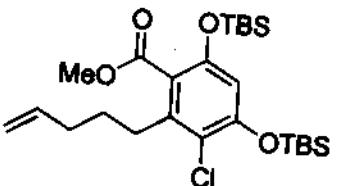
Date 20050221
Time 11:45
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpp30
TD 65536
SOLVENT Aceton
NS 3060
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 8192
DW 15.900 usec
DE 6.00 usec
TE 298.0 K
D1 0.1500001 sec
d11 0.0300000 sec
DELTA 0.05000000 sec
MCREST 0.0000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -4.90 dB
SF01 125.7697360 MHz

===== CHANNEL f2 =====
CPDPG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 9.54 dB
PL13 10.00 dB
SF02 500.1325000 MHz

F2 - Processing parameters
SI 65536
SF 125.7576758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1P 210.000 ppm
F1 26409.11 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPCM 10.50000 ppm/cm
H2CM 1320.45557 Hz/cm



Current Data Parameters

NAME	01
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20050811
Time	20.55
INSTRUM	dix400
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	4789.272 Hz
FIDRES	0.146157 Hz
AQ	3.4210291 sec
RG	256
DW	104.400 usec
DE	5.50 usec
TE	297.2 K
D1	1.0000000 sec
MCREST	0.0000000 sec
MCWRK	0.0150000 sec

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

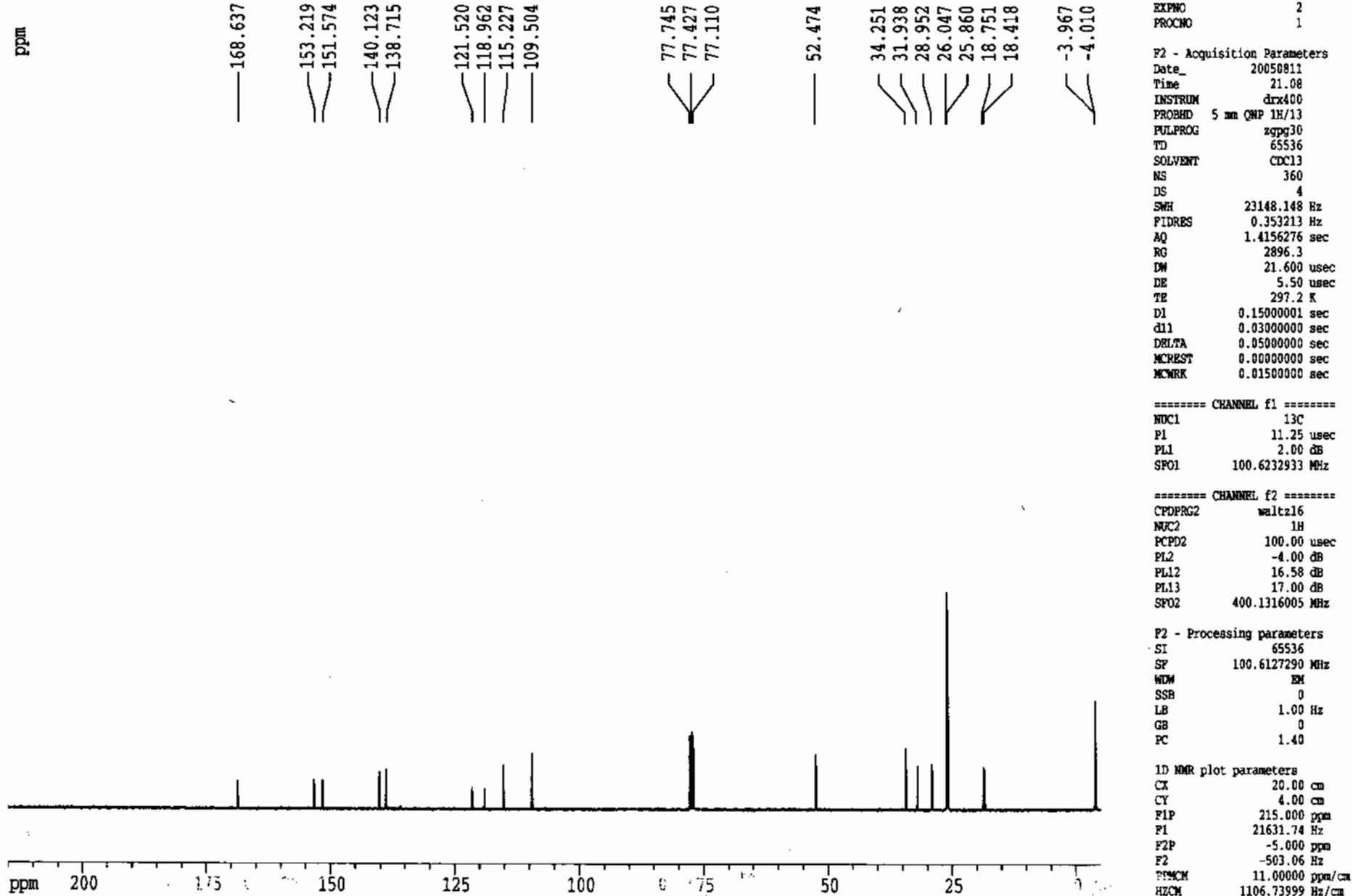
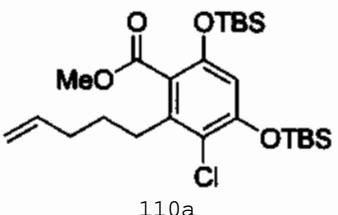
NUC1	1H
P1	9.35 usec
PL1	-4.00 dB
SFO1	400.1320007 MHz

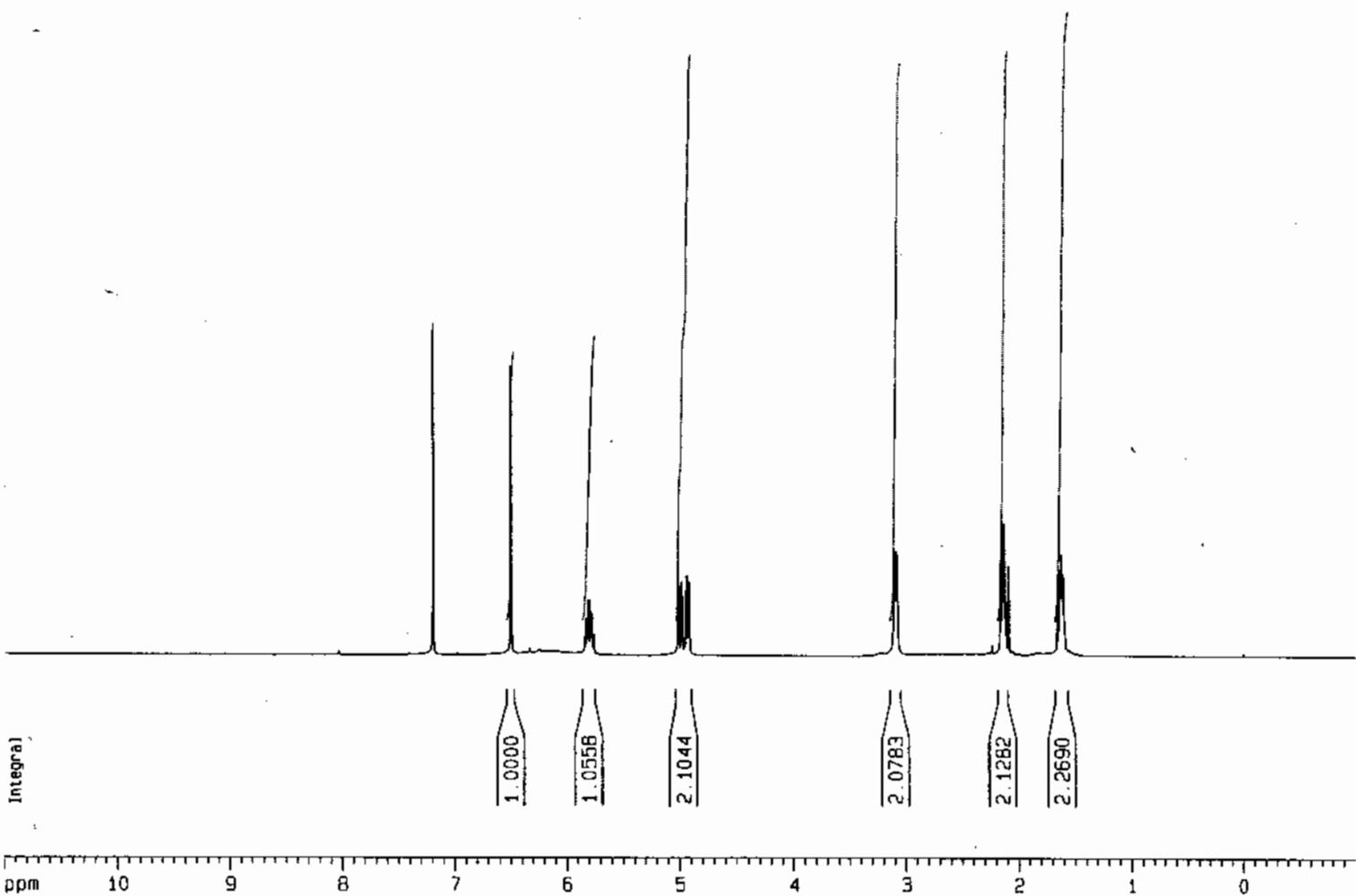
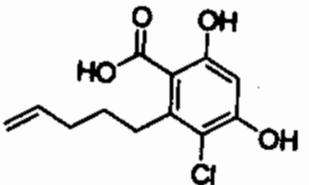
F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	11.000 ppm
F1	4401.43 Hz
F2P	-1.000 ppm
F2	-400.13 Hz
PPMCM	0.60000 ppm/cm
HZCM	240.07800 Hz/cm





Current Data Parameters
 NAME d2
 EXPNO 1
 PROCN0 1

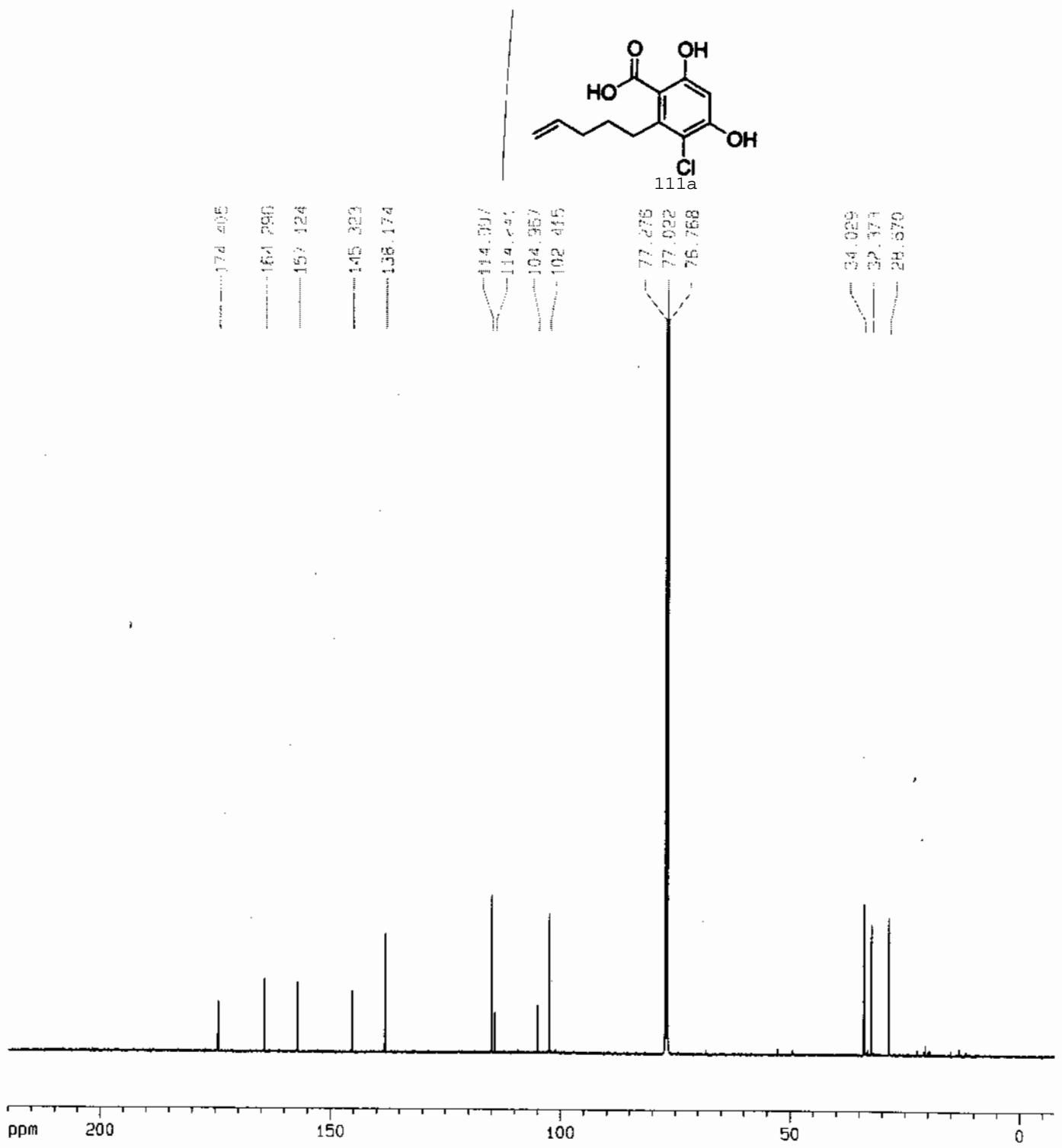
F2 - Acquisition Parameters
 Date 20050809
 time 10.20
 INSTRUM spect
 PROBHD 5 mm CPOUL 13C
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 64
 DW 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 NCOREST 0.0000000 sec
 NCWAK 0.0150000 sec

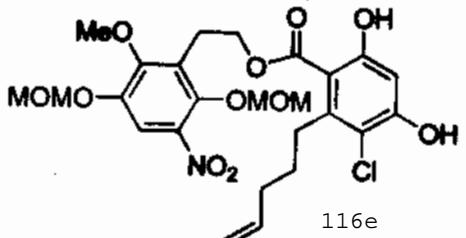
----- CHANNEL f1 -----
 NUC1 1H
 P1 15.00 usec
 PL1 -5.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300480 MHz
 MDW EH
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 NC2 0F
 SF 500.1300000 MHz
 MDW DSINE
 SSB 0
 LB 0.30 Hz
 GB 0

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 5501.43 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 300.07803 Hz/cm





116e

Current Data Parameters
 NAME wmw0504033
 EXPNO 1
 PROCN0 1

F2 - Acquisition Parameters
 Date_ 20050403
 Time 17.48
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 161.3
 DW 104.400 usec
 DE 5.50 usec
 TE 297.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral

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

1.0000

1.0643

1.0954

1.0251

2.1767

2.1836

2.2155

2.1636

3.2508

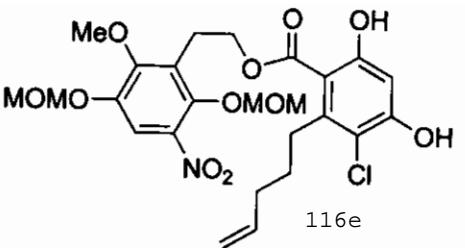
6.2700

2.2247

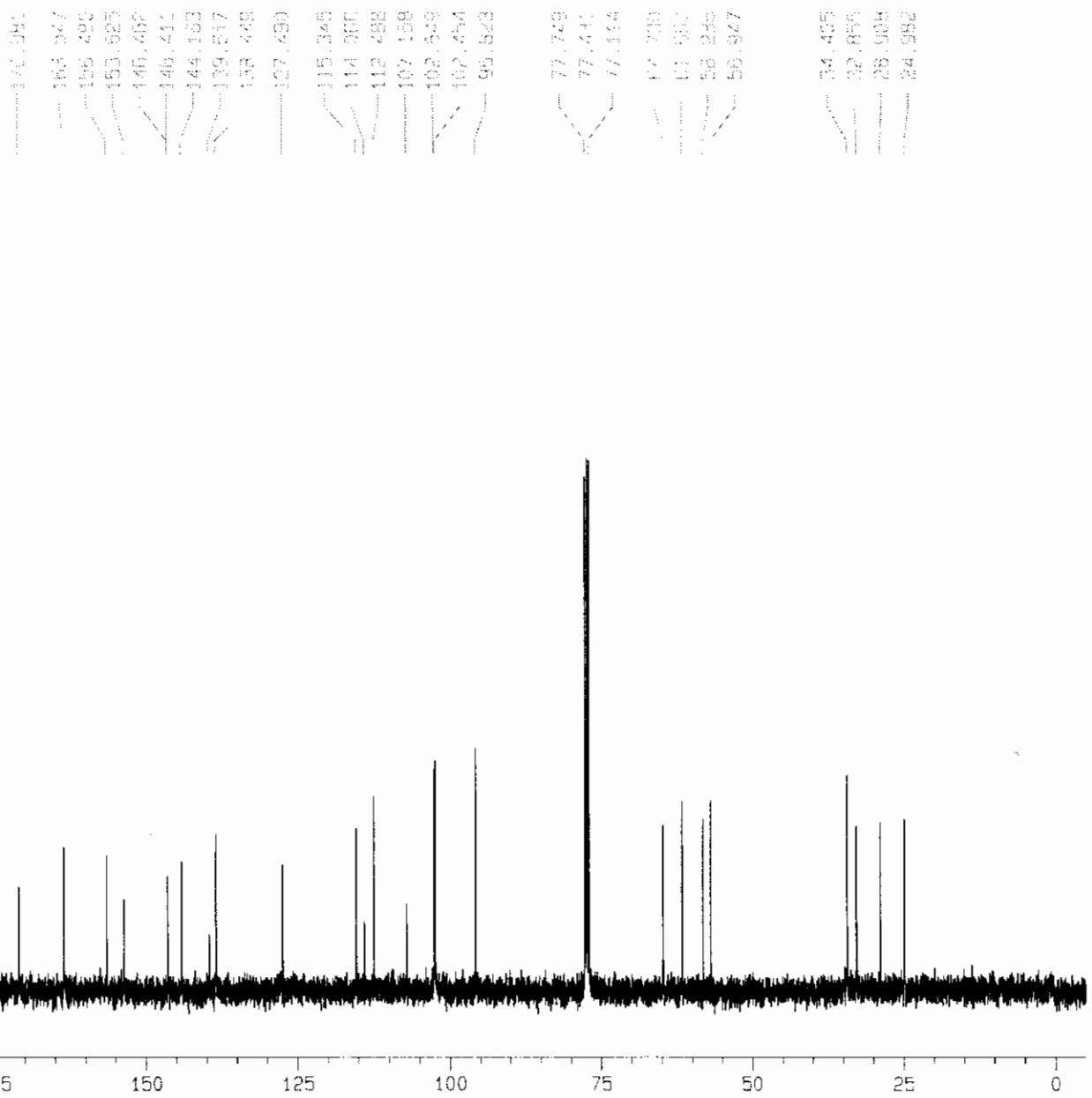
2.0518

2.2265

2.3135



ppm



Current Data Parameters
 NAME mmw0504031
 EXPNO 2
 PROCN0 1

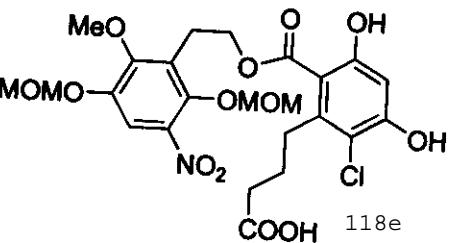
F2 - Acquisition Parameters
 Date_ 20050403
 Time 16.54
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 350
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 4096
 DW 21.600 usec
 DE 5.50 usec
 TE 297.2 K
 D1 0.1500001 sec
 d11 0.0300000 sec
 DELTA 0.0500000 sec
 MCREST 0.0000000 sec
 MCWAK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD02 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



Current Data Parameters
 NAME wmw0504061
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050406
 Time 21.12
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 181
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

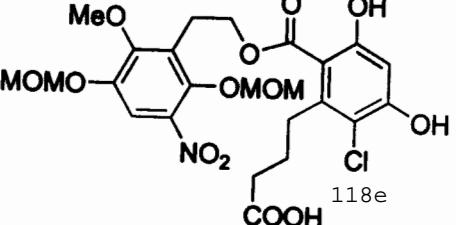
F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

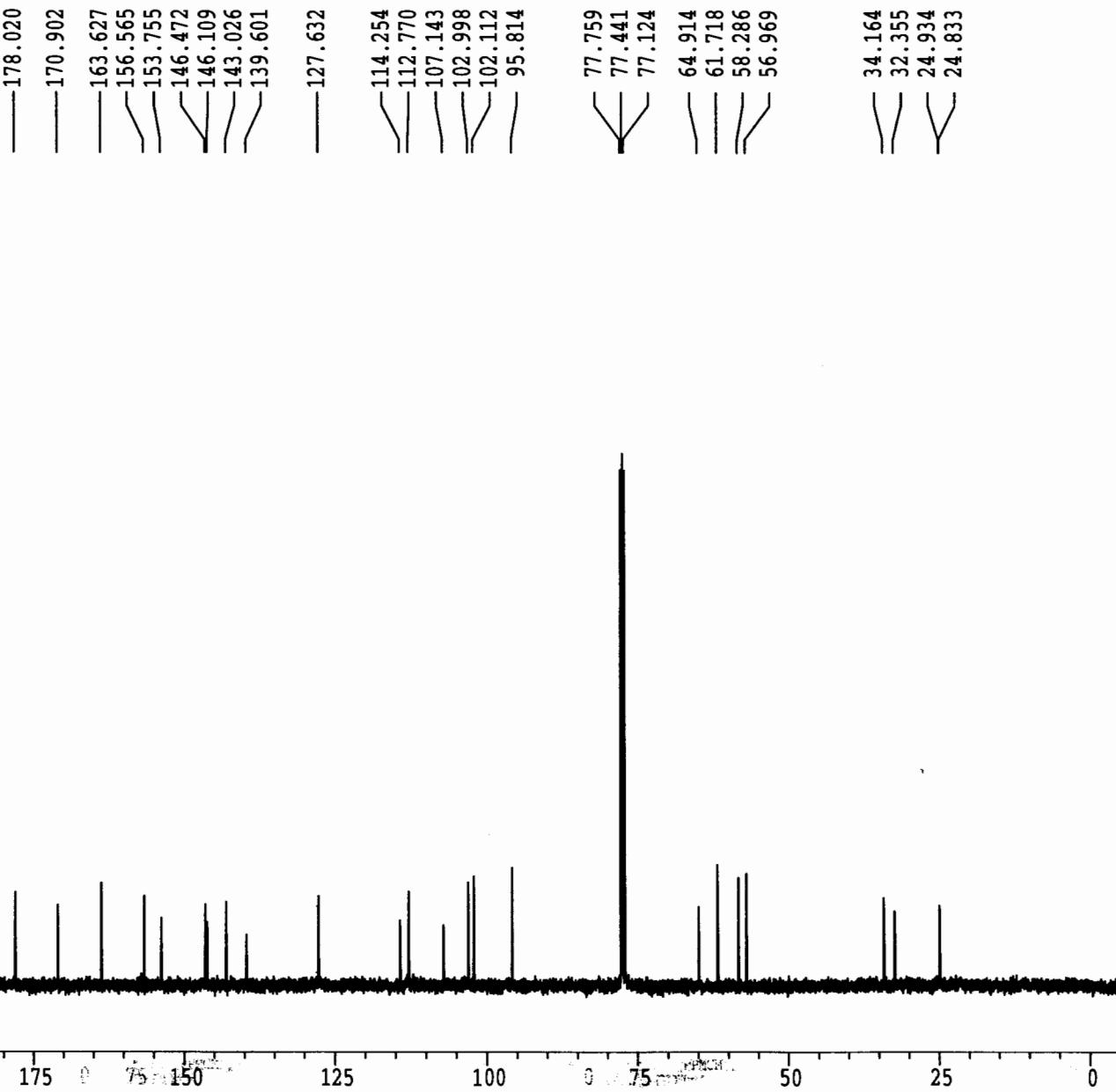
Integral



4-(2-chloro-3,5-dihydroxy-6-((2-methoxy-3,6-bis(methoxymethoxy)-5-nitrophenoxy)carbonyl)phenyl)butanoic acid



ppm



Current Data Parameters
 NAME mmw0504061
 EXPNO 2
 PROCN0 1

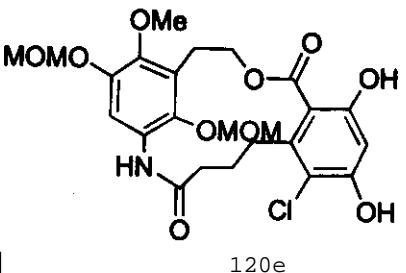
F2 - Acquisition Parameters
 Date_ 20050406
 Time 21.32
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 505
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 4597.6
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



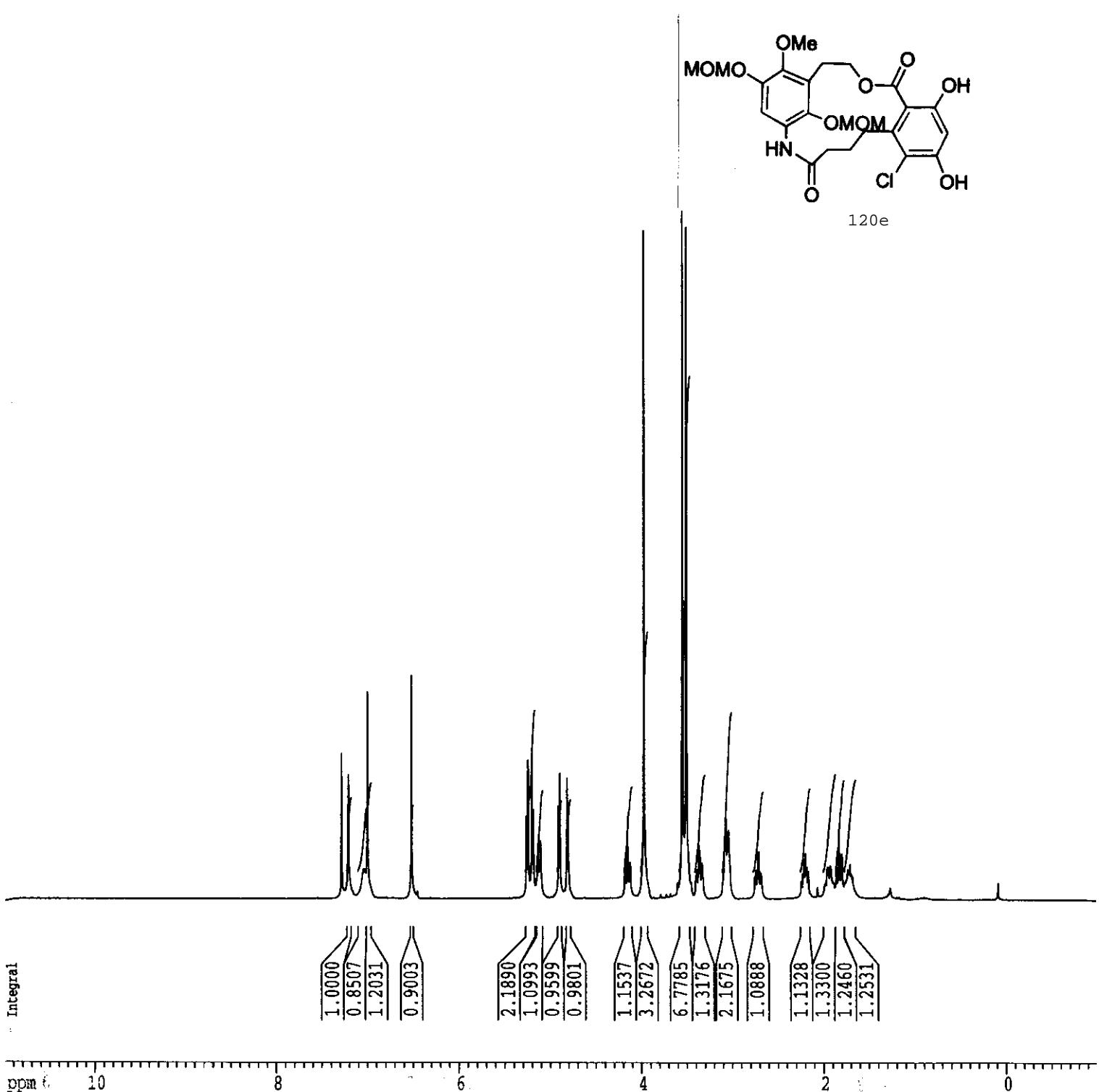
Current Data Parameters
 NAME wwww050415
 EXPNO 1
 PROCNO 1

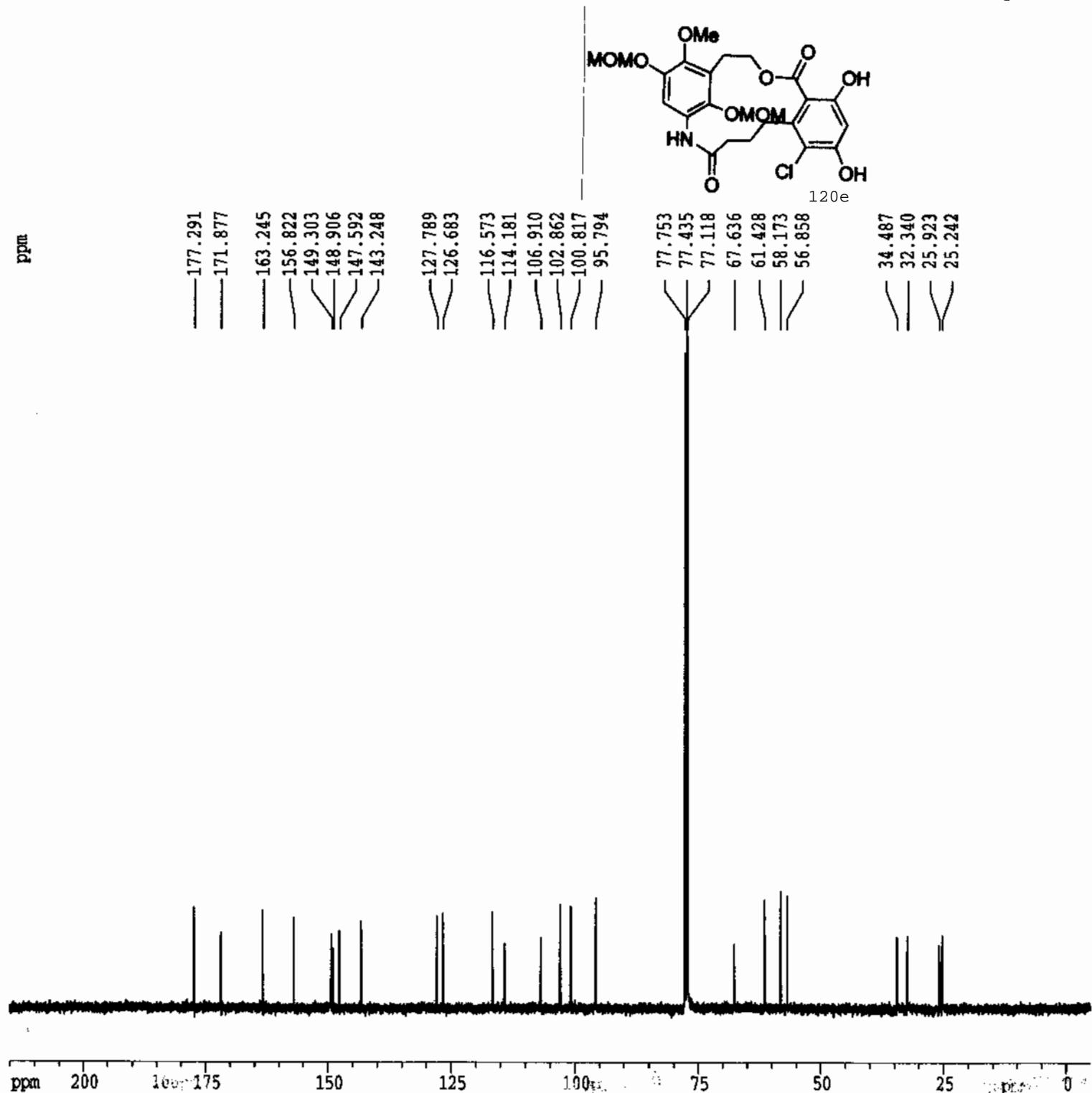
P2 - Acquisition Parameters
 Date_ 20050415
 Time 14.54
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 203.2
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm





Current Data Parameters
 NAME mmw050415
 EXPNO 3
 PROCNO 1

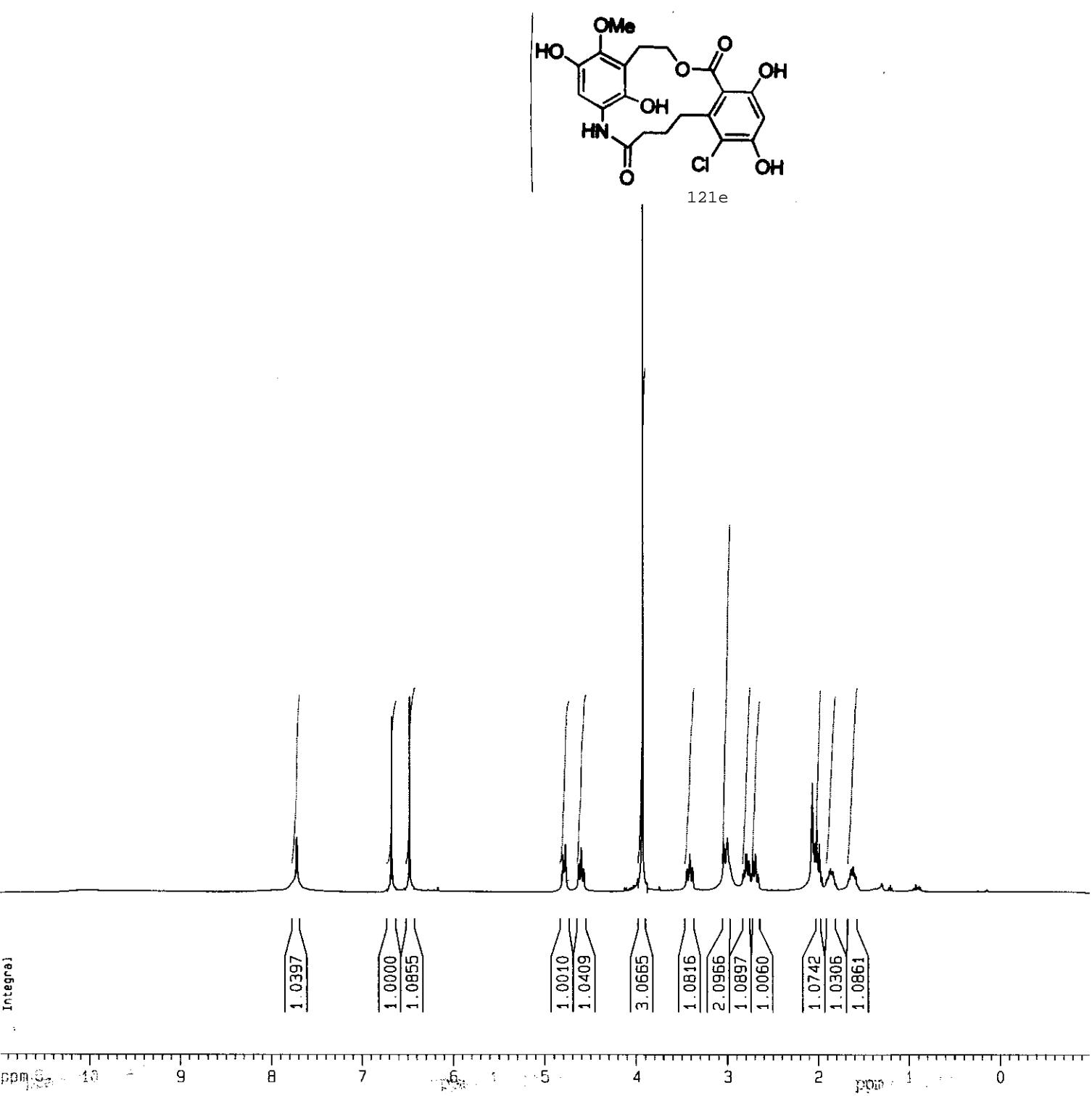
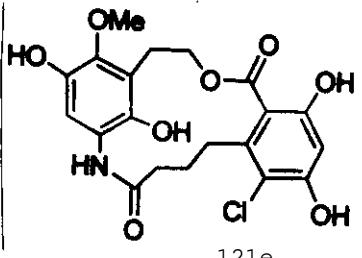
F2 - Acquisition Parameters
 Date_ 20050420
 Time 20.24
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 4597.6
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCRWKR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SPO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SPO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.00 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



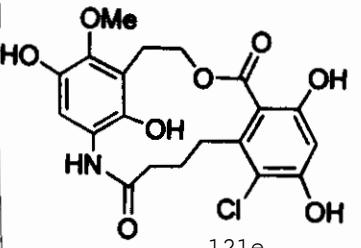
Current Data Parameters
 NAME wmw0505262
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050526
 Time 16.06
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT *acetone-d6*
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIORES 0.146157 Hz
 AQ 3.4210291 sec
 RG 287.4
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

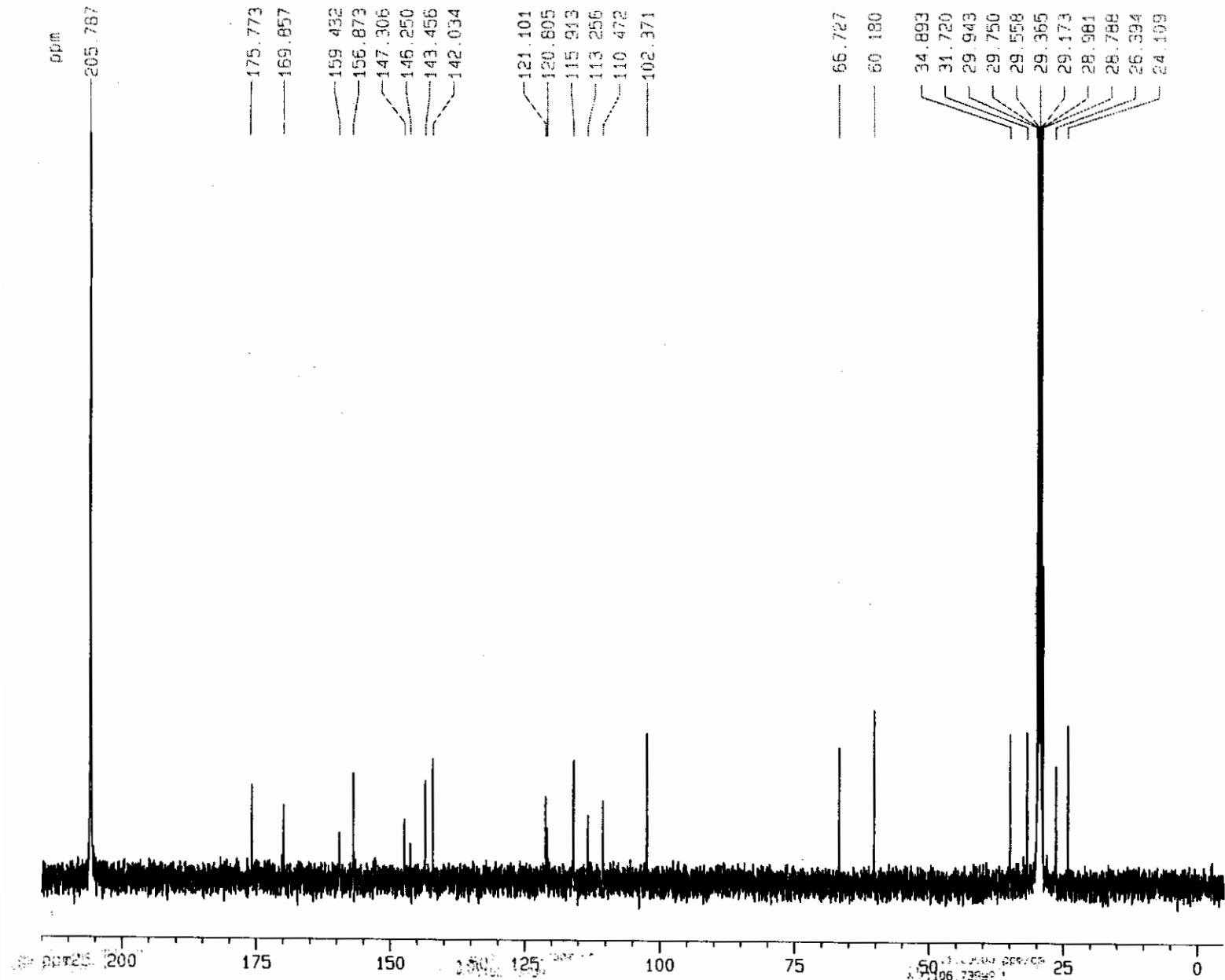
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WMW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm



121e



Current Data Parameters
 NAME mm0505262
 EXPNO 2
 PROCN0 1

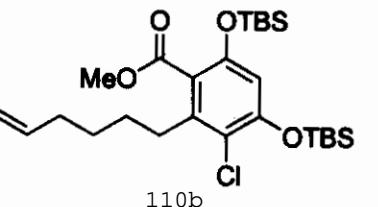
F2 - Acquisition Parameters
 Date_ 20050526
 Time 16.08
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT acetone-~~water~~
 NS 873
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 5792.6
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ^{1H}
 PCP02 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 MW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 60.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMW 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



Current Data Parameters
 NAME rcIV-93a
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050521
 Time 17.03
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 20.00 cm
 F1P 10.985 ppm
 F1 4395.28 Hz
 F2P -0.985 ppm
 F2 -393.99 Hz
 PPMCM 0.59846 ppm/cm
 HZCM 239.46359 Hz/cm

Integral

ppm

10

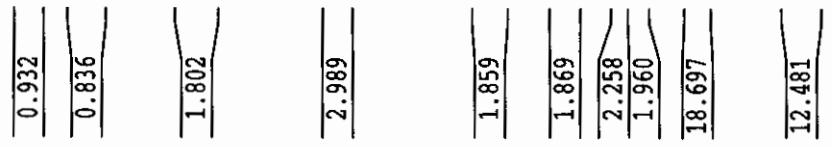
8

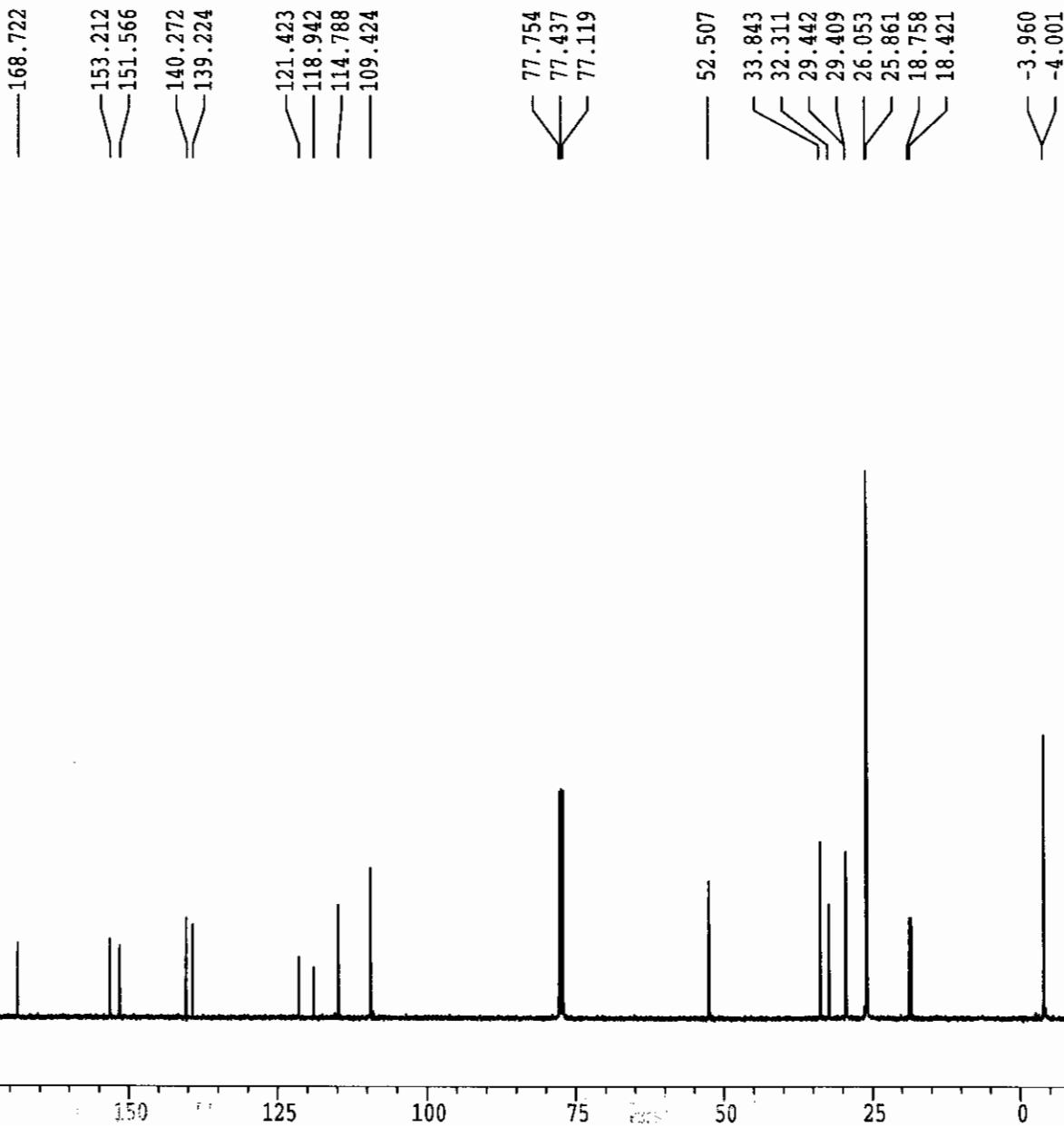
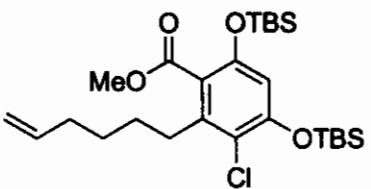
6

4

2

0





Current Data Parameters
 NAME rcIV-93a-C13
 EXPNO 1
 PROCNO 1

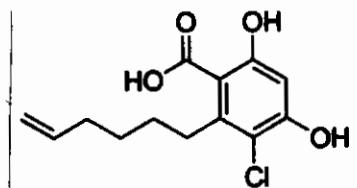
P2 - Acquisition Parameters
 Date_ 20050521
 Time 17.21
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 3251
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SPO1 100.6232933 MHz

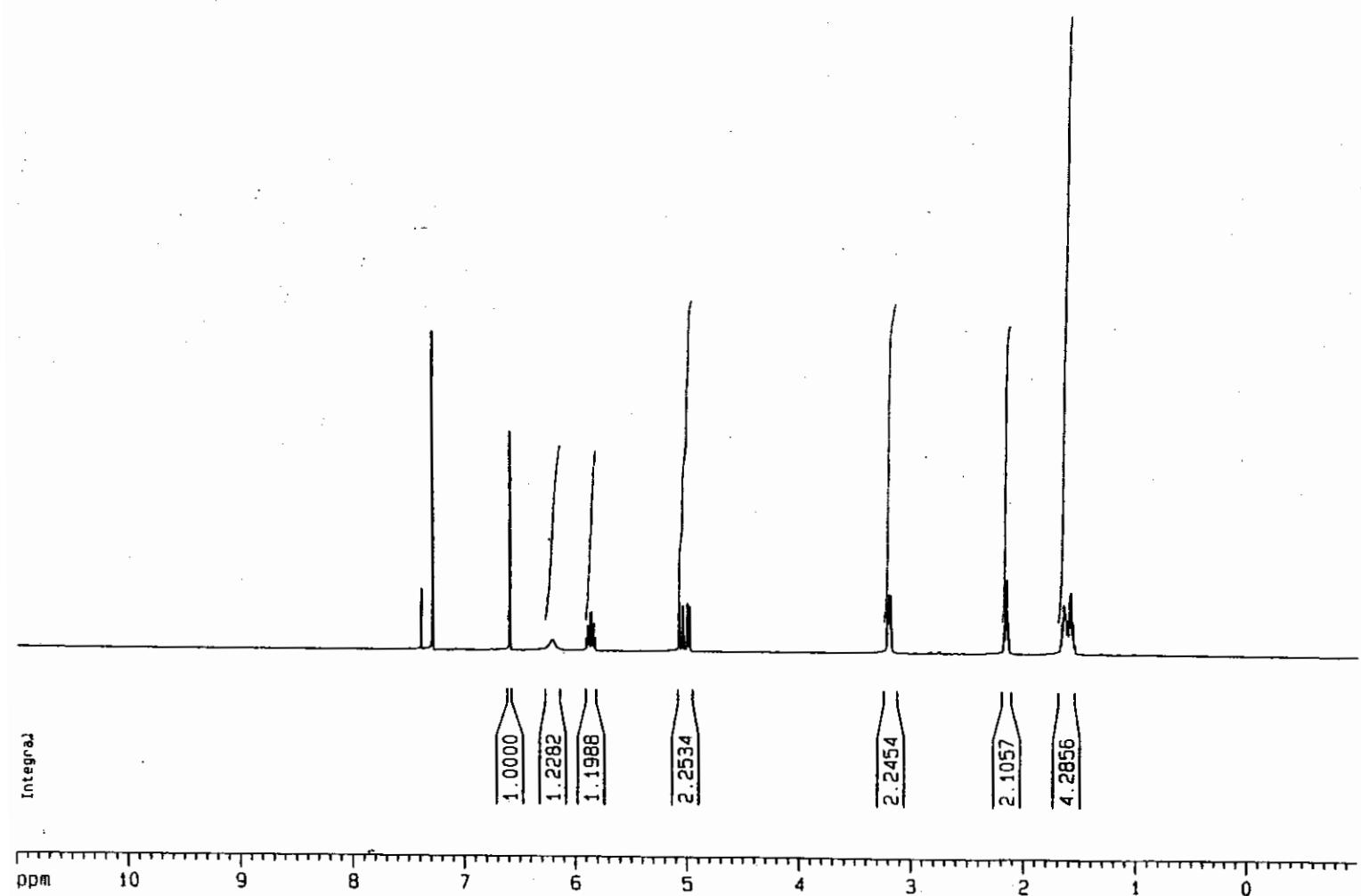
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

P2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 220.036 ppm
 F1 22138.42 Hz
 F2P -10.036 ppm
 F2 -1009.73 Hz
 PPMCM 11.50359 ppm/cm
 Hz/cm² 1157.40747 Hz/cm²



111b



Current Data Parameters
 NAME d1
 EXPNO 1
 PROCNO 1

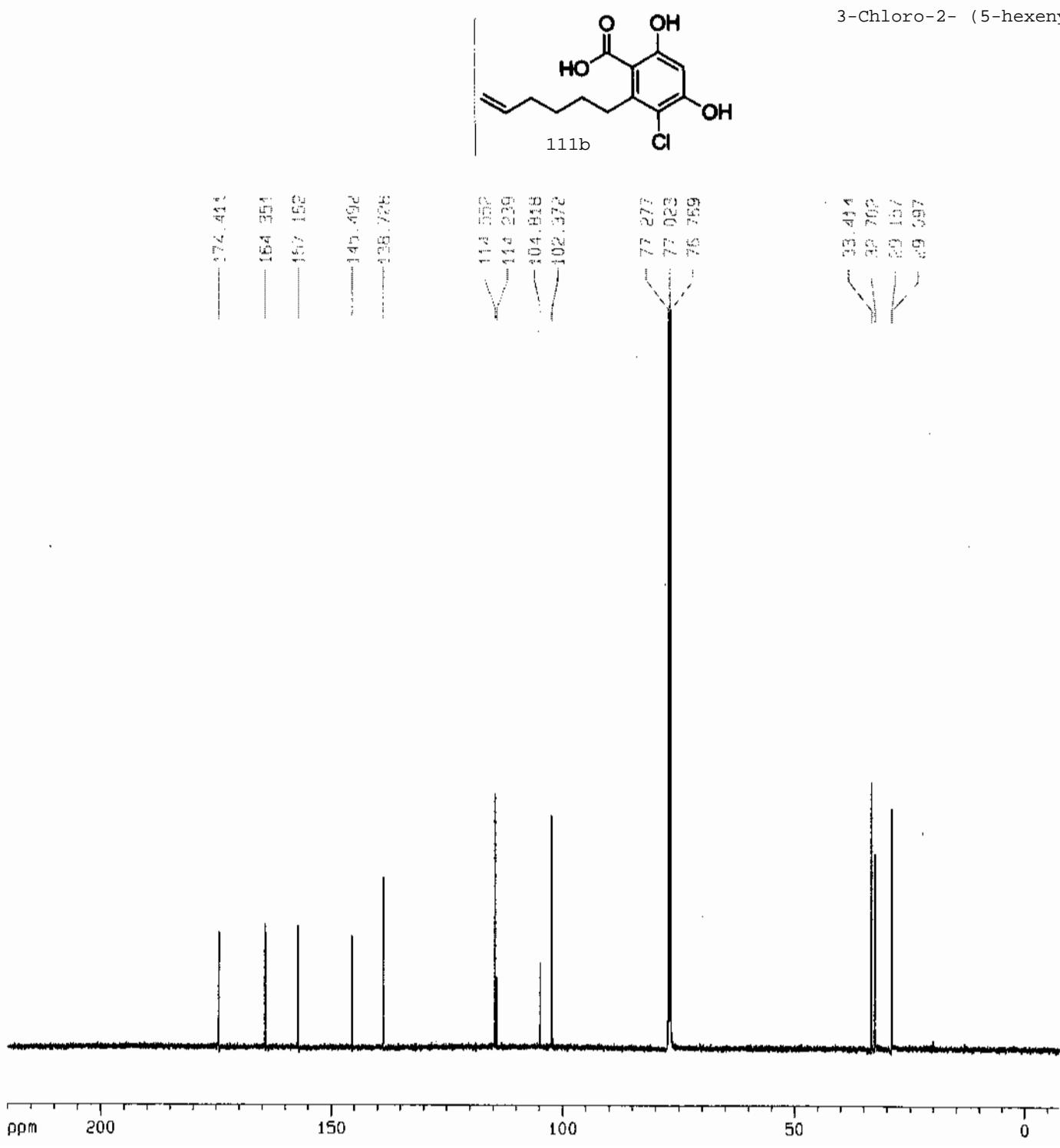
F2 - Acquisition Parameters
 Date_ 20050809
 Time 10.01
 INSTRUM spect
 PROBHD 5 mm CPQUL 13C
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 64
 DM 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 NCWRIK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 PI 15.00 usec
 PL1 -5.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 MW EN
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 0F
 SF 500.1300000 MHz
 MW OSINE
 SSB 0
 LB 0.30 Hz
 GB 0

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 5501.43 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMW 0.60000 ppm/cm
 HZCN 300.07800 Hz/cm



Current Data Parameters
 NAME d1
 EXPNO 2
 PROCNO 1

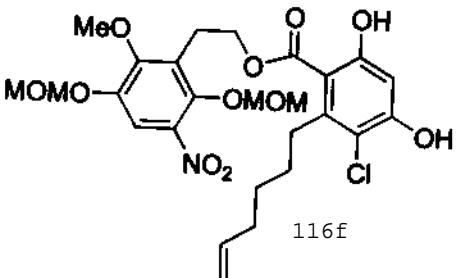
F2 - Acquisition Parameters
 Date_ 20050809
 Time 10.13
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT COC13
 NS 579
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420724 sec
 RG 8192
 DW 15.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.15000001 sec
 D11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -4.90 dB
 SF01 125.7697360 MHz

===== CHANNEL f2 =====
 CPDPG2 wait216
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 9.54 dB
 PL13 10.00 dB
 SF02 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577890 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 30.00 cm
 F1P 242.517 ppm
 F1 30498.43 Hz
 F2P -7.539 ppm
 F2 -948.11 Hz
 PPMM 12.50282 ppm/cm
 HZCM 1572.32690 Hz/cm



Current Data Parameters
 NAME www0505041
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050504
 Time 14.46
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

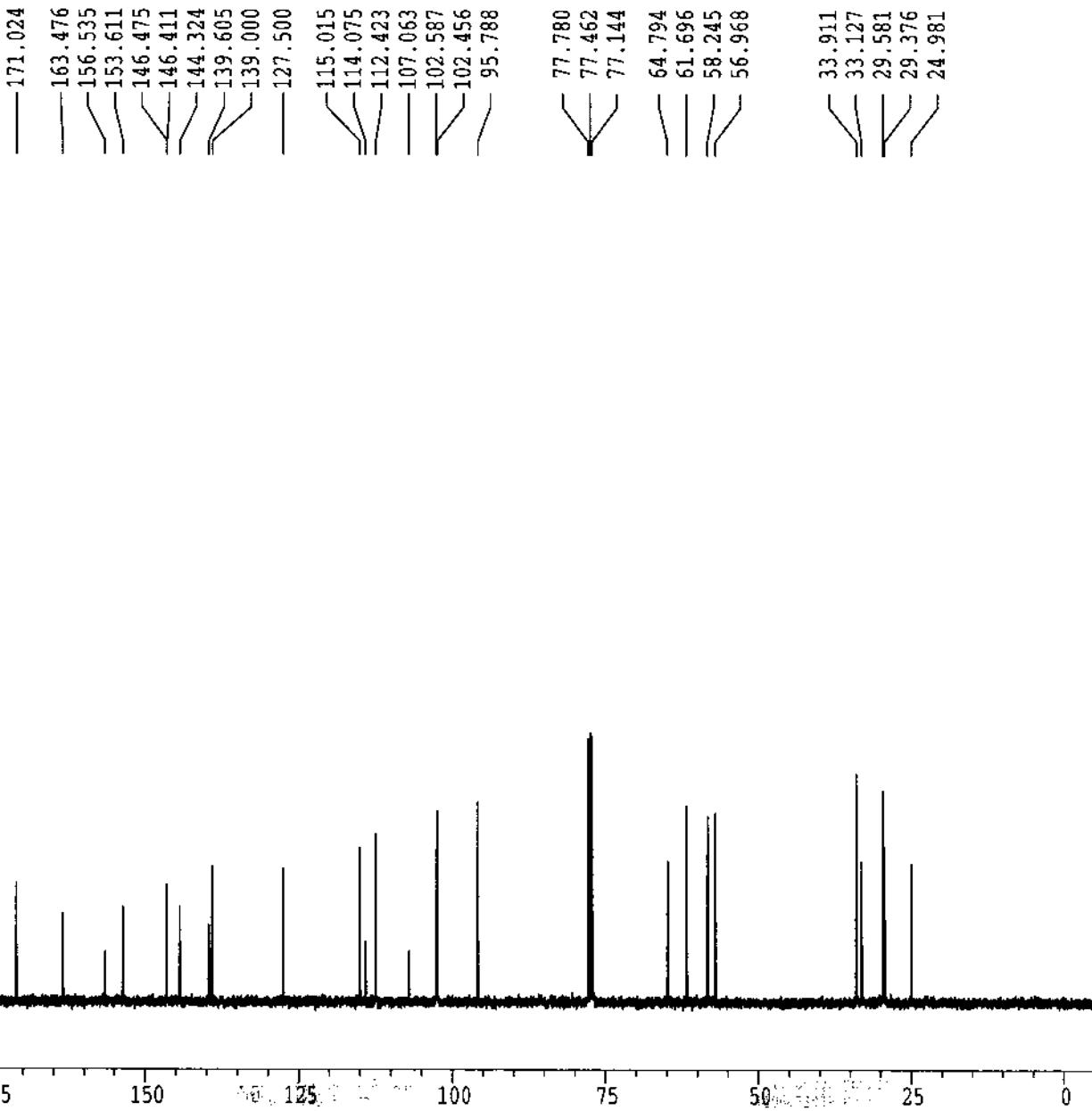
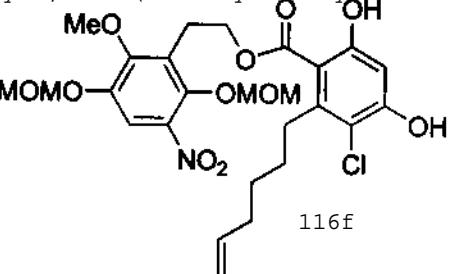
1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral

ppm

10 8 6 4 2 0

1.0054
 1.0120
 1.0755
 2.0832
 1.9921
 2.1659
 2.0050
 2.9293
 6.1012
 2.0152
 1.9690
 2.0577
 2.0793
 2.0025



Current Data Parameters

NAME wmm0505041
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date 20050504
Time 15.22
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 380
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 6502
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.15000001 sec
G11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MWKR 0.01500000 sec

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

NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

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

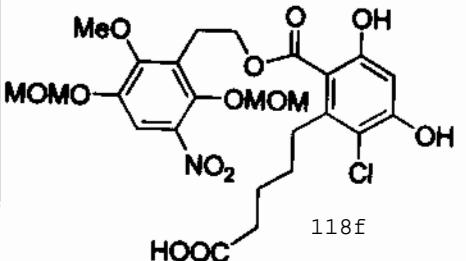
CPDPG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 65536
SP 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 4.00 cm
PIP 215.00 ppm
P1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm



Current Data Parameters
 NAME wmv0505093
 EXPNO 1
 PROCNO 1

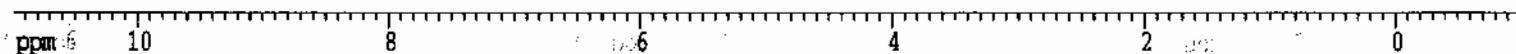
F2 - Acquisition Parameters
 Date 20050509
 Time 19.07
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 181
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

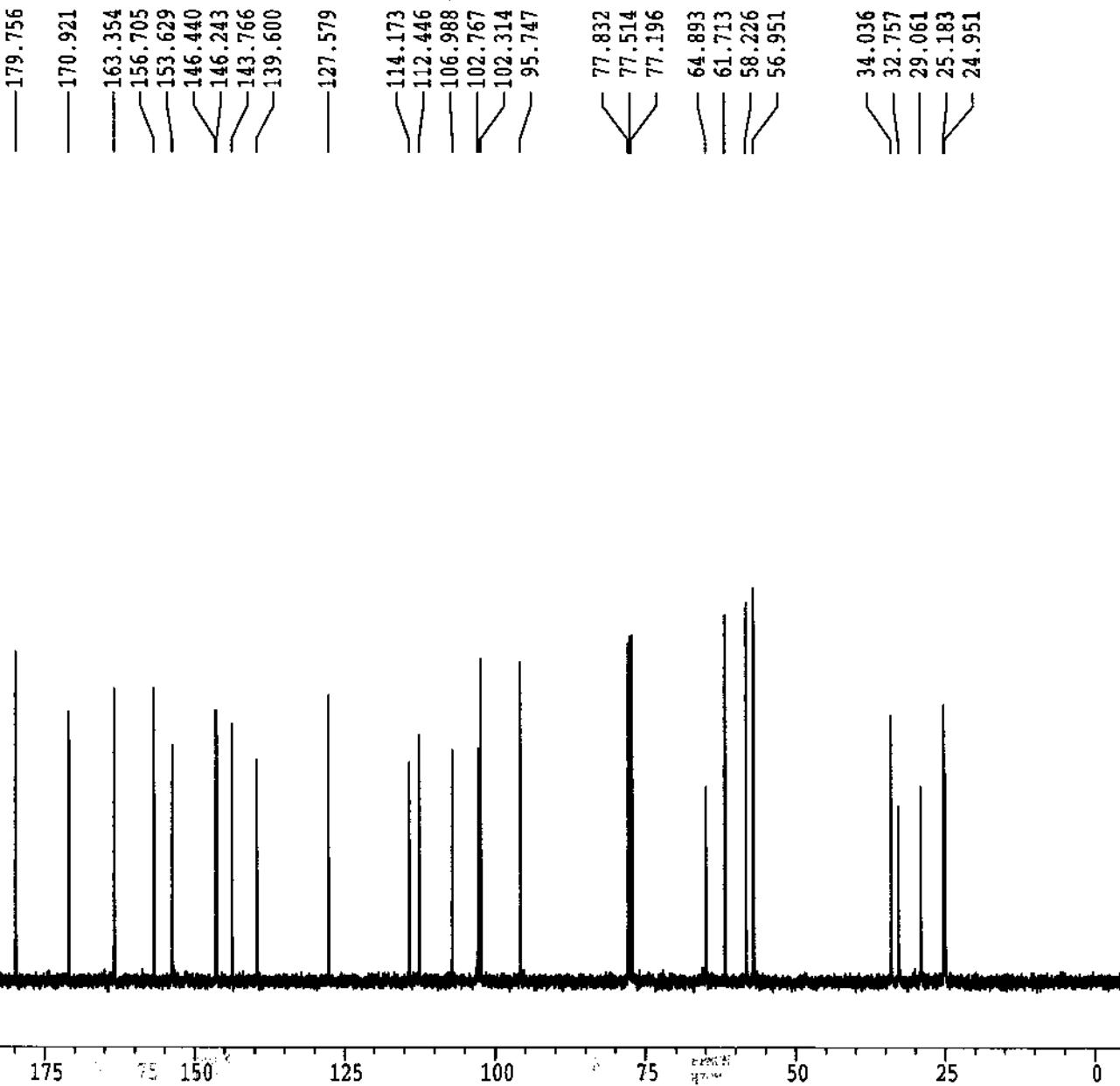
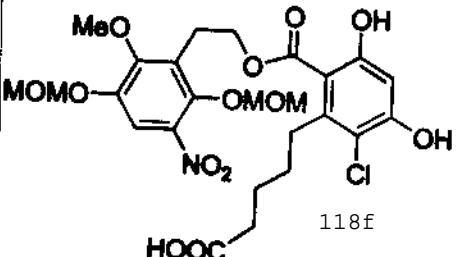
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral





Current Data Parameters
 NAME www0505093
 EXPNO 2
 PROCHNO 1

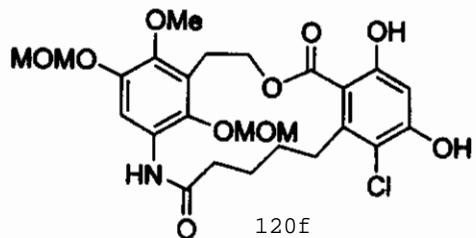
F2 - Acquisition Parameters
 Date_ 20050509
 Time 19.25
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 189
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 3649.1
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



Current Data Parameters
 NAME wmmw05050173
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050517
 Time 16.35
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 161.3
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

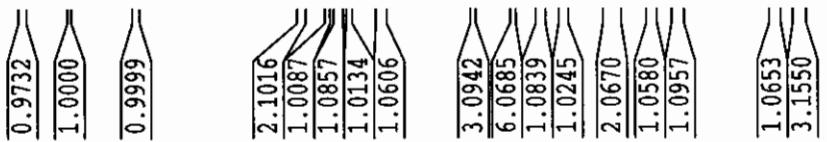
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

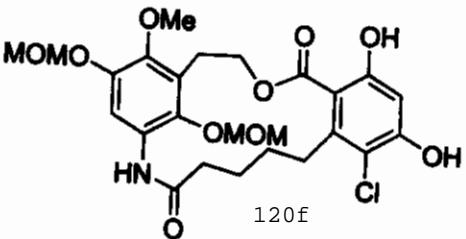
1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral

ppm



10 9 8 7 6 5 4 3 2 1 0



ppm

176.726
171.827
163.938
156.795
148.912
148.815
147.567
144.141

127.227
127.018
116.169
114.185
106.433
102.681
100.869
95.680

77.758
77.643
77.441
77.123
65.627
61.564
57.674
56.712

34.195
31.565
28.446
25.013
24.765

Current Data Parameters
NAME wmm05050173
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050517
Time 17.42
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2005
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 6502
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.1500001 sec
d11 0.03000000 sec
DETA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

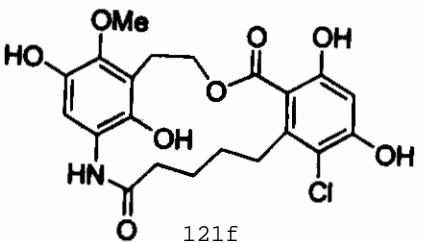
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 25.00 cm
F1P 215.00 ppm
P1 21631.74 Hz
F2P -5.000 ppm
P2 -503.06 Hz
PPCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm

200 175 150 125 100 75 50 25 0



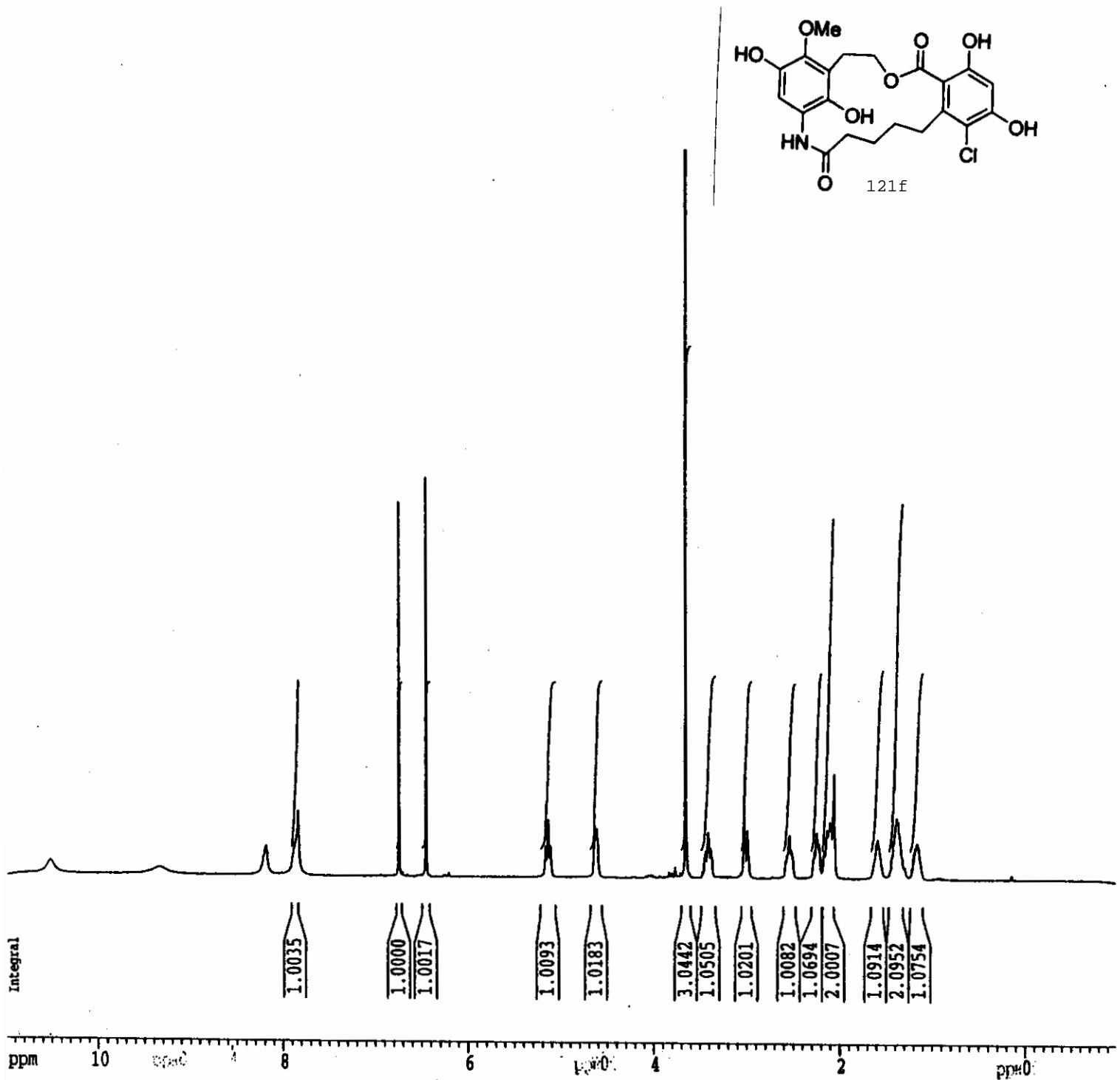
Current Data Parameters
 NAME wwww0505263
 EXPNO 1
 PROCNO 1

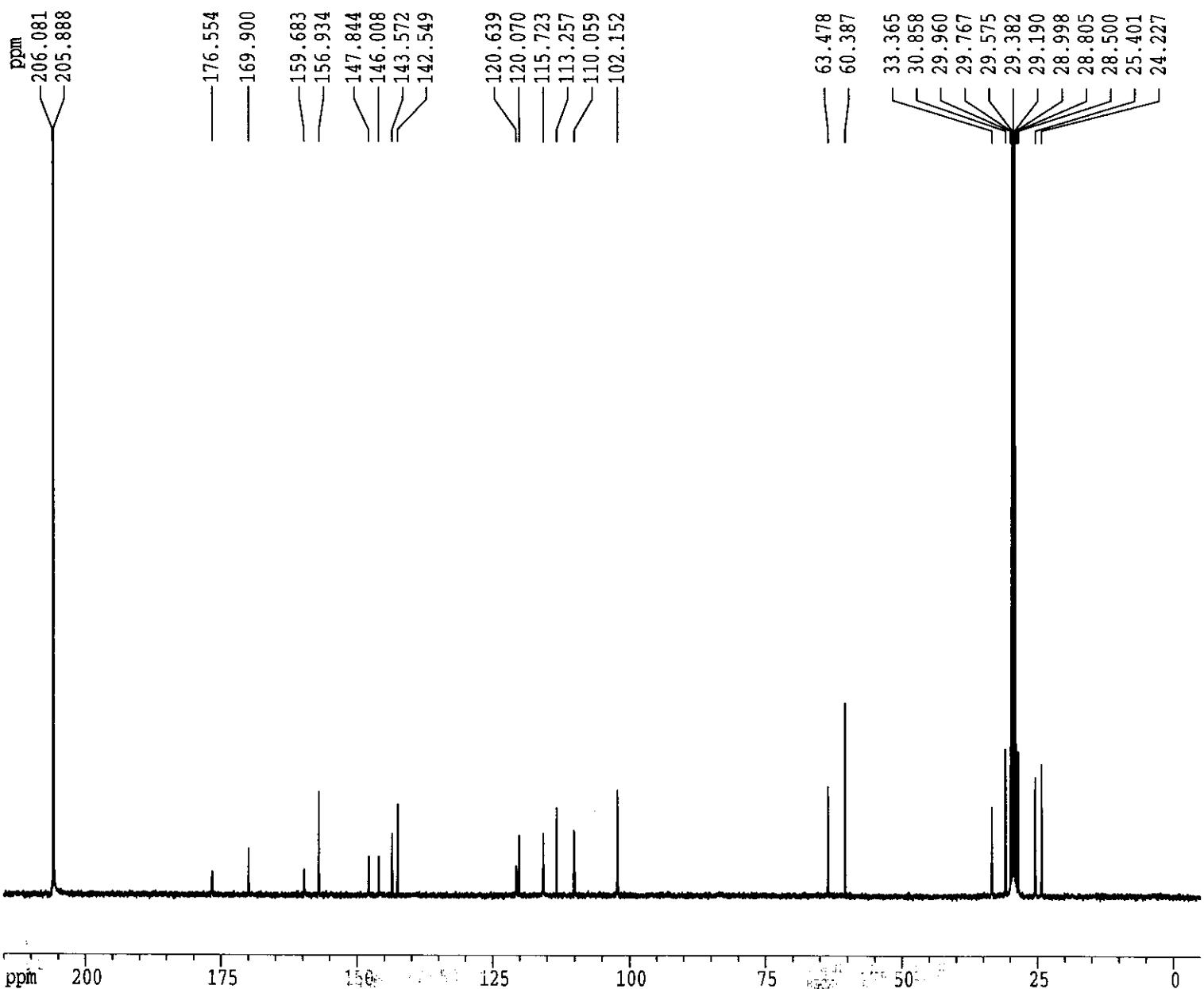
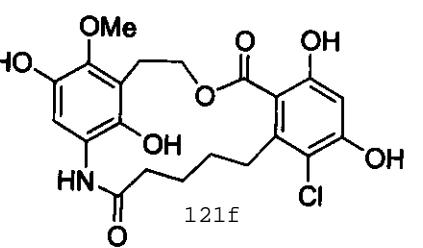
F2 - Acquisition Parameters
 Date_ 20050526
 Time 20.59
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT Aceton
 NS 16
 DS 2
 SWH 4789.272 Hz
 PIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 143.7
 DW 104.400 usec
 DE 5.50 usec
 TB 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL F1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SPO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 20.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm





Current Data Parameters
NAME wmw0505263

EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

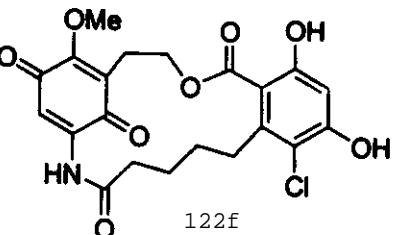
Date_ 20050526
Time 21.41
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2376
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 4096
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.1500001 sec
d11 0.0300000 sec
DELTA 0.0500000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== CHANNEL f2 =====
CPDPG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1P 215.000 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPCM 11.00000 ppm/cm
H2CM 1106.73999 Hz/cm



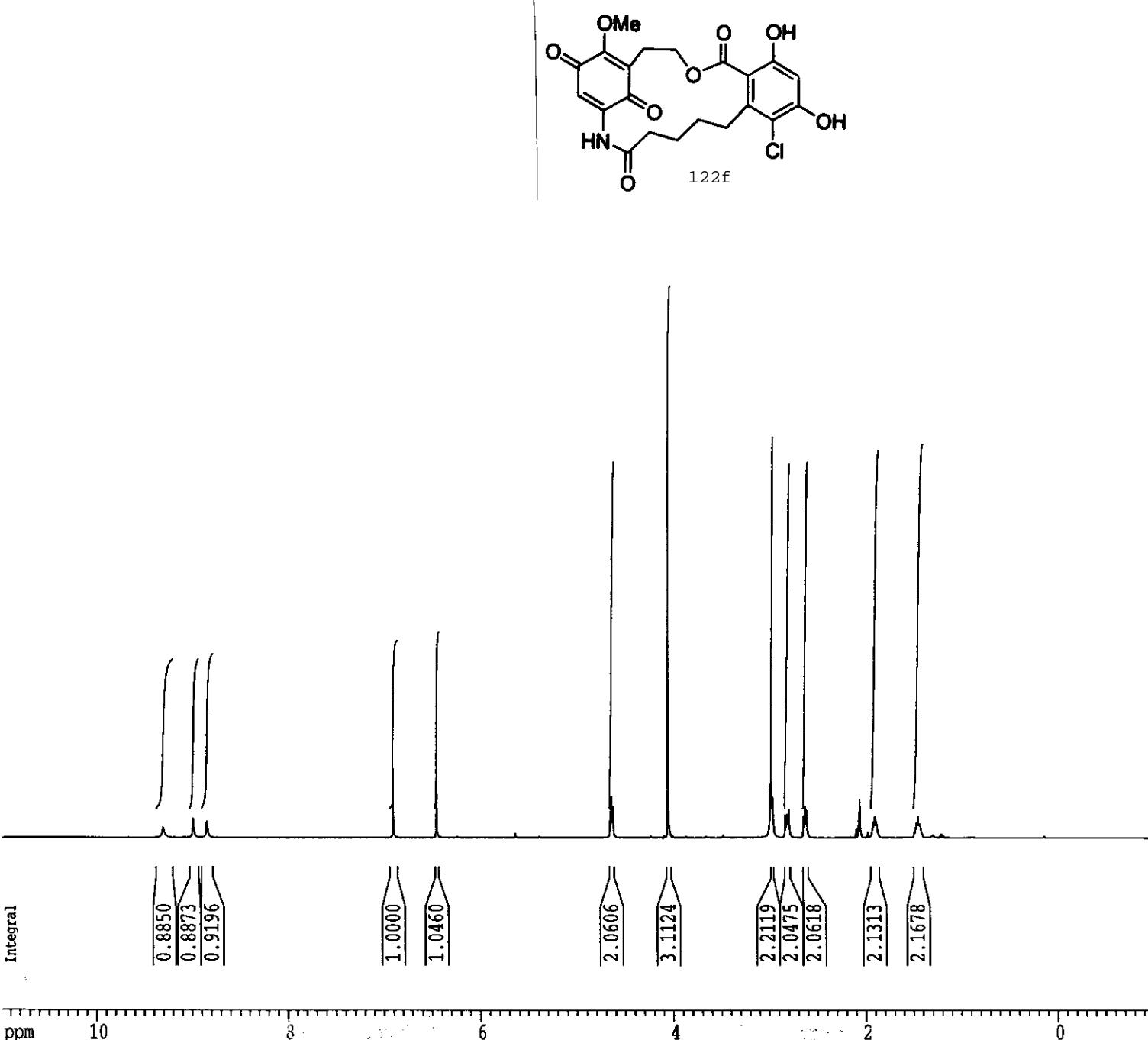
Current Data Parameters
 NAME mw506033
 EXPNO 1
 PROCN 1

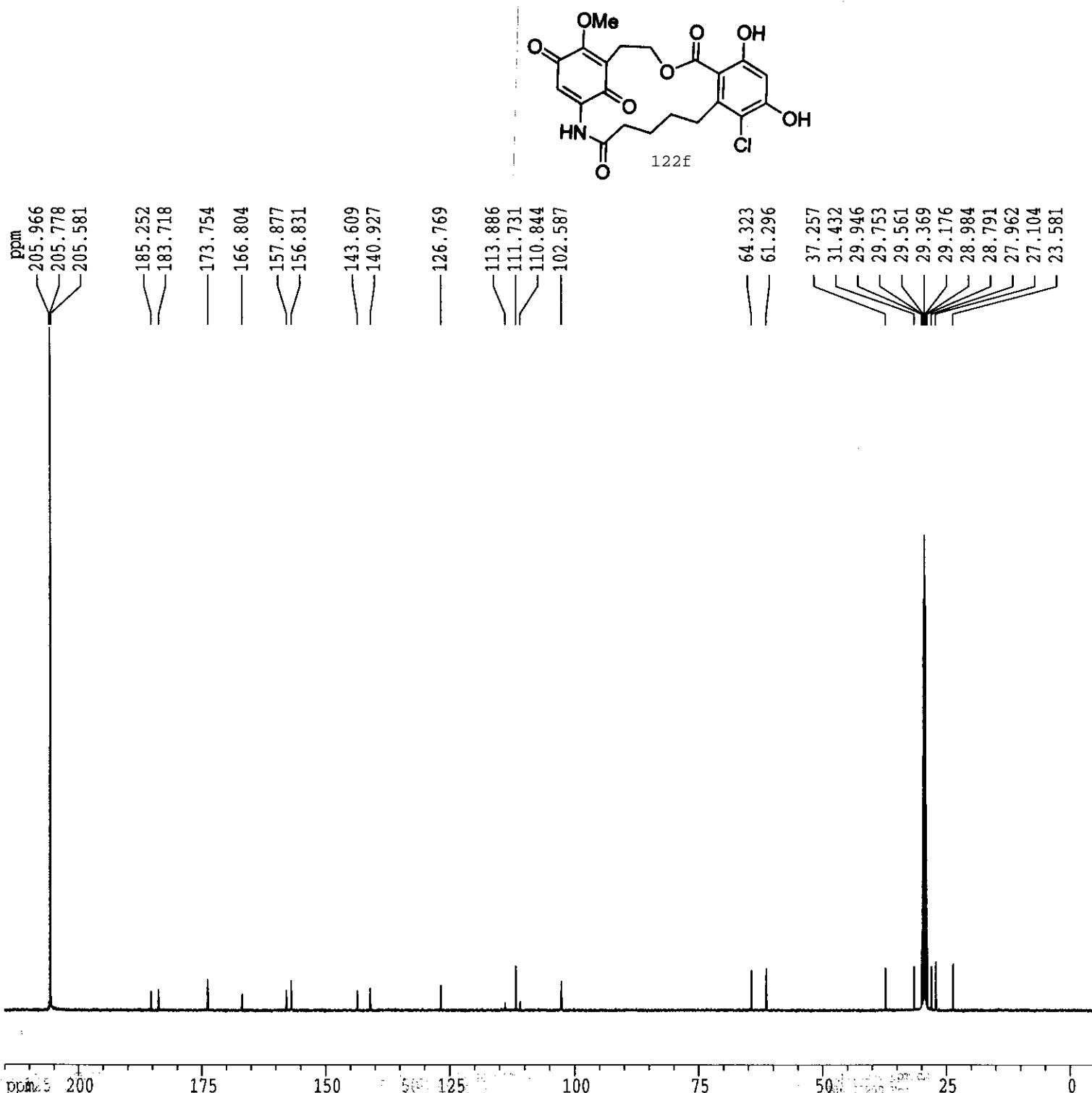
F2 - Acquisition Parameters
 Date_ 20050602
 Time 16.21
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 203.2
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 10.985 ppm
 F1 4395.28 Hz
 F2P -0.985 ppm
 F2 -393.99 Hz
 PPMCM 0.59846 ppm/cm
 HZCM 239.46362 Hz/cm





Current Data Parameters
 NAME mw506033
 EXPNO 2
 PROCN0 1

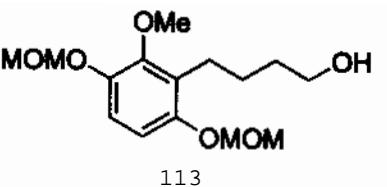
F2 - Acquisition Parameters
 Date_ 20050602
 Time 17.04
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpp30
 TD 65536
 SOLVENT CDCl3
 NS 2318
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 3251
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.1500001 sec
 d11 0.0300000 sec
 DELTA 0.0500000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SP 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 4106.73999 Hz/cm



Current Data Parameters
 NAME wmm1013
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051013
 Time 18.24
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 64
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 P2P -1.000 ppm
 P2 -400.13 Hz
 PPMCM 0.60000 ppm/
 HZCM 240.07800 Hz/c

Integral

ppm

10

9

8

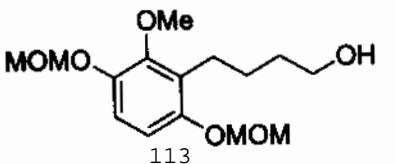
6

4

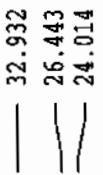
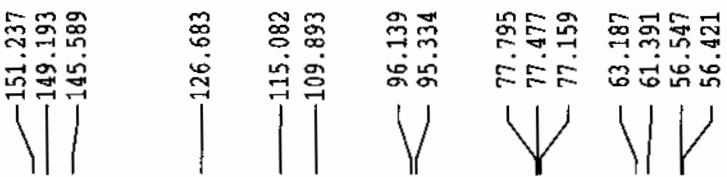
2

0





ppm



Current Data Parameters
 NAME mmw1013
 EXPNO 2
 PROCNO 1

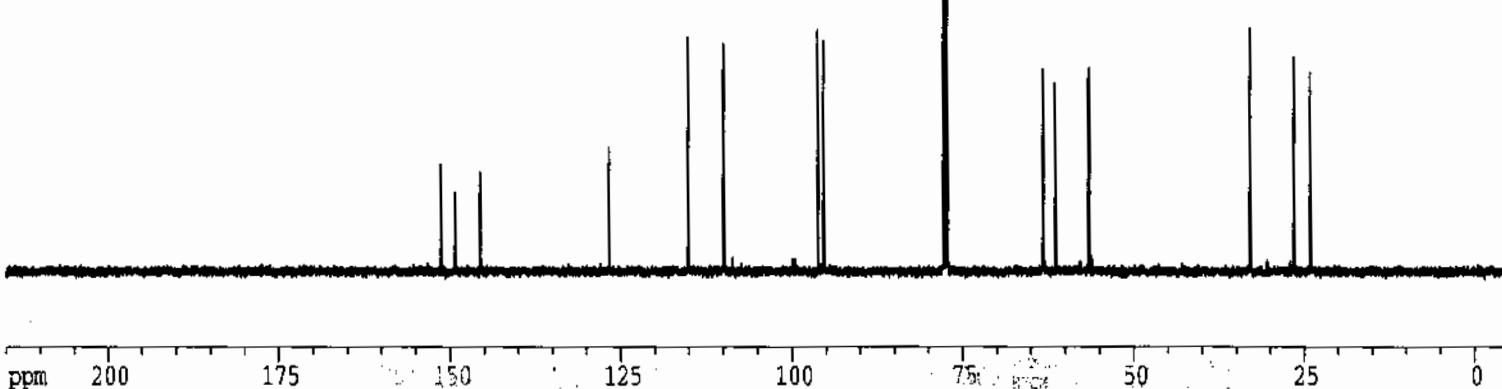
F2 - Acquisition Parameters
 Date 20051013
 Time 18.33
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 287
 DS 4
 SWH 23148.148 Hz
 PIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 4096
 DW 21.600 usec
 DE 5.50 usec
 TE 294.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

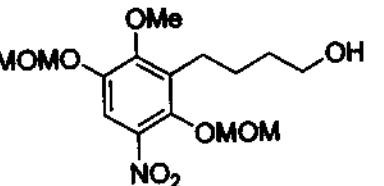
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SFO1 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 215.000 ppm
 P1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPNCM 11.00000 ppm
 CP 106.73999 Hz/





Current Data Parameters
 NAME www12042
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051205
 Time 10.57
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 90.5
 DW 104.400 usec
 DE 5.50 usec
 TE 295.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

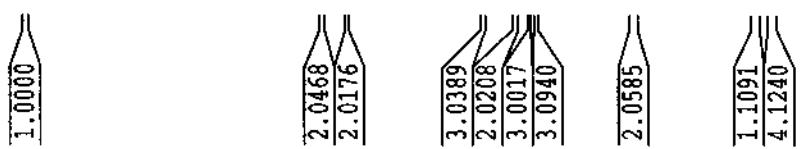
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

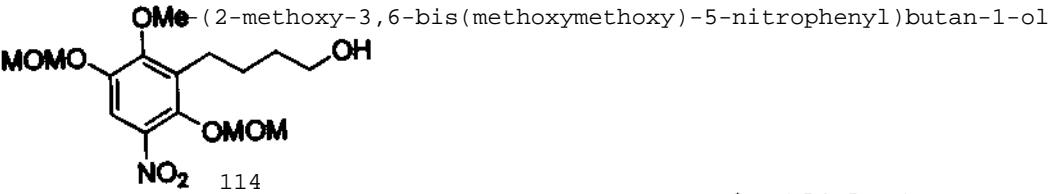
F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW RM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 7.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

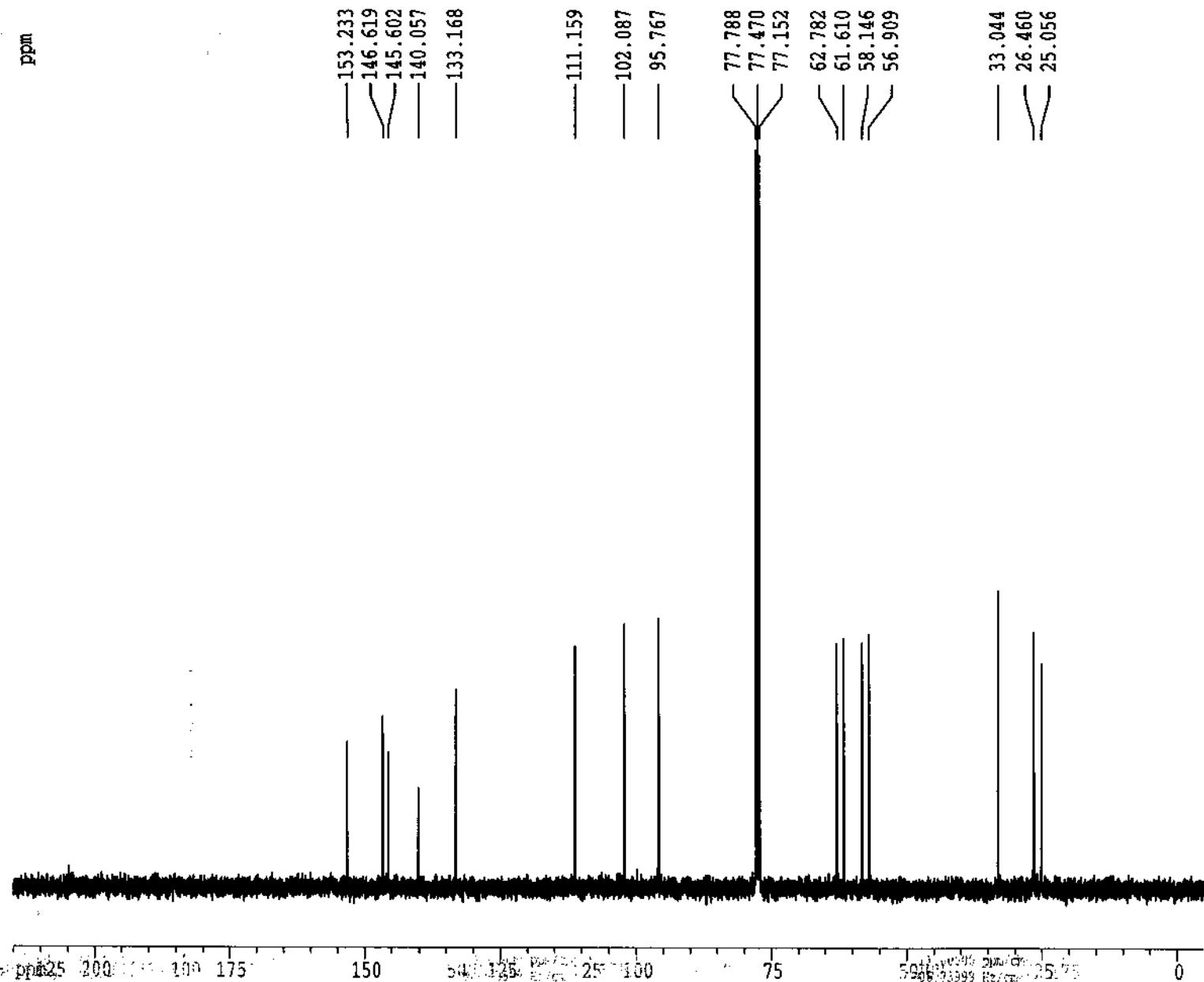
Integral

ppm 10 8 6 4 2 0





ppm



Current Data Parameters
 NAME www12042
 EXPNO 2
 PROCHNO 1

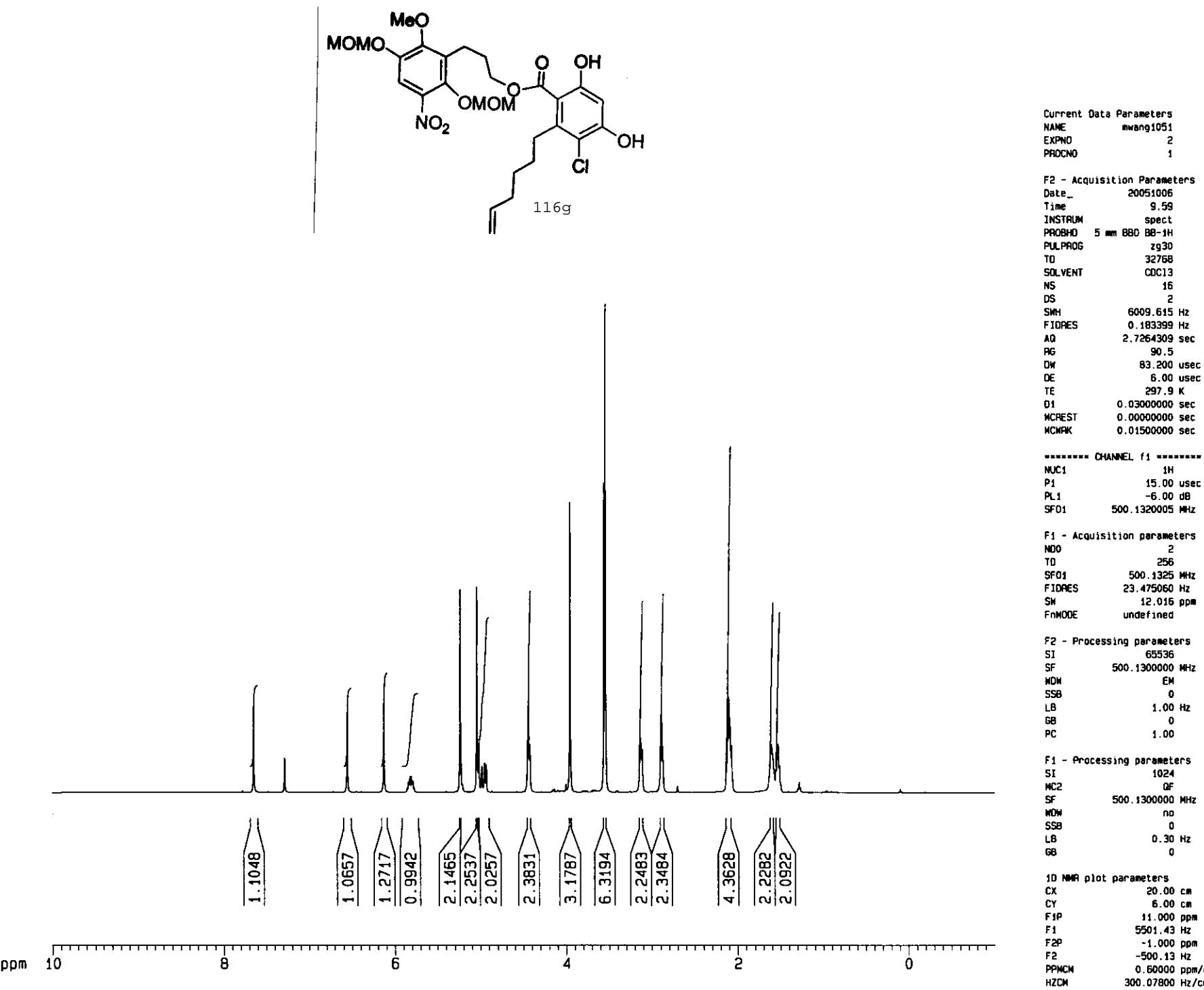
F2 - Acquisition Parameters
 Date_ 20051205
 Time 11.08
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 415
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 3649.1
 DW 21.600 usec
 DE 5.50 usec
 TE 295.2 K
 D1 0.1500001 sec
 d11 0.0300000 sec
 DELTA 0.0500000 sec
 MCREST 0.0000000 sec
 MWKR 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

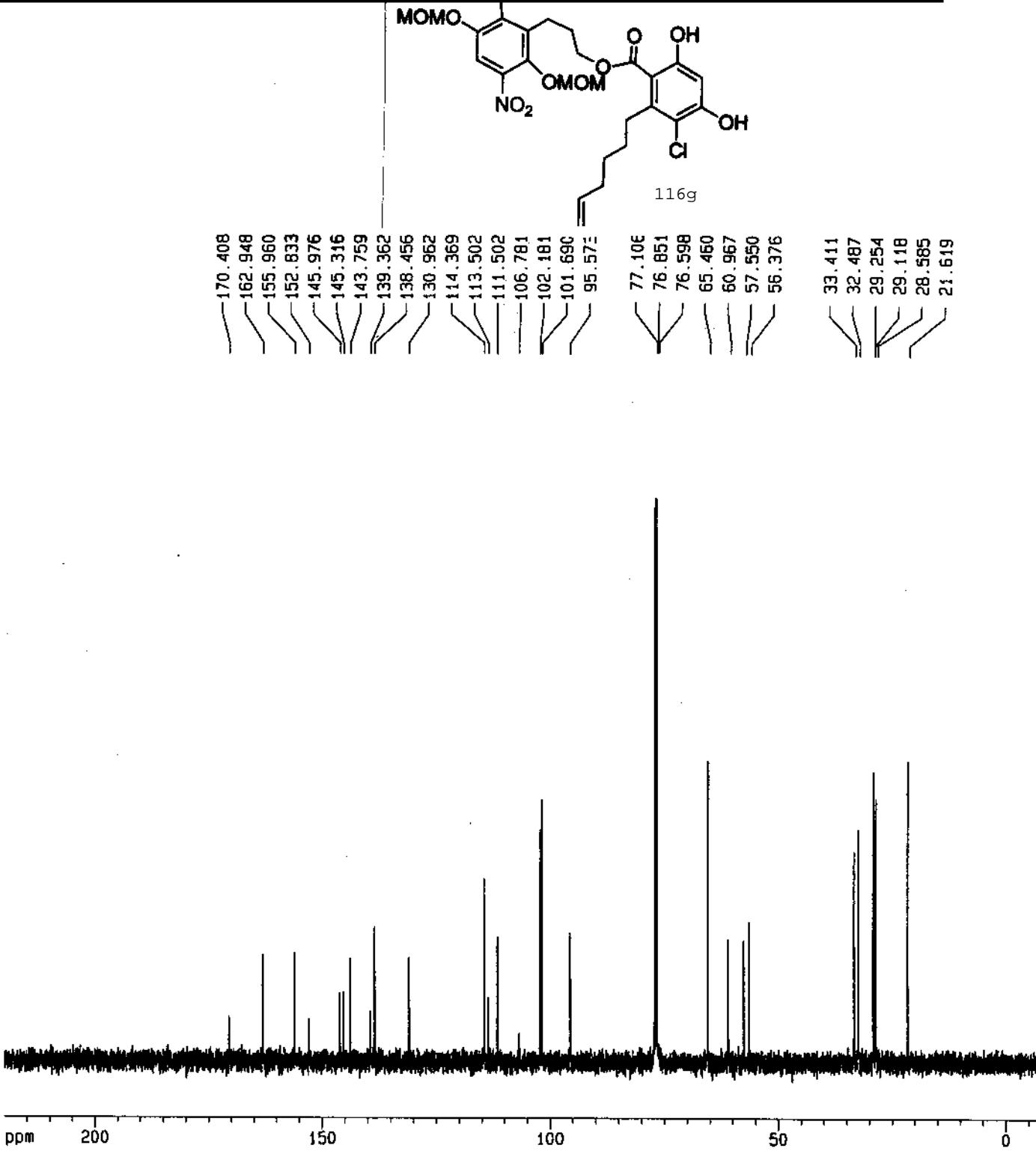
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SP 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPDM 11.00000 ppm, 17.00000 ppm
 HZCM 14.00000 Hz, 17.00000 Hz



ppm



Current Data Parameters

NAME: mwang1061
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters

Date: 20051006
Time: 10:15
INSTRUM: spect
PROBHD: 5 mm BB6 88-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 629
DS: 4
SWH: 31446.544 Hz
FIDRES: 0.479336 Hz
AQ: 1.0420883 sec
RG: 4192
DW: 15.900 usec
DE: 6.00 usec
TE: 300.5 K
D1: 0.1500000 sec
d11: 0.0500000 sec
DELTA: 0.0500000 sec
INCEST: 0.0000000 sec
NCMRK: 0.0150000 sec

***** CHANNEL F1 *****

NUC1: ¹³C
PI: 10.00 usec
PL1: -4.90 dB
SF01: 125.7897360 MHz

***** CHANNEL F2 *****

CPDPPG2: waltz16
NUC2: ¹H
PCPD2: 80.00 usec
PL2: -6.00 dB
PL12: 8.54 dB
PL13: 10.00 dB
SF02: 500.1325000 MHz

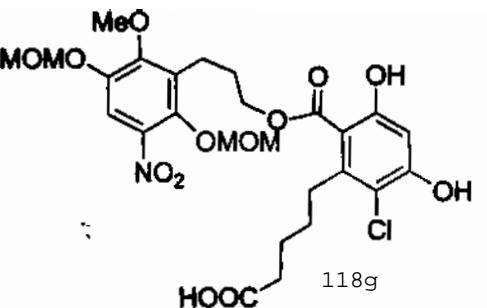
F1 - Acquisition parameters

N00: 2
TD: 256
SF01: 500.1325 MHz
FIDRES: 23.475060 Hz
SW: 12.015 ppm
Fn MODE: undefined

F2 - Processing parameters
SI: 65536
SF: 125.7578000 MHz
MW: EH
MW0: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

F1 - Processing parameters
SI: 1024
NC2: 0F
SF: 500.1300000 MHz
MW: no
MW0: 0
LB: 0.30 Hz
GB: 0

1D NMR plot parameters
CX: 20.00 cm
CY: 10.00 cm
F1P: 242.517 ppm
F1: 30498.43 Hz
F2P: -7.539 ppm
F2: -948.11 Hz
PPM0: 12.50282 ppm/cm
HZCM: 1572.32703 Hz/cm



Current Data Parameters
 NAME wmv109-4
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051010
 Time 21.10
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 203.2
 DW 104.400 usec
 DE 5.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

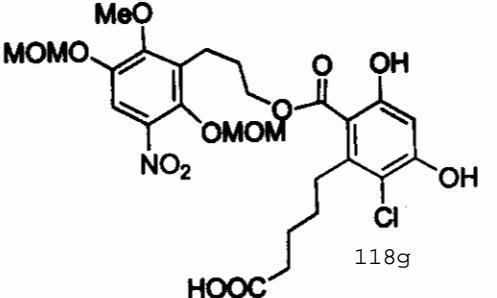
F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

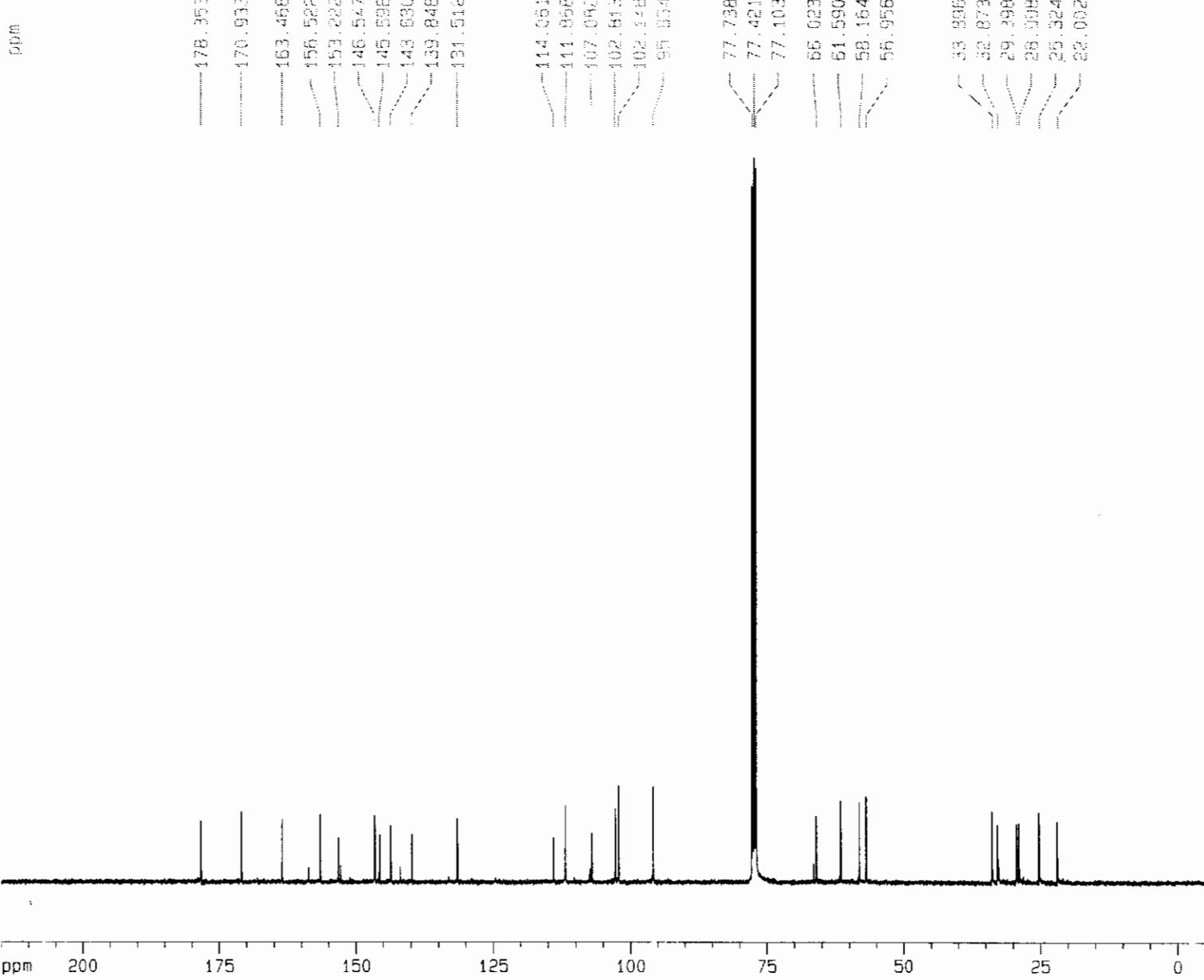
Integral

ppm 10 8 6 4 2 0





ppm



Current Data Parameters

NAME mmw109-4
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20051010
Time 23.04
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 20070
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 7298.2
DW 21.600 usec
DE 5.50 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SF01 100.6232933 MHz

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

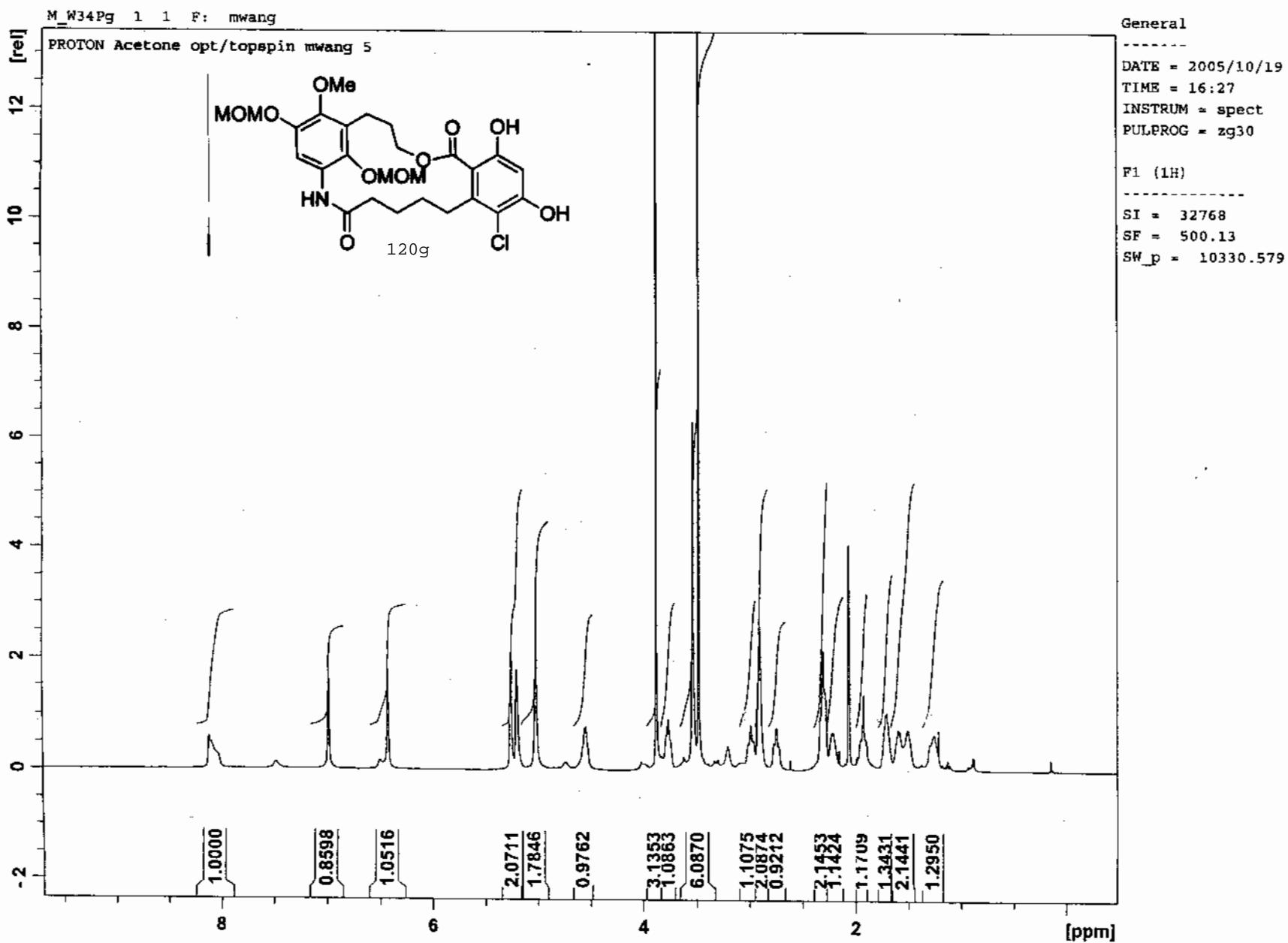
CPDPG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SF02 400.1316005 MHz

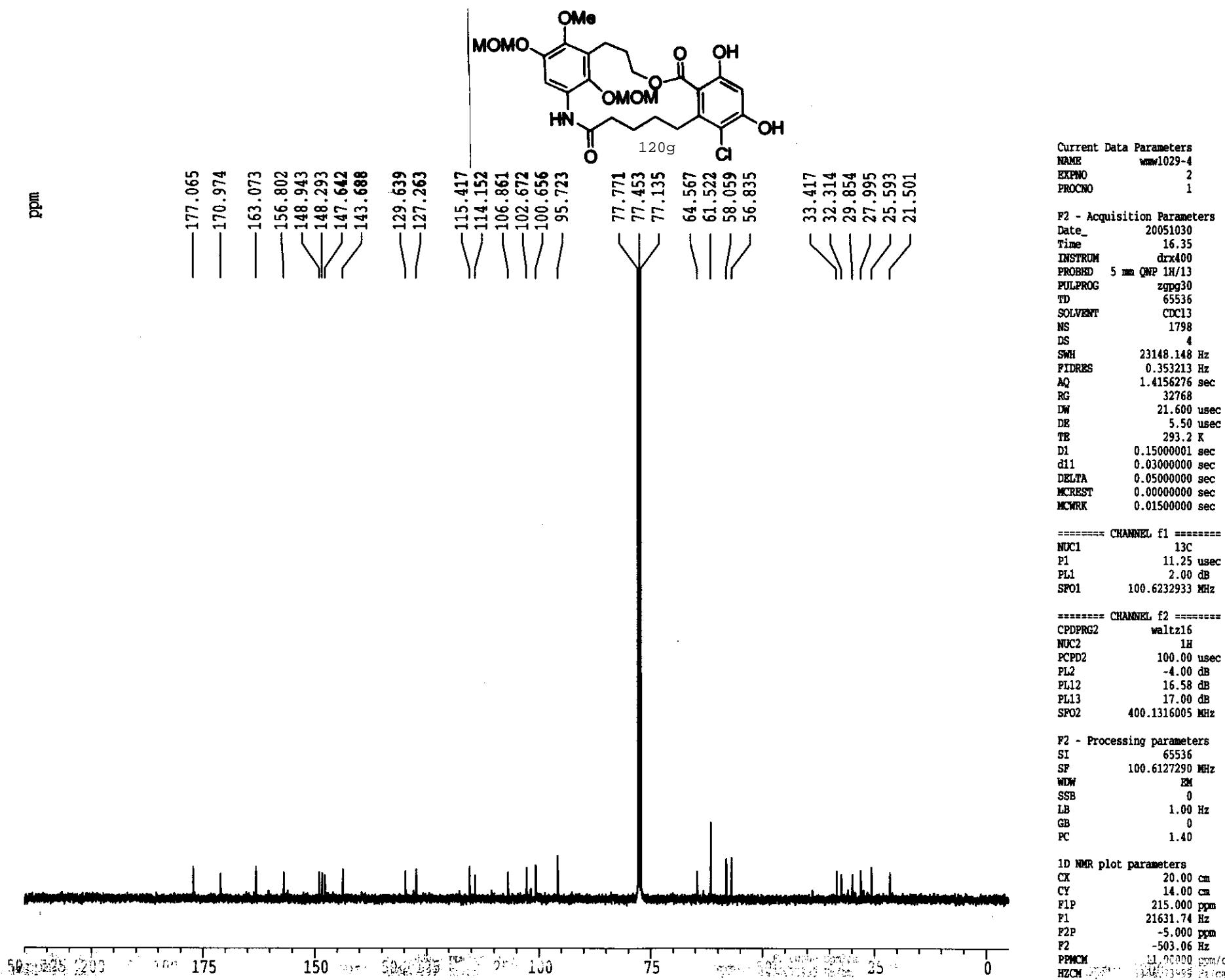
F2 - Processing parameters

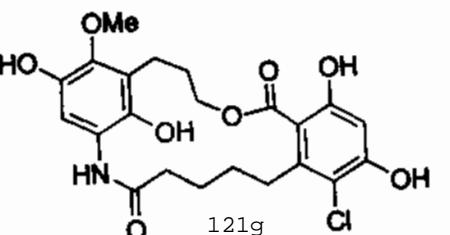
S1 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 12.00 cm
F1P 215.000 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm







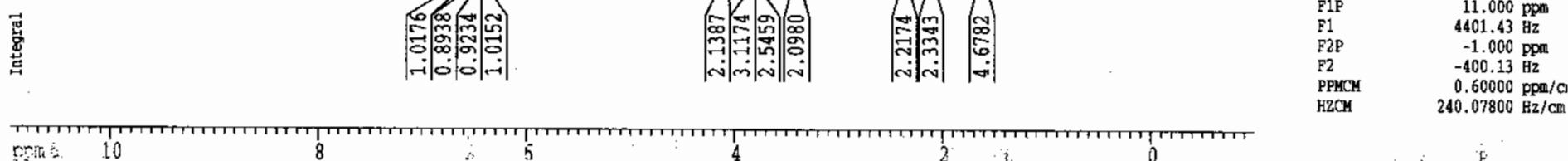
Current Data Parameters
 NAME 2-wmW342
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051109
 Time 15.32
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 645.1
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

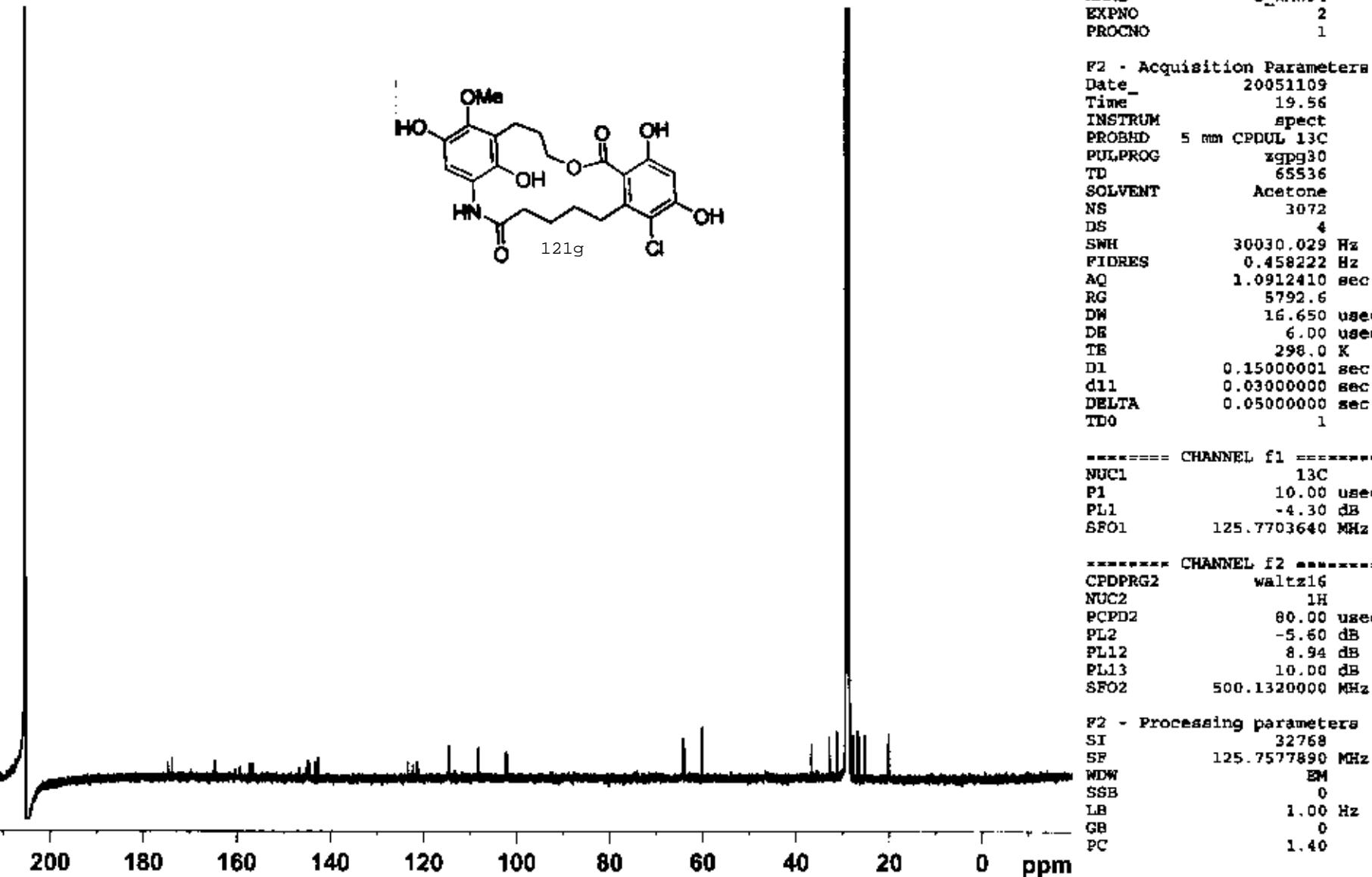
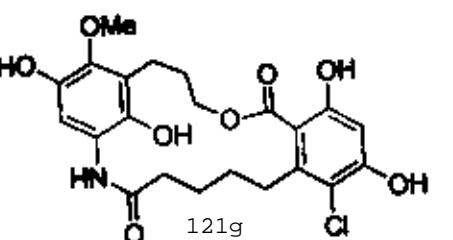
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

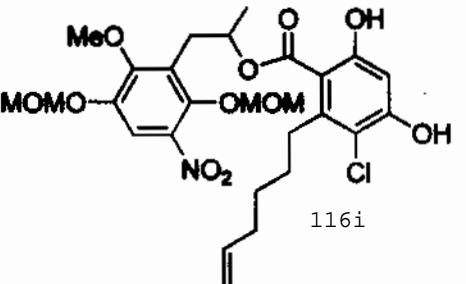
F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm



Macrocycle
Current Data Parameters
NAME 2_WMW34
EXPNO 2
PROCNO 1





Current Data Parameters
 NAME www07131
 EXPNO 1
 PROCNO 1

P2 - Acquisition Parameters
 Date_ 20050713
 Time 20.34
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 143.7
 DW 104.400 usec
 DE 5.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 11.000 ppm
 P1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPWCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral

ppm

10

8

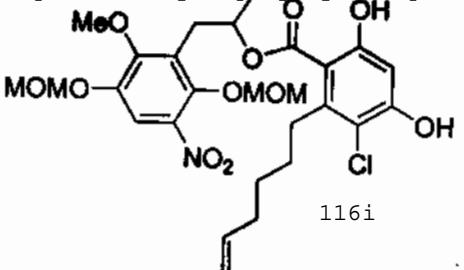
6

4

2

0

7



Current Data Parameters

NAME wnm07131
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050713
Time 20.38
INSTRUM dnx400
PROBHD 5 mm QNP 1H/13C
PULPROG zgppg30
TD 65536
SOLVENT CDCl3
NS 1021
DS 4
SWR 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 1448.2
DW 21.600 usec
DE 5.50 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

***** CHANNEL f2 *****

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

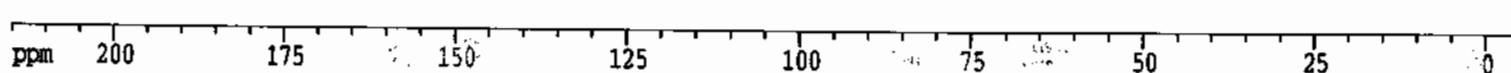
F2 - Processing parameters

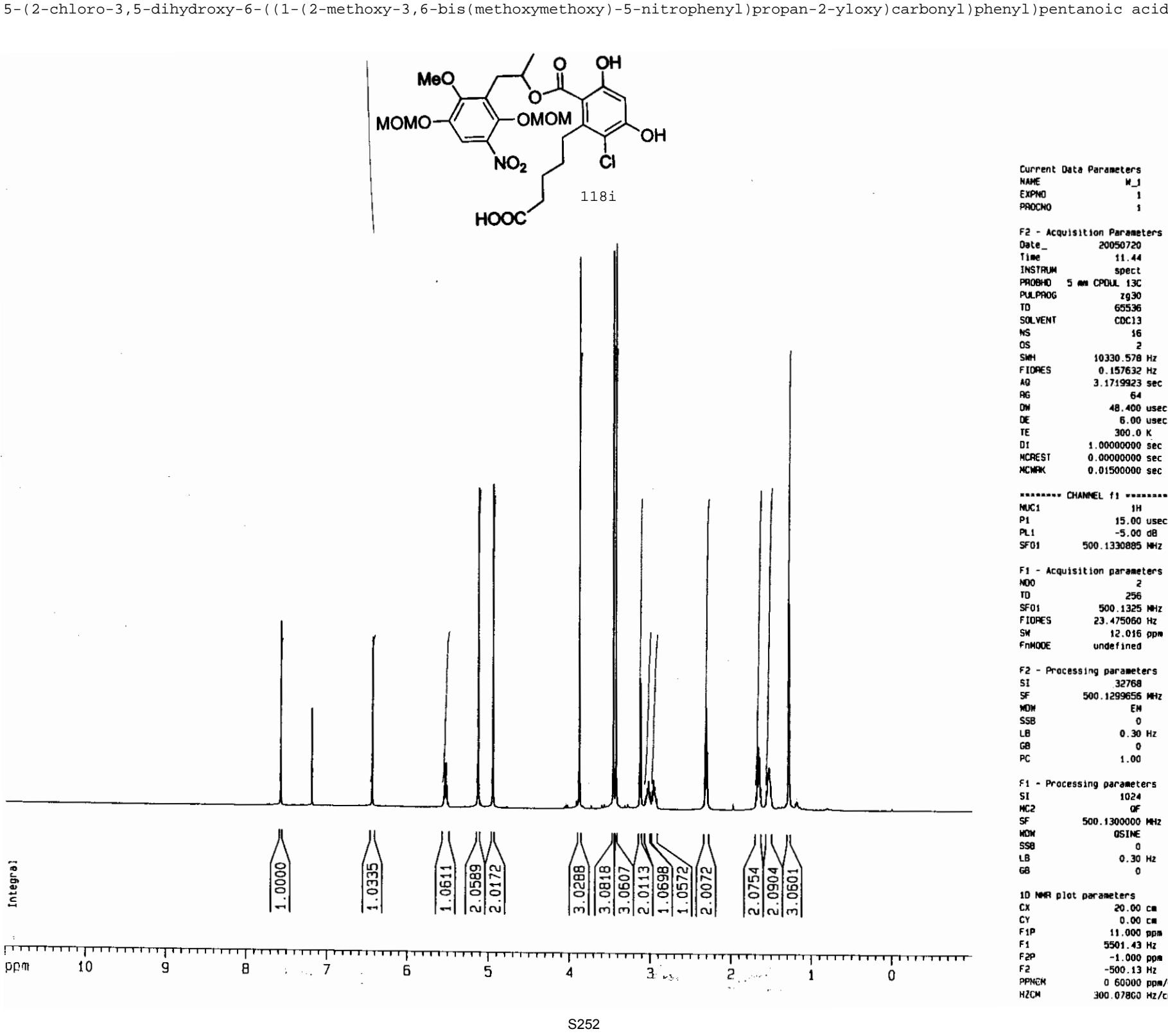
SI 65536
SP 100.6127290 MHz
WDM EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

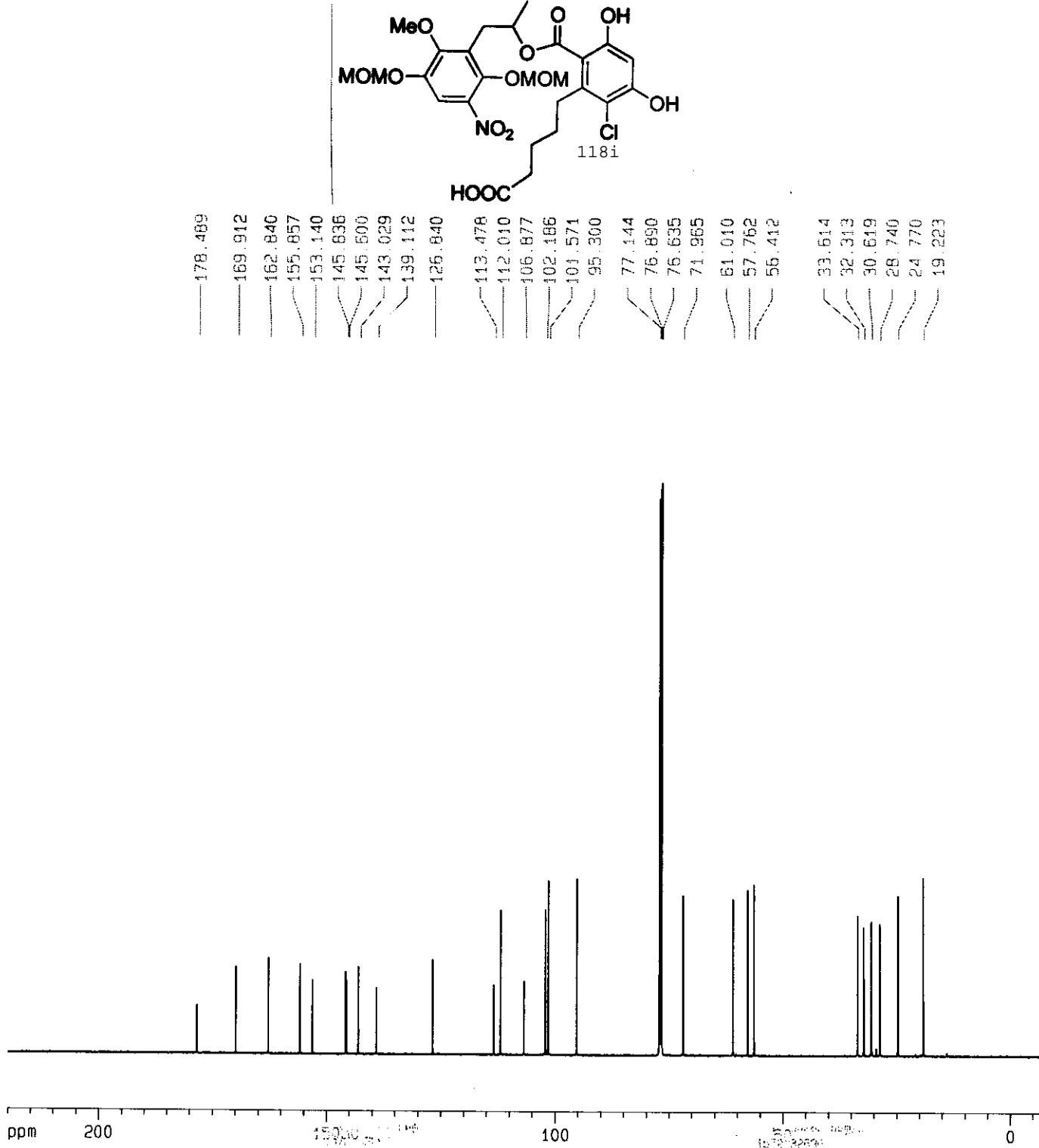
1D NMR plot parameters

CX 20.00 cm
CY 6.00 cm
F1P 215.000 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCH 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm

ppm







Current Data Parameters
 NAME W_1
 EXPNO 2
 PROCN0 1

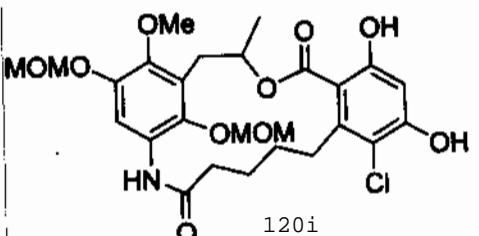
F2 - Acquisition Parameters
 Date 20050720
 Time 12.17
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1536
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420724 sec
 RG 8192
 DW 15.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.1500001 sec
 D11 0.0300000 sec
 DELTA 0.0500000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 -4.90 dB
 SF01 125.7697360 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 9.54 dB
 PL13 10.00 dB
 SF02 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 242.517 ppm
 F1 30498.43 Hz
 F2P -7.539 ppm
 F2 -948.11 Hz
 PPMLN 12.50292 ppm/cm
 HZCM 12.50292 Hz/cm



Current Data Parameters
 NAME mwang 2
 EXPNO 11
 PROCNU 1

F2 - Acquisition Parameters
 Date_ 20050729
 Time 10.33
 INSTRUM spect
 PROBHD 5 mm CPOUL 13C
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 64
 DW 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 DT 1.0000000 sec
 MCPLST 0.0000000 sec
 MCWAK 0.0150000 sec

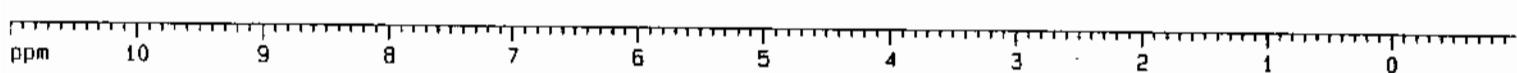
----- CHANNEL f1 -----
 NUC1 1H
 PI 15.00 usec
 PL1 -5.00 dB
 SF01 500.1330685 MHz

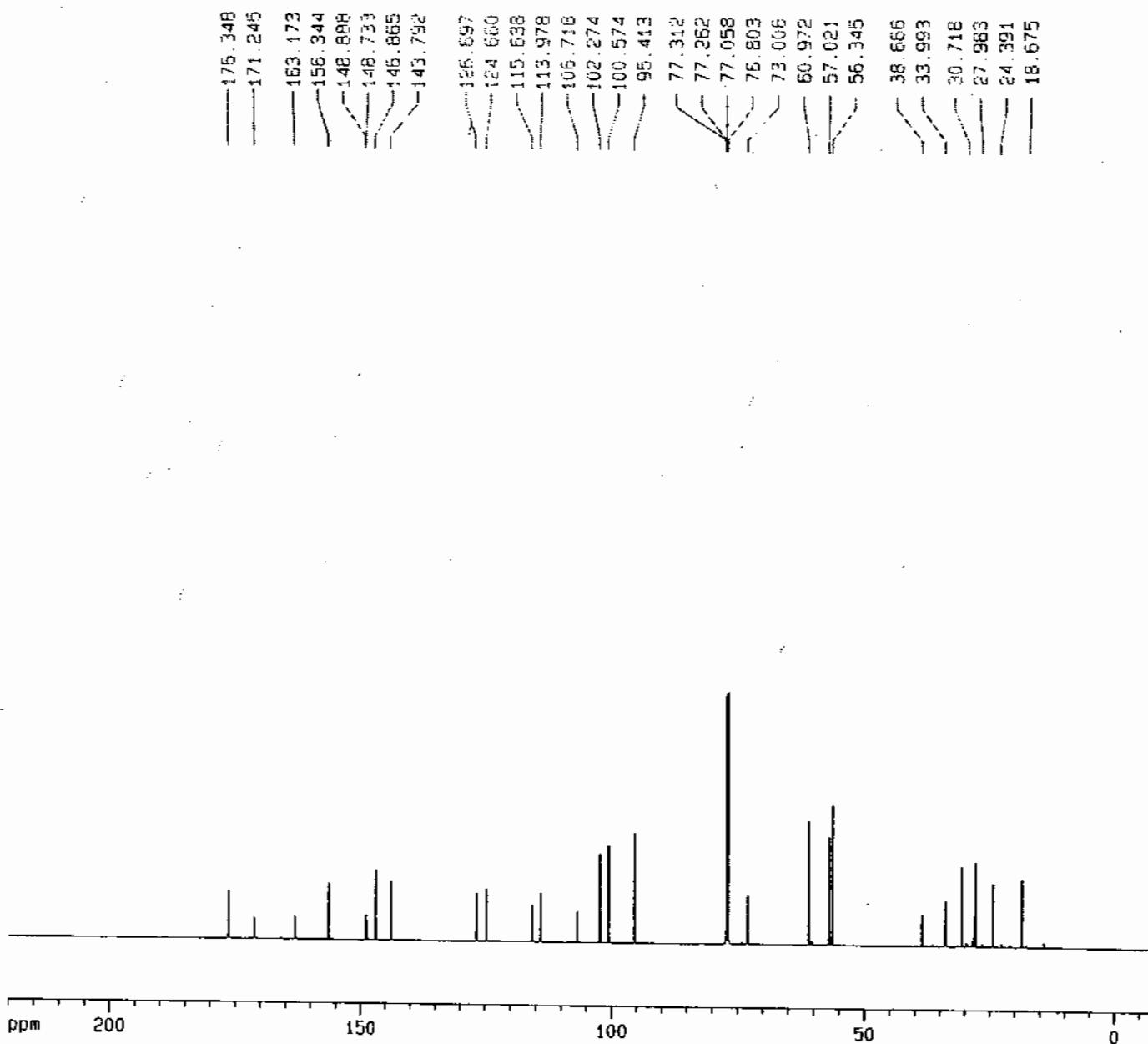
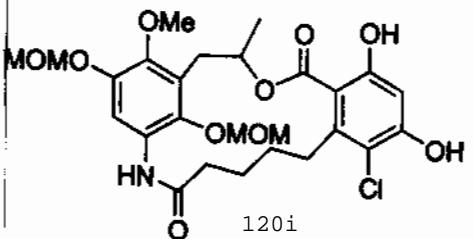
F2 - Processing parameters
 SI 32768
 SF 500.1300425 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 NC2 0F
 SF 500.1300000 MHz
 WDN QSINE
 SSB 0
 LB 0.30 Hz
 GB 0

1D NMR plot parameters
 CX 20.00 cm
 CY 20.00 cm
 F1P 11.000 ppm
 F1 5501.43 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCN 0.60000 ppm/
 HZCM 300.07803 Hz/cm

Integral





Current Data Parameters
 NAME Wang2
 EXPNO 12
 PROCHD 1

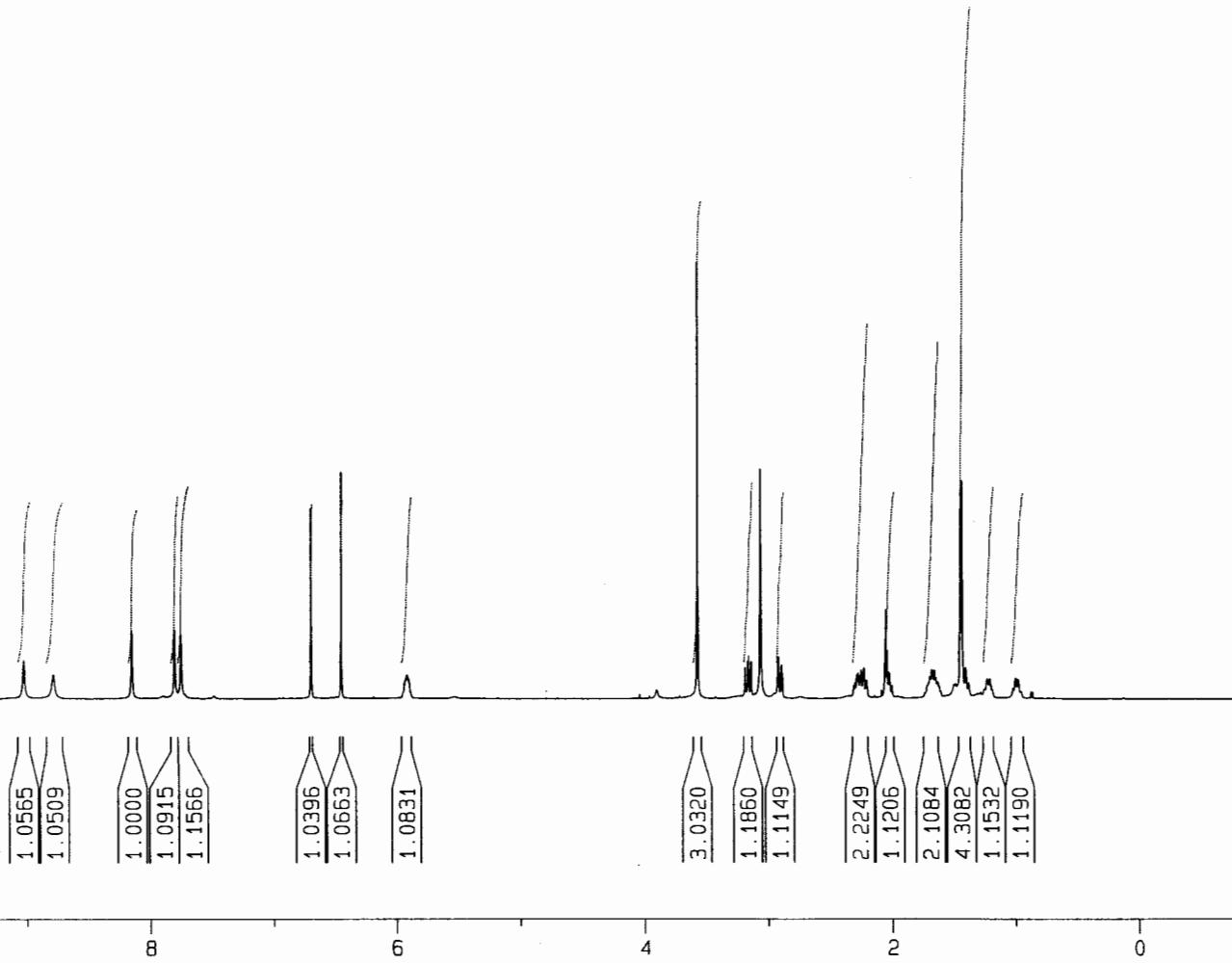
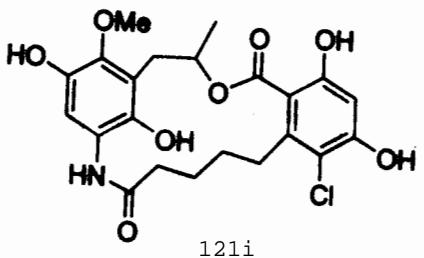
F2 - Acquisition Parameters
 Date 20050729
 Time 11.08
 INSTRUM spect
 PROBHD 5 mm CPOUL f3C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1664
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420724 sec
 RG 8192
 DW 15.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCPREST 0.00000000 sec
 MCWRFK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 10.00 usec
 PL1 -4.90 dB
 SF01 125.7697360 MHz

***** CHANNEL f2 *****
 CPDPG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -5.00 dB
 PL12 9.54 dB
 PL13 10.00 dB
 SF02 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577890 MHz
 MW EM
 SSB 0
 LB 1.00 Hz
 BB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 242.517 ppm
 F1 30498.43 Hz
 F2P -7.539 ppm
 F2 -948.11 Hz
 PPWCH 12.50282 ppm/cm
 HZCM 1572.32690 Hz/cm



Current Data Parameters
 NAME WMWHQ24i
 EXPNO 11
 PROCNO 1

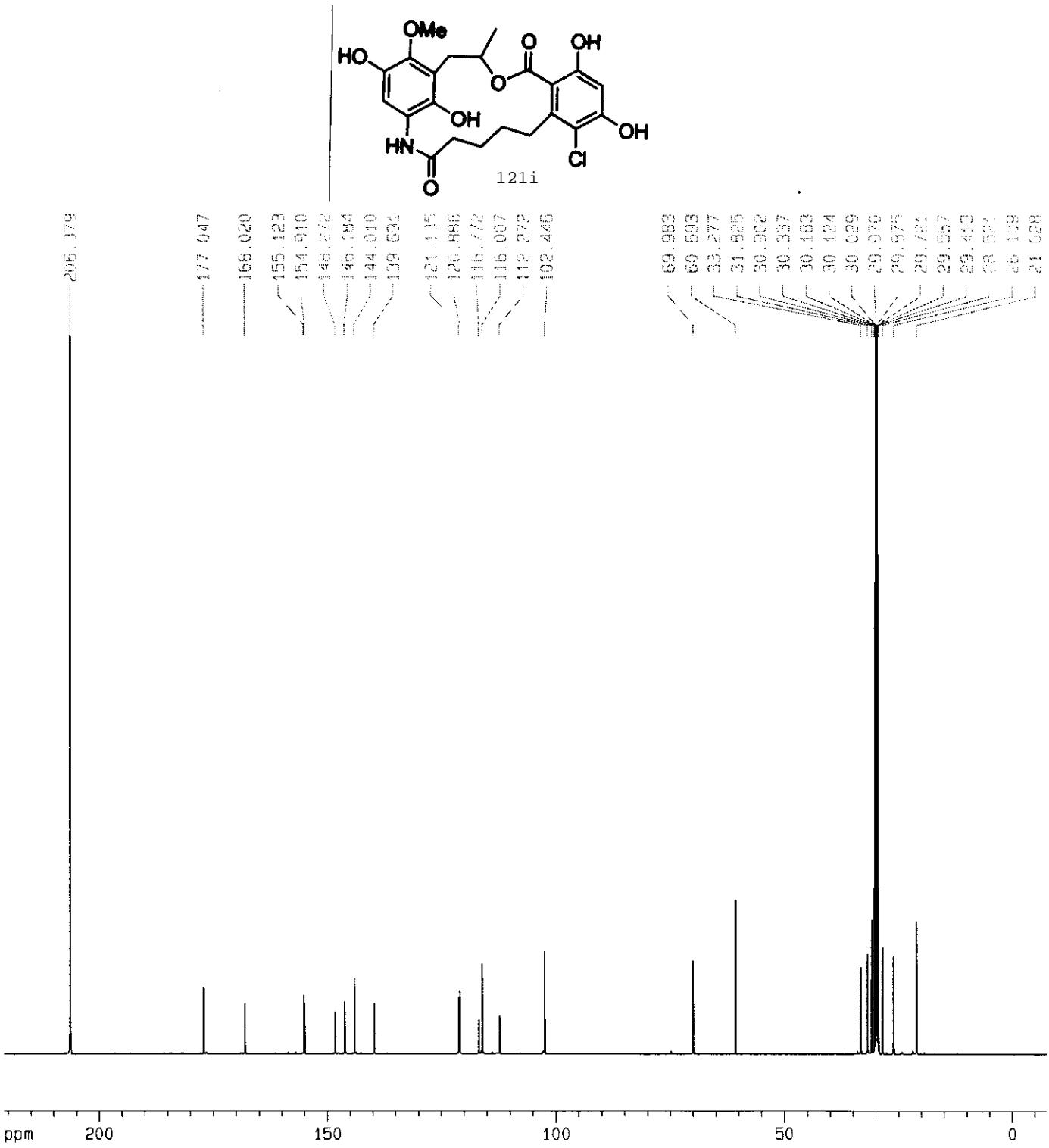
F2 - Acquisition Parameters
 Date_ 20050802
 Time 15.26
 INSTRUM spect
 PROBHD 5 mm CPDUL 13C
 PULPROG zg30
 TD 65536
 SOLVENT Aceton
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 64
 DW 40.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -5.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300087 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 500.1300000 MHz
 WDW QSINE
 SSB 0
 LB 0.30 Hz
 GB 0

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 10.979 ppm
 F1 5490.98 Hz
 F2P -0.781 ppm
 F2 -390.59 Hz
 PPVCM 0.58800 ppm/cm
 HZCM 294.07846 Hz/cm



Current Data Parameters

NAME WMNHQ241
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters

Date 20050802
Time 15.59
INSTRUM spect
PROBHD 5 mm CPOUL 13C
PULPROG zgpg30
TD 65536
SOLVENT Aceton
NS 1536
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420724 sec
RG 8192
DW 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 ¹³C
P1 10.00 usec
PL1 -4.90 dB
SF01 125.7697360 MHz

***** CHANNEL f2 *****

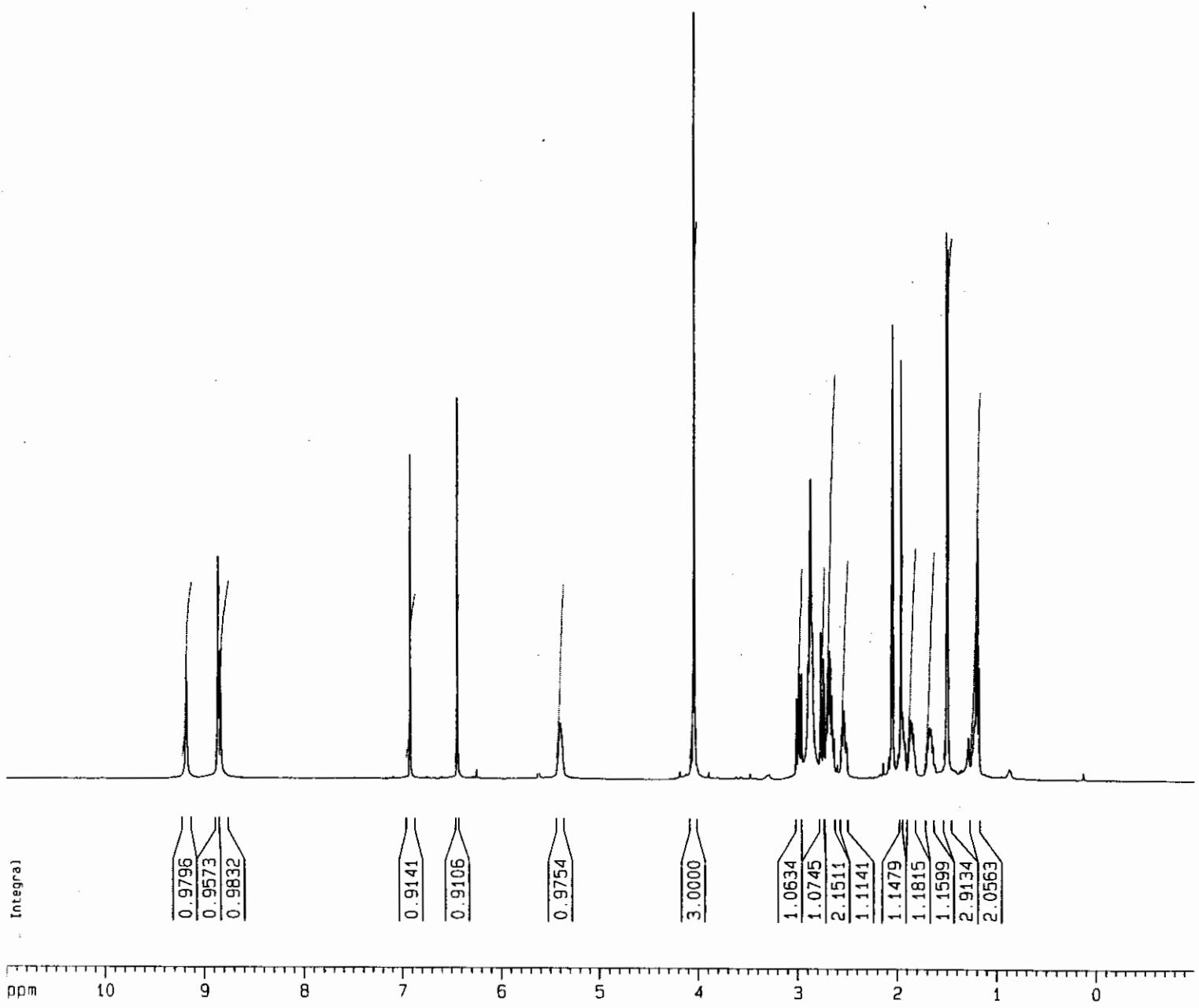
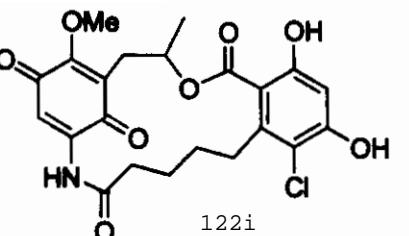
CPDPG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 9.54 dB
PL13 10.00 dB
SF02 500.1325000 MHz

F2 - Processing parameters

SI 65536
SF 125.7576758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 0.00 cm
F1P 242.517 ppm
F1 30498.40 Hz
F2P -7.539 ppm
F2 -948.11 Hz
PPMCM 12.50282 ppm/cm
HZCM 1572.32544 Hz/cm



Current Data Parameters
 NAME WMHQ24i
 EXPNO 11
 PROCNO 1

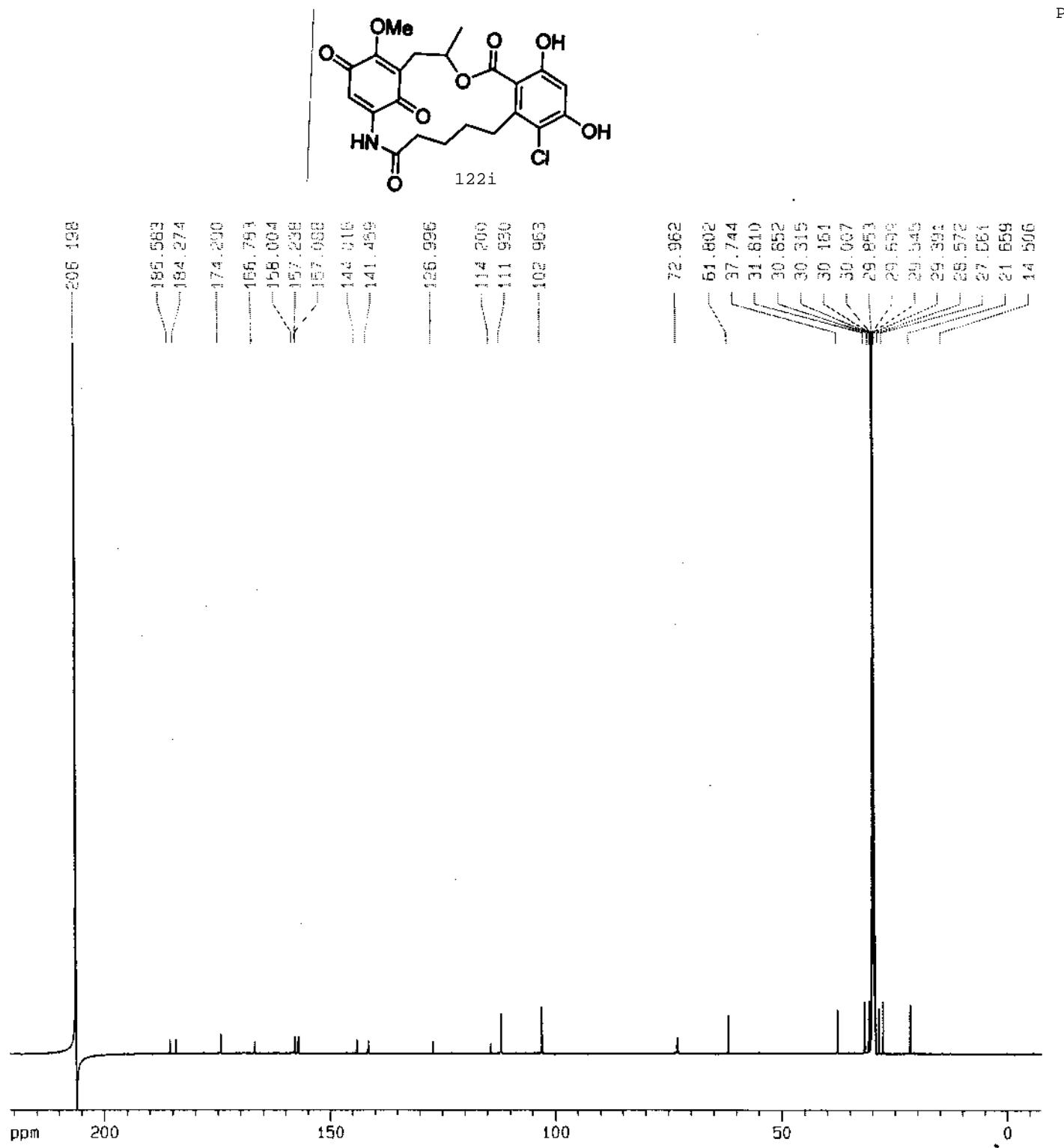
F2 - Acquisition Parameters
 Date_ 20050802
 Time 16.47
 INSTRUM spect
 PROBHD 5 mm CPOUL 13C
 PULPROG zg30
 TD 65536
 SOLVENT Aceton
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 64
 DW 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 15.00 usec
 PL1 -5.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300106 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 0F
 SF 500.1300000 MHz
 WDW GSINE
 SSB 0
 LB 0.30 Hz
 GB 0

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 11.000 ppm
 F1 5501.43 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCH 0.60000 ppm/
 HZCM 300.07800 Hz/cr



Current Data Parameters

NAME MMWQ241
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050802
Time 17.20
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT Aceton
NS 1536
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420724 sec
RG 8192
DW 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 0.1500001 sec
d11 0.0300000 sec
DELTA 0.0500000 sec
MCREST 0.0000000 sec
MCWAIR 0.0150000 sec

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

NUC1 13C
P1 10.00 usec
PL1 -4.90 dB
SF01 125.7697360 MHz

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

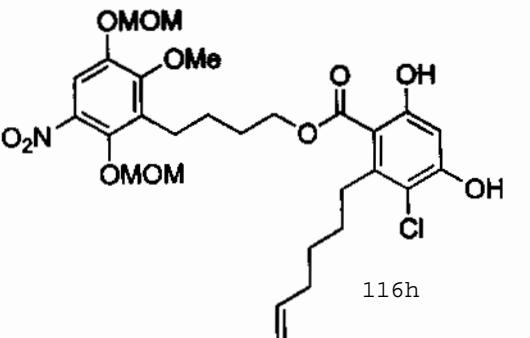
CPDPFG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 9.54 dB
PL13 10.00 dB
SF02 500.1325000 MHz

F2 - Processing parameters

SI 65536
SF 125.7576758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 30.00 cm
F1P 242.517 ppm
F1 30498.40 Hz
F2P -7.539 ppm
F2 -946.11 Hz
PPMCH 12.50282 ppm/cm
HZCM 1572.32544 Hz/cm



Current Data Parameters
 NAME wmw12043
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20051205
 Time 15.52
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 203.2
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

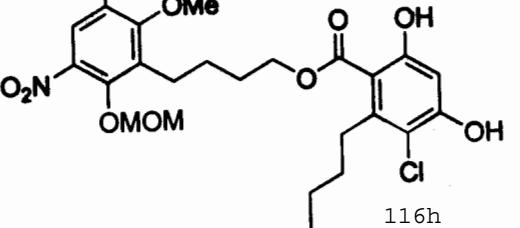
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SP 400.1300091 MHz
 WDW EM
 SSE 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 P2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral





171.283

163.576
156.456
153.169
146.599
145.723
144.217
139.983
139.023
132.401115.043
114.013
111.380
107.009
102.619
102.206
95.77577.757
77.439
77.122
66.072
61.581
58.171
56.94734.043
33.210
29.654
28.918
26.668
24.958

Current Data Parameters

NAME wnw12043
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date 20051205
Time 16.03
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpp30
TD 65536
SOLVENT CDCl3
NS 1483
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 2048
DW 21.600 usec
DE 5.50 usec
TE 294.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SF01 100.6232933 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SF02 400.1316005 MHz

F2 - Processing parameters

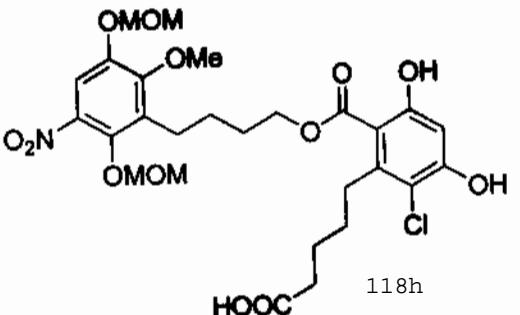
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 20.00 cm
F1P 215.00 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
PPMHC 1106.73999 Hz/cm

ppm

200 175 150 125 100 75 50 25 0



Current Data Parameters
 NAME wmm12132
 EXPNO 1
 PROCNO 1

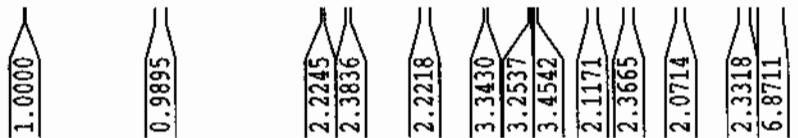
F2 - Acquisition Parameters
 Date 20051216
 Time 9.32
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 256
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

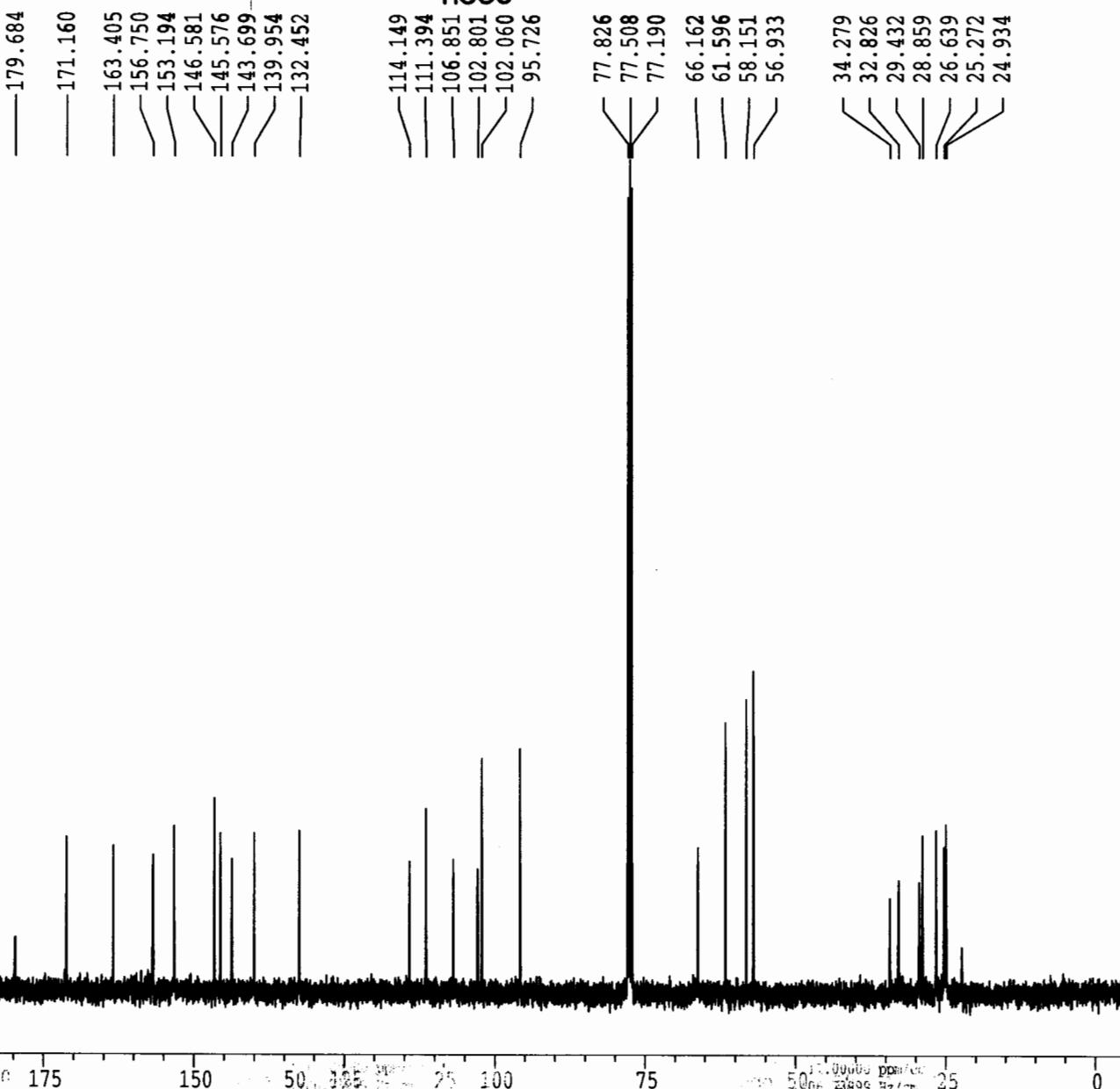
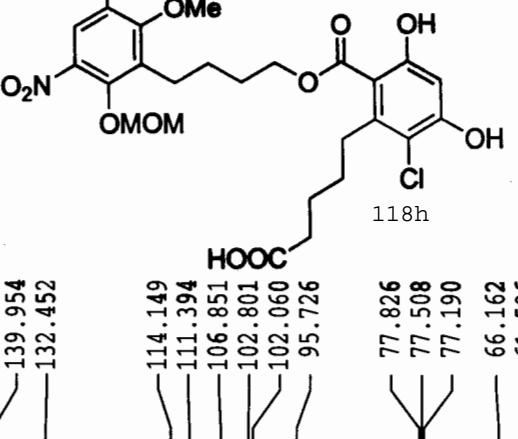
1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm

Integral



ppm

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



Current Data Parameters
 NAME wmw12133
 EXPNO 2
 PROCNO 1

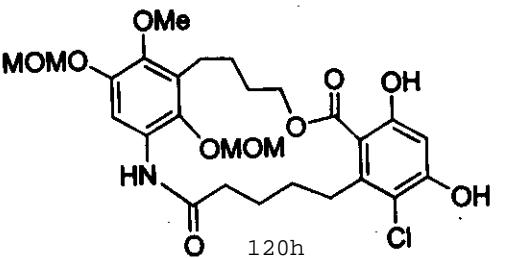
F2 - Acquisition Parameters
 Date_ 20051216
 Time 10.45
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 343
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 3251
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.1500001 sec
 d11 0.0300000 sec
 DELTA 0.0500000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -4.00 dB
 PL12 16.58 dB
 PL13 17.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SP 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 215.000 ppm
 F1 21631.74 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/
 HZCM 9.34 / 1106.2499 Hz/cm



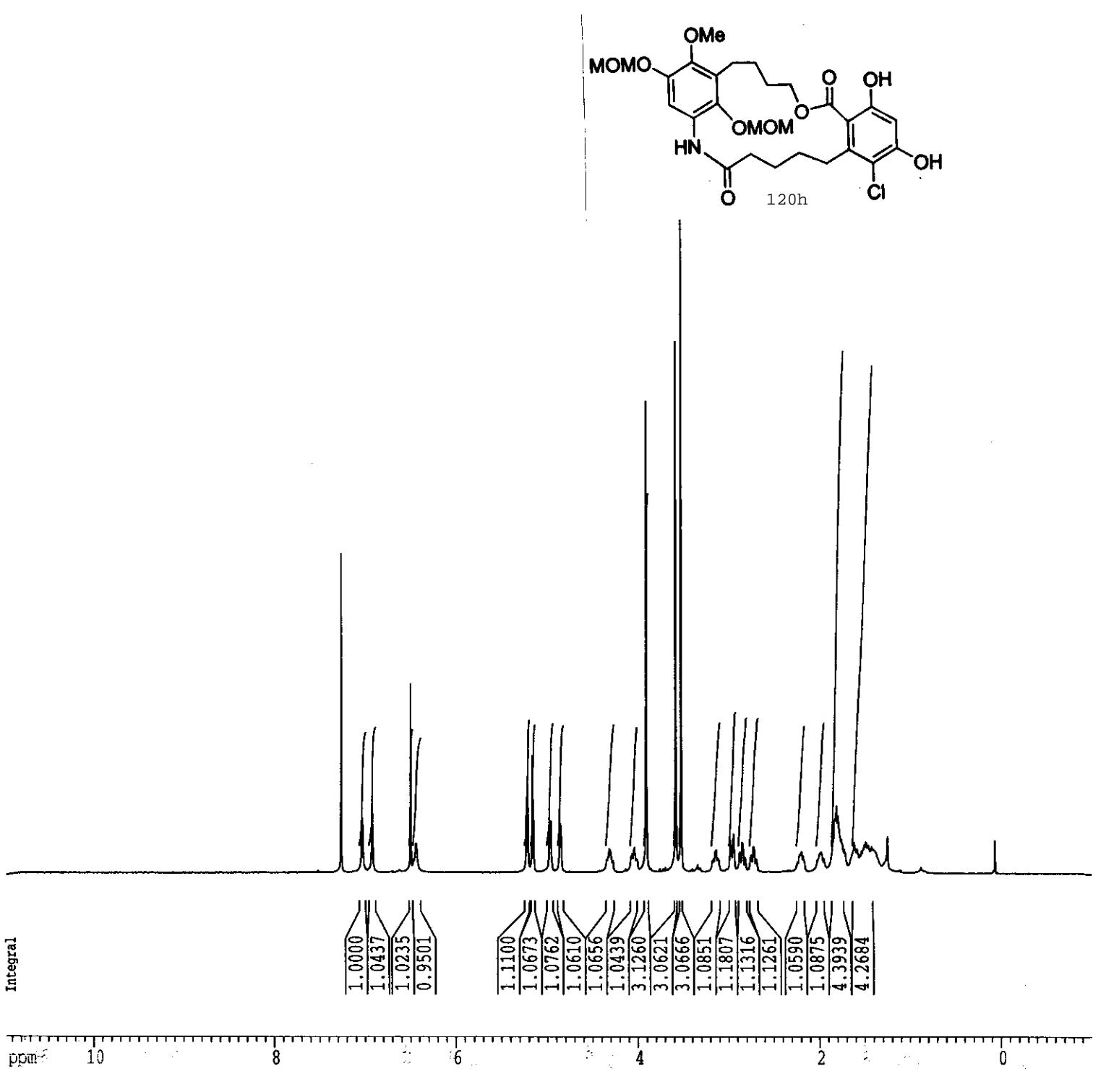
Current Data Parameters
 NAME wmm12212
 EXPNO 1
 PROCNO 1

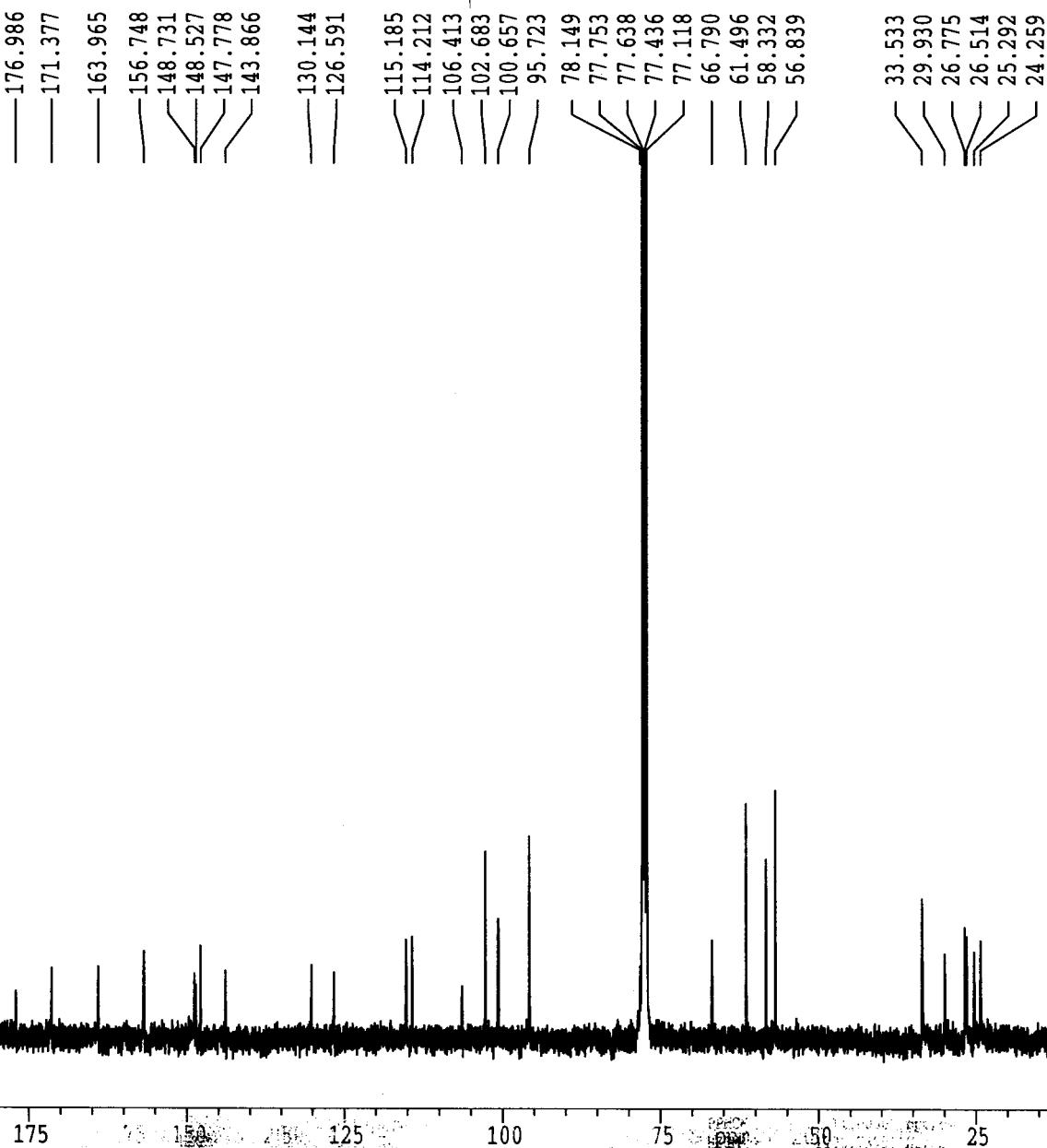
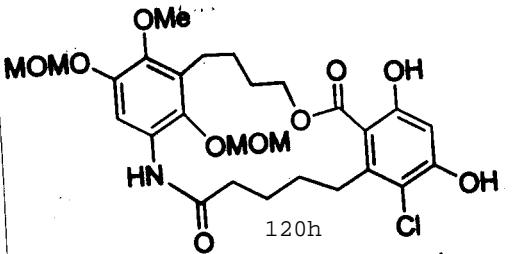
F2 - Acquisition Parameters
 Date_ 20051221
 Time 20.13
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 456.1
 DW 104.400 usec
 DE 5.50 usec
 TE 293.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 11.000 ppm
 F1 4401.43 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 240.07800 Hz/cm





Current Data Parameters

NAME www12212
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date 20051221
Time 20.41
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgppg30
TD 65536
SOLVENT CDCl3
NS 23552
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 2048
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELT1A 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

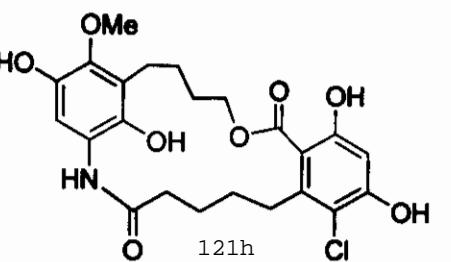
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 100.00 cm
F1P 215.000 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
PPMFT 1106.73999 Hz/cm



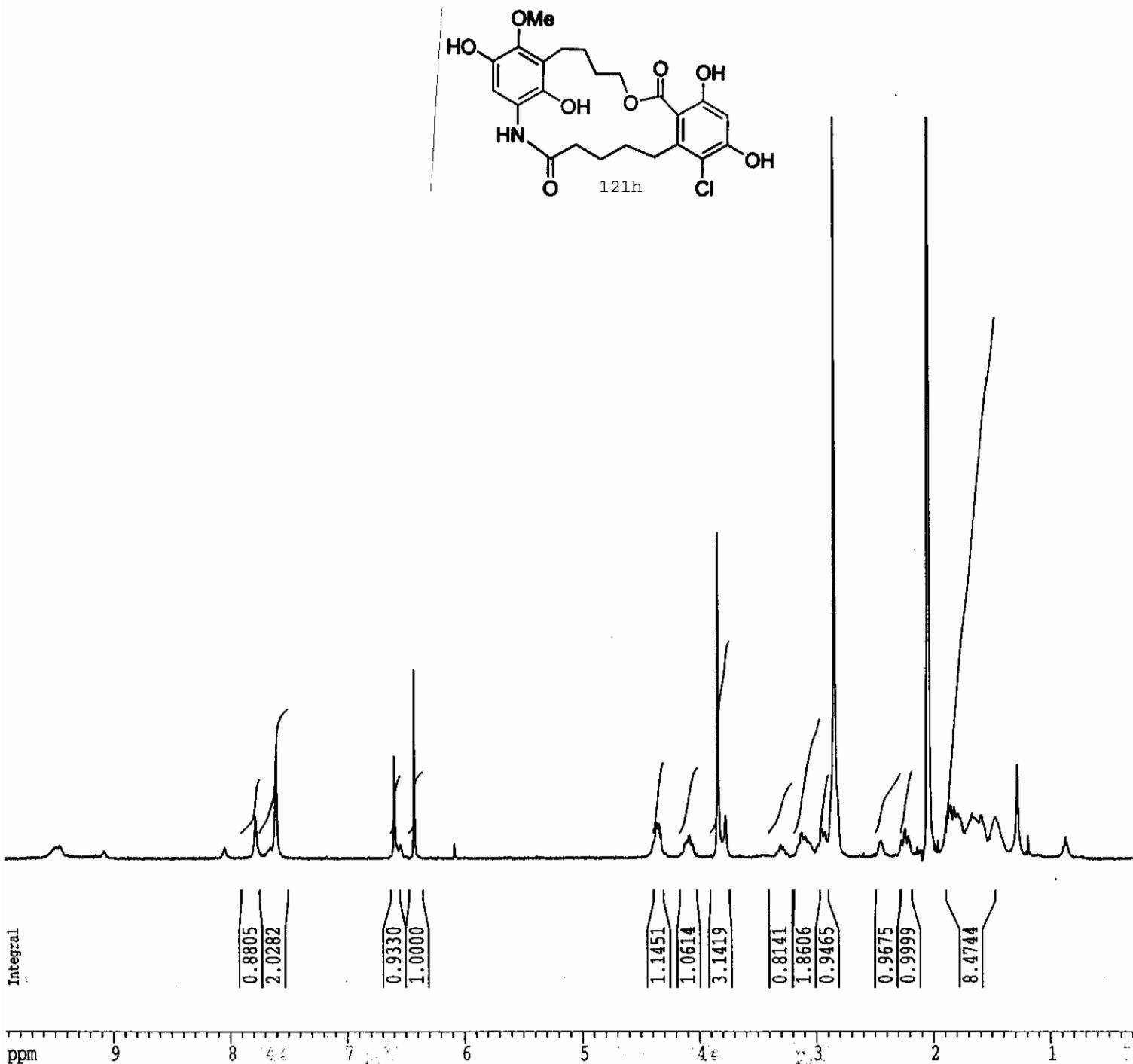
Current Data Parameters
 NAME wmw601042
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060104
 Time 15.10
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT Aceton
 NS 46
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 645.1
 DW 104.400 usec
 DE 5.50 usec
 TE 294.2 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 24.00 cm
 F1P 9.927 ppm
 F1 3972.10 Hz
 F2P 0.239 ppm
 F2 95.78 Hz
 PPMCM 0.48438 ppm/cm
 HZCM 193.81583 Hz/cm



mwang_w_0601 2 1 /opt/topspin sarah

