

Radester, A Novel Inhibitor of the Hsp90 Protein Folding Machinery

Gang Shen and Brian S. J. Blagg^{*}

*Department of Medicinal Chemistry and the Center for Protein Structure and Function
1251 Wescoe Hall Drive, Malott 4070, The University of Kansas,
Lawrence, KS 66045-7563*

bblagg@ku.edu

Supplementary Information

Spectra for Compounds

Current Data Parameters
 NAME sg224
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20031202
 Time 22.32
 INSTRUM drx400
 PROBHD 5 mm Multinuc1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SNH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 161.3
 DM 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

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

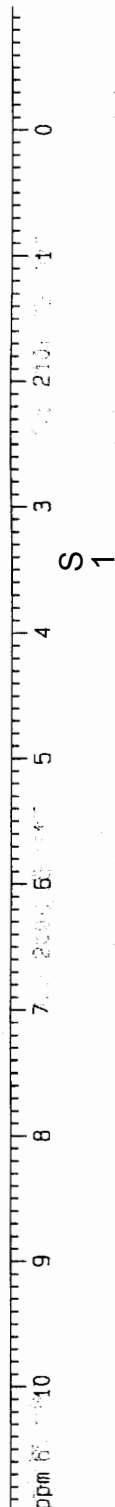
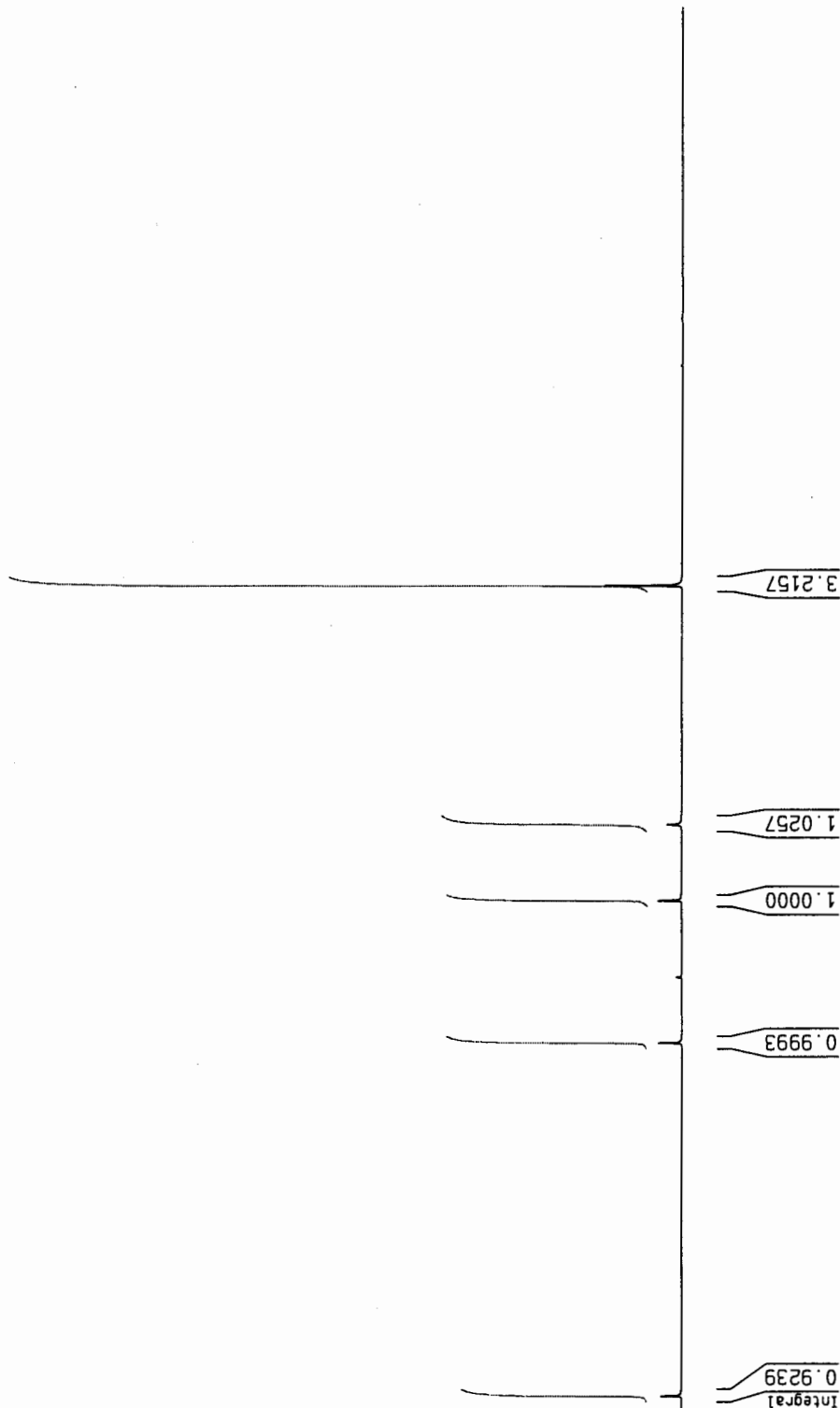
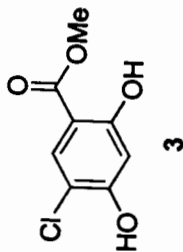
NUC1 1H
 P1 7.70 usec
 PL1 -6.00 dB
 SF01 400.1320007 MHz

F2 - Processing parameters

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

1D NMR plot parameters

CX 20.00 cm
 CY 1.10 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 sg225
 EXPNO 2
 PROCNO 1

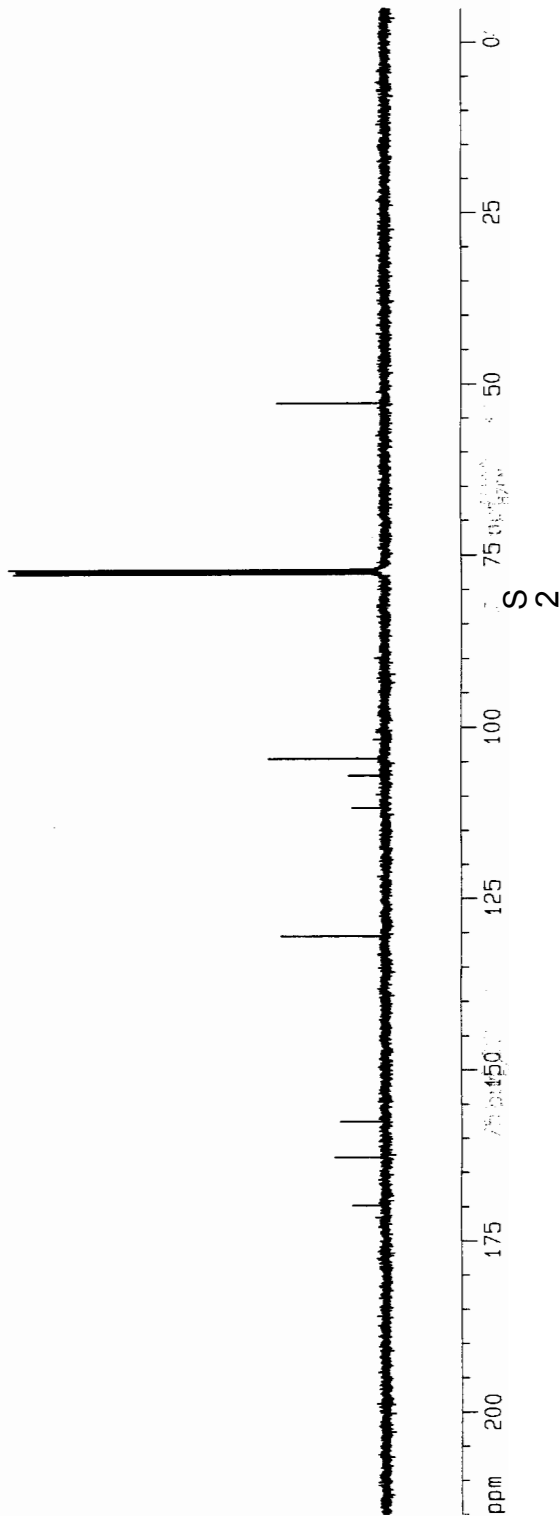
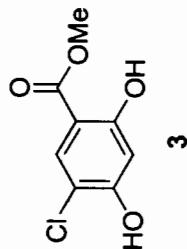
F2 - Acquisition Parameters
 Date_ 20031202
 Time 22.34
 INSTRUM drx400
 PROBD 5 mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 263
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DM 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

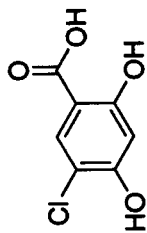
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPOPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SFD2 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

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





4

Current Data Parameters
NAME sg229
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

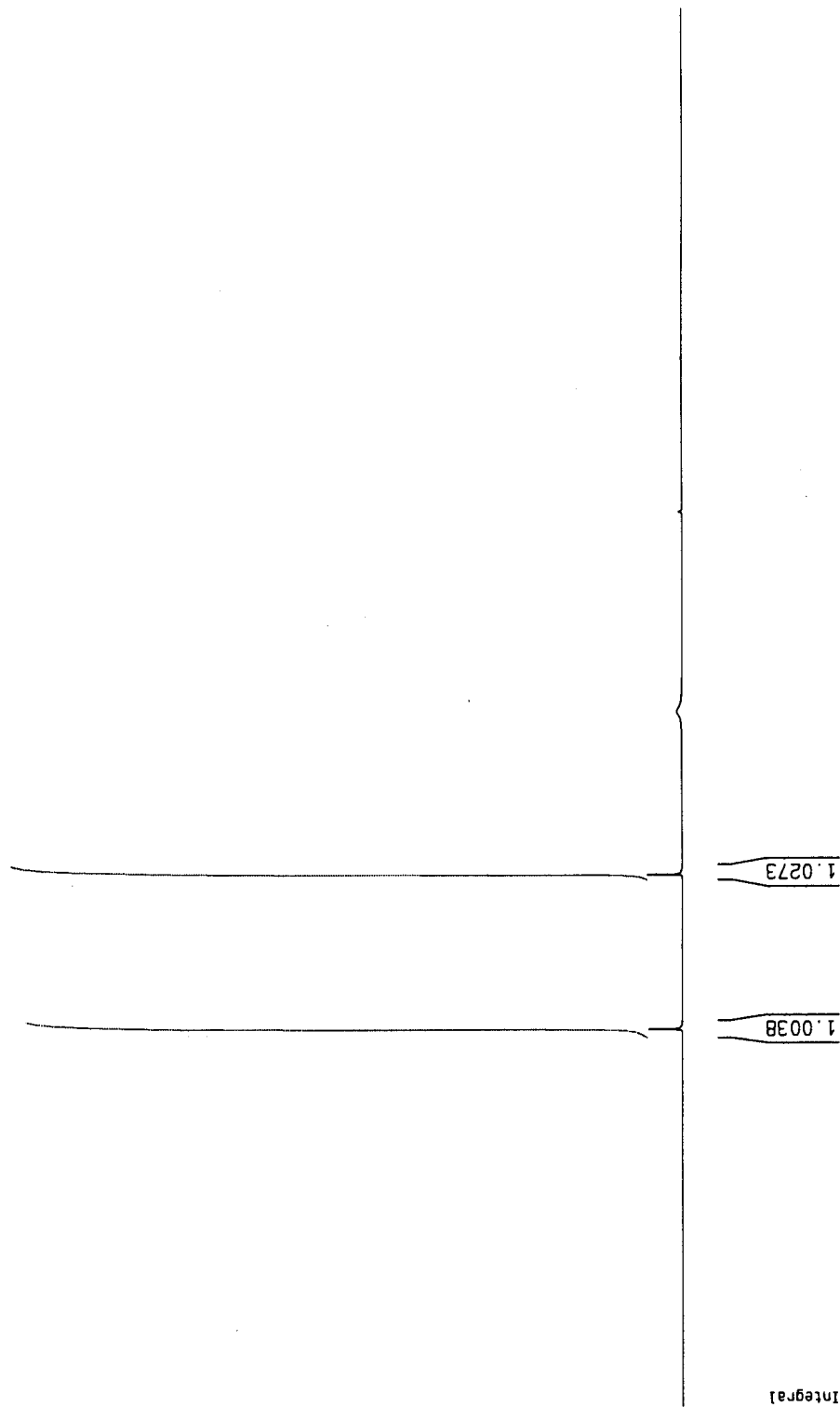
Date_ 20031202
Time 23.32
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 114
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

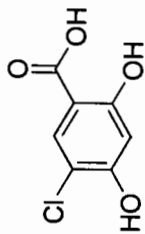
===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
SF01 400.1320007 MHz

F2 - Processing parameters

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

1D NMR plot parameters
CX 20.00 cm
CY 0.50 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





4

Current Data Parameters
NAME sg228
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

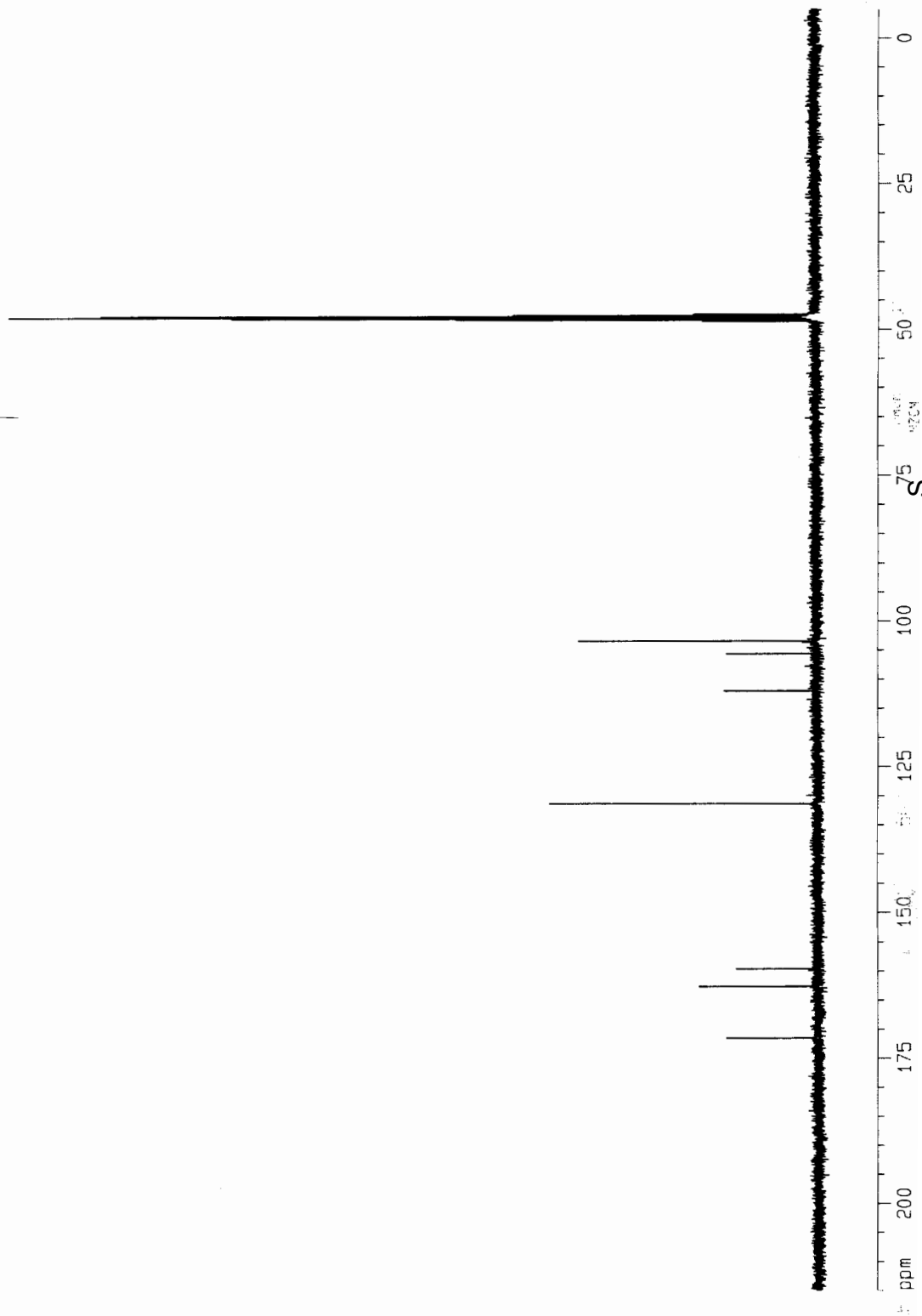
Date_ 20031202
Time 23.30
INSTRUM drx400
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT MeOH
NS 93
DS 2
SWH 231.48.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 812.7
DM 21.600 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.0002000 sec

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

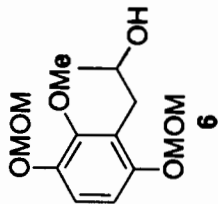
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 18.00 dB
PL13 18.00 dB
SF02 400.1316005 MHz

F2 - Processing parameters
S1 32768
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
PPMCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm



S 4



Current Data Parameters
 NAME sg420
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050305
 Time 16.47
 INSTRUM drx400
 PROBD 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 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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

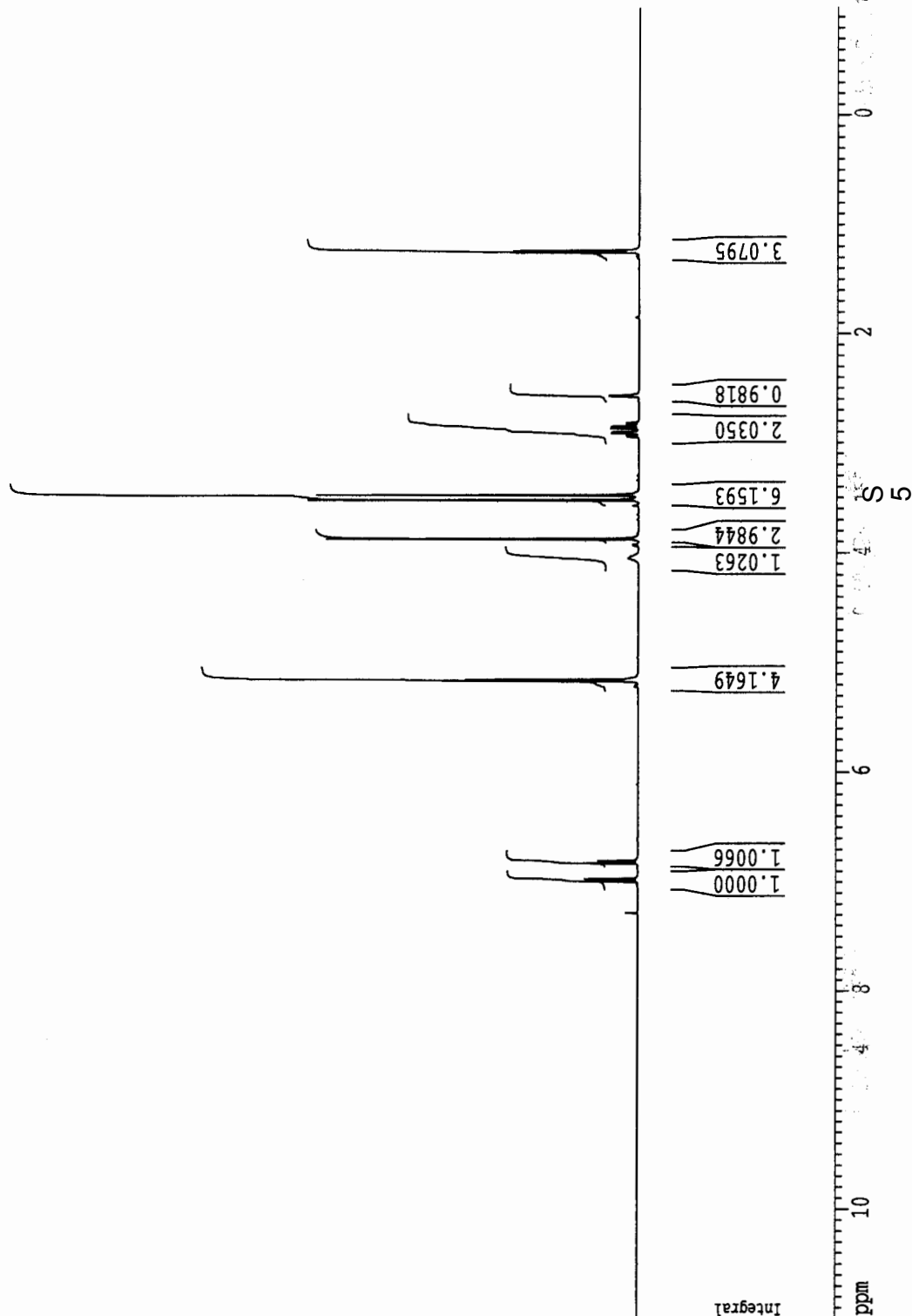
NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SF01 400.1320007 MHz

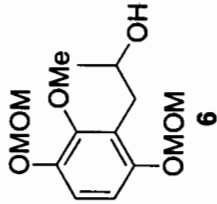
F2 - Processing parameters

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

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 sg420
EXPNO 2
PROCNO 1

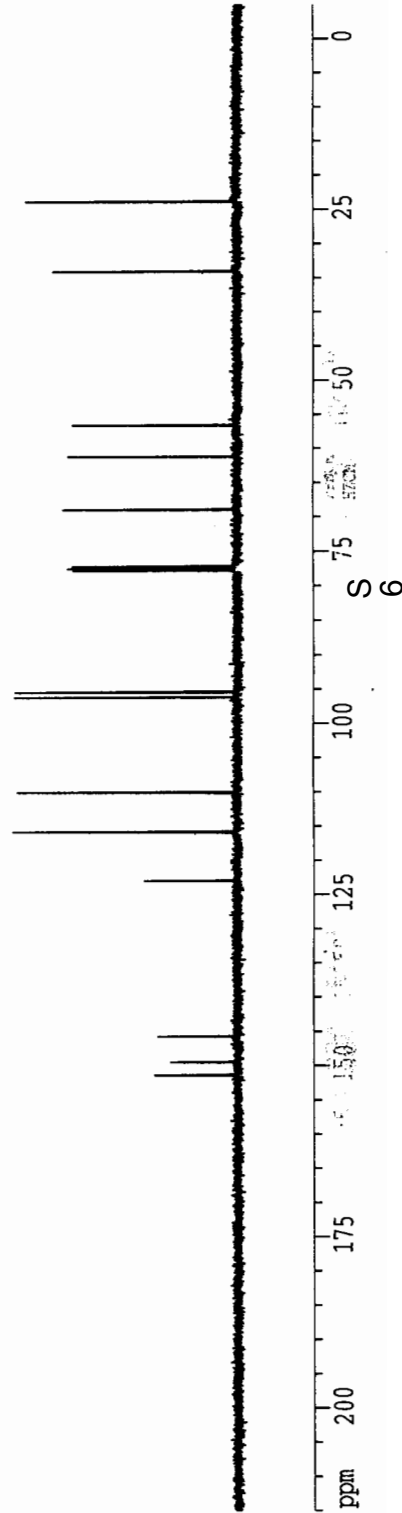
F2 - Acquisition Parameters
Date_ 20050305
Time 16:51
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 170
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

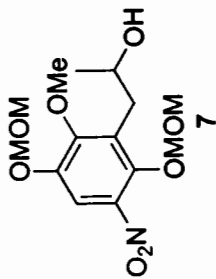
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== 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 3.00 cm
FIP 215.000 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
P1MCM 11.00000 ppm/cm
P2MCM 1106.73999 Hz/cm





Current Data Parameters
 NAME sg421
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050305
 Time 18.14
 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 1.00000000 sec
 MCREST 0.00000000 sec
 MCWPK 0.01500000 sec

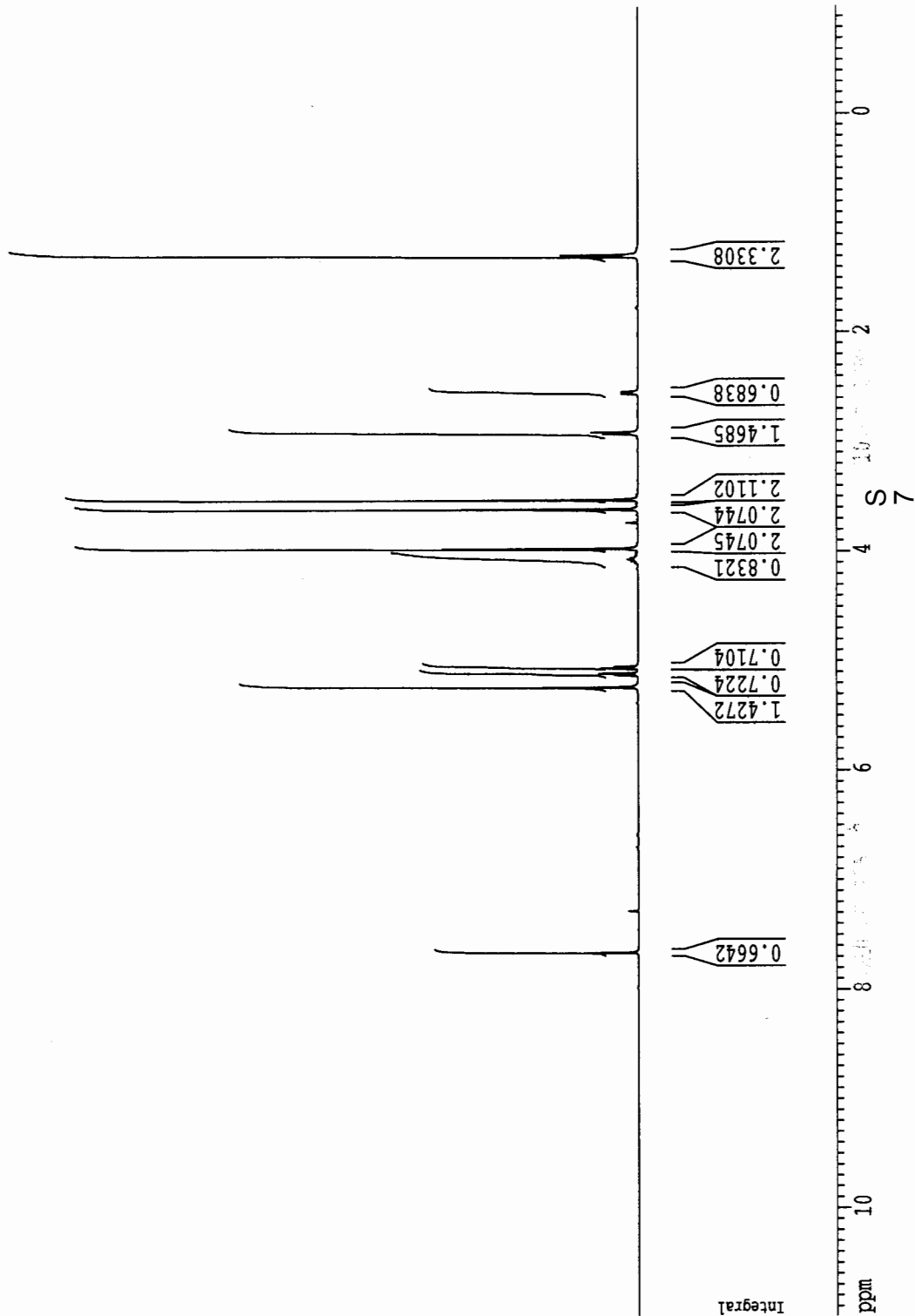
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 -4.00 dB
 SFO1 400.1320007 MHz

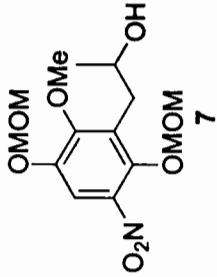
F2 - Processing parameters

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 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





Current Data Parameters
NAME S9421
EXPNO 2
PROCNO 1

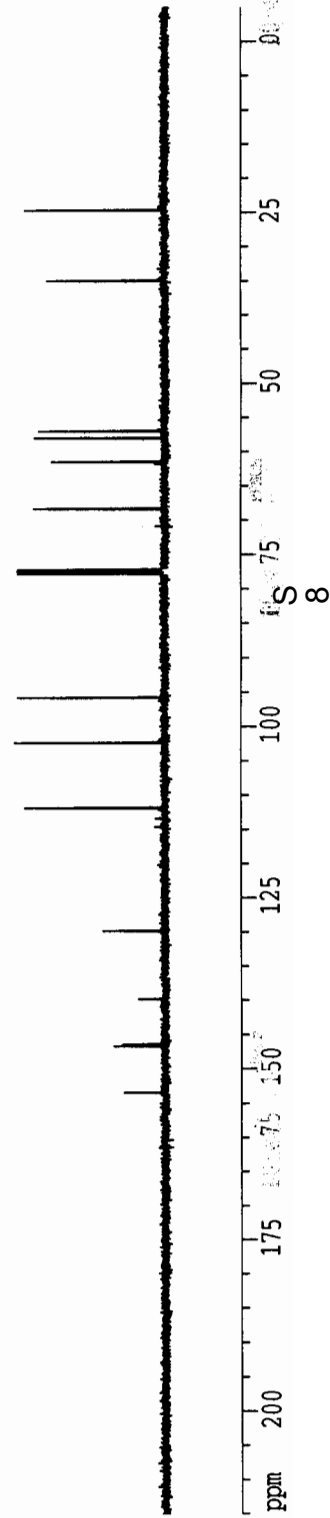
F2 - Acquisition Parameters
Date_ 20050305
Time 18.16
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 144
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 5.50 usec
TE 293.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

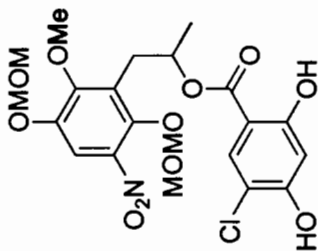
===== CHANNEL f1 =====
NUC1 13C
P1 11.25 usec
PL1 2.00 dB
SFO1 100.6232933 MHz

===== 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 2.00 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





8

Current Data Parameters
NAME gs-572
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050307
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 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

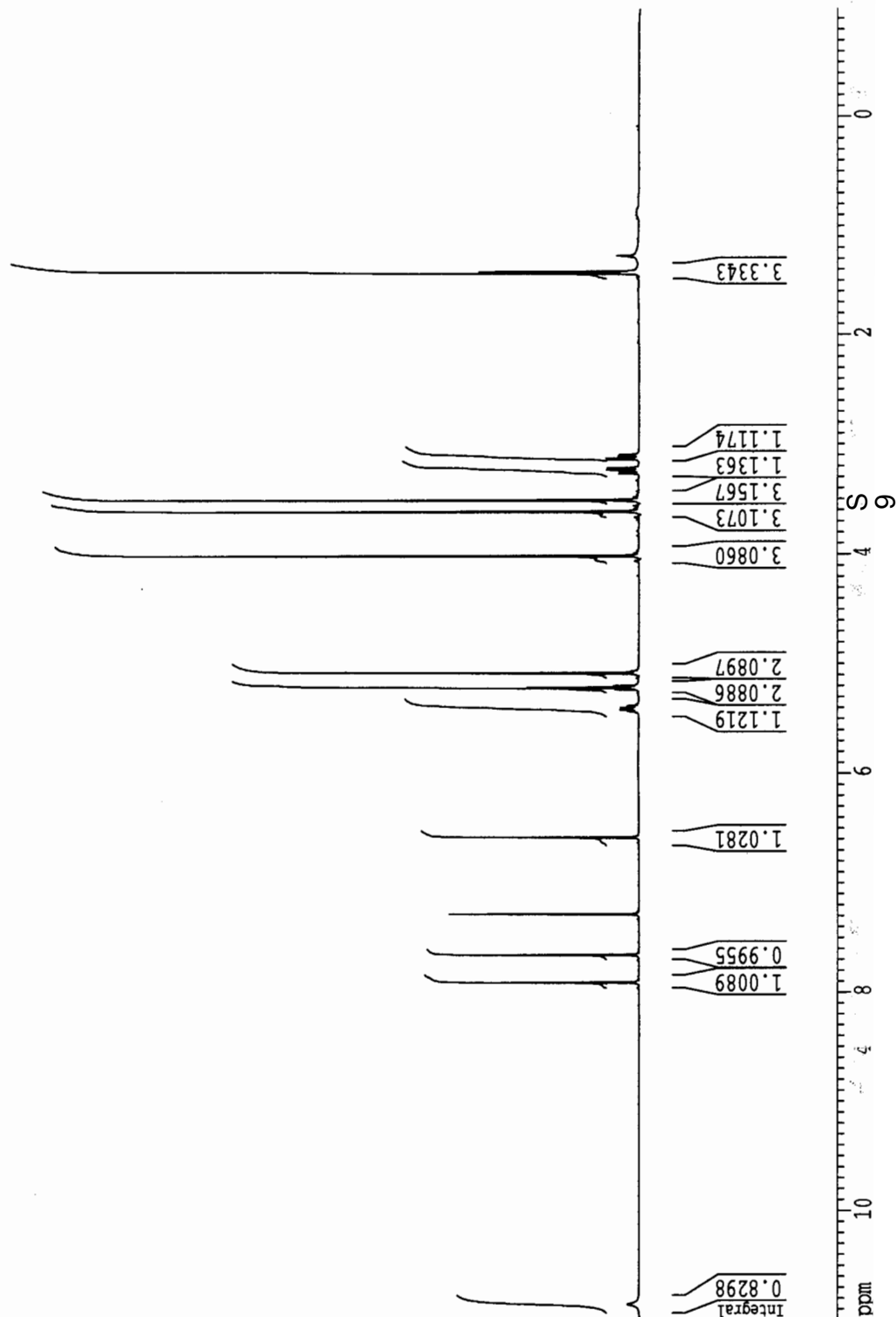
===== CHANNEL f1 =====
NUC1 1H
P1 9.35 usec
PL1 -4.00 dB
SFO1 400.1320007 MHz

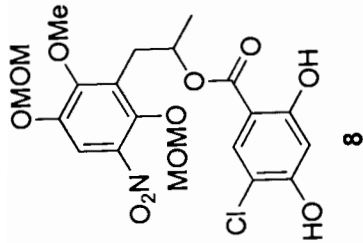
F2 - Processing parameters

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

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 gs-572
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

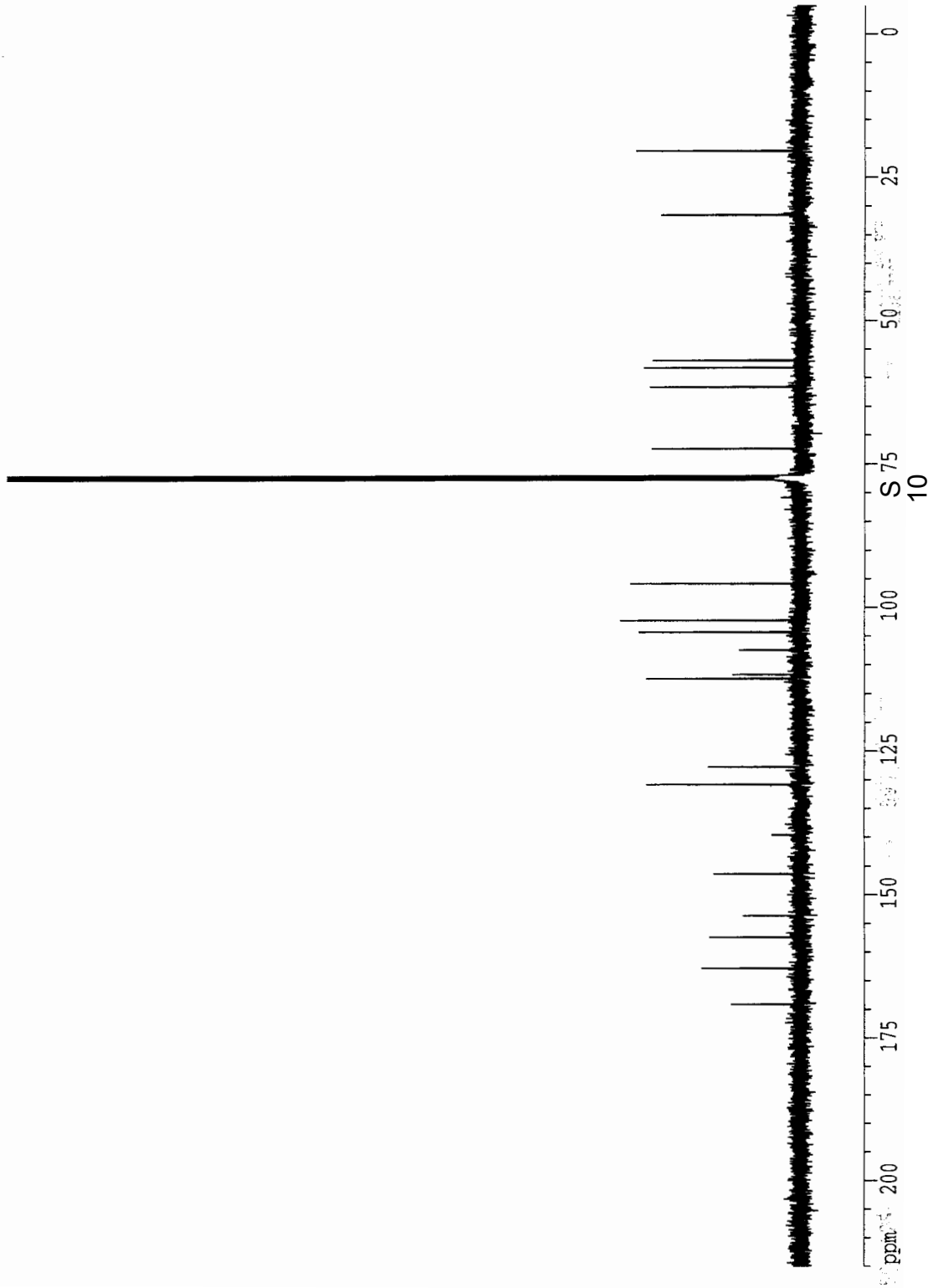
Date_ 20050307
 Time 12.53
 INSTRUM dirx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1928
 DS 4
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 5.50 usec
 TE 293.2 K
 D1 0.15000001 sec
 d11 0.03000000 sec
 DELTA 0.05000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

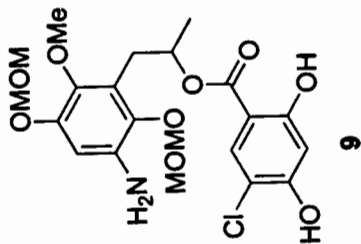
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.25 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 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
 FIP 215.000 ppm
 F1 21631.74 Hz
 F2 -5.000 ppm
 F2 -503.06 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm



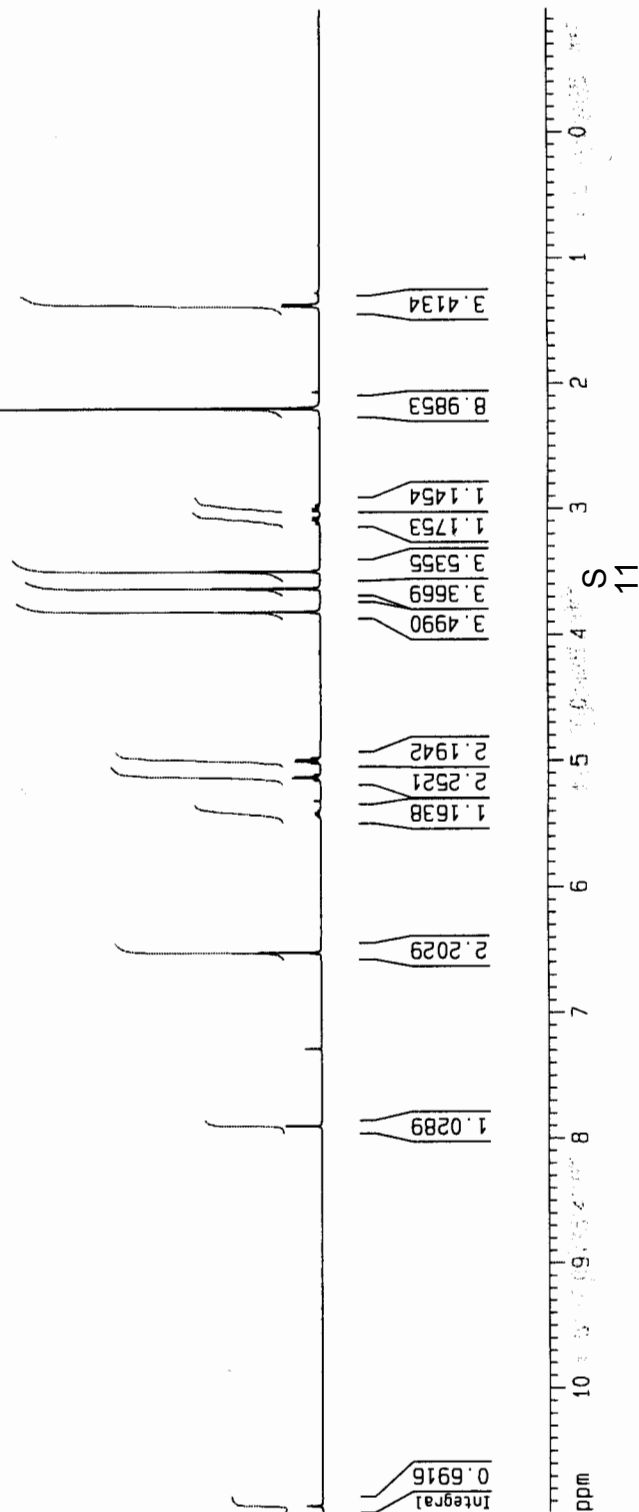


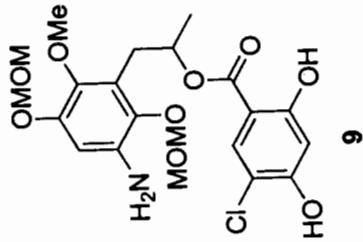
Current Data Parameters
 NAME sg-162
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20031007
 Time 16.48
 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 101.6
 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
 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
 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 sg-163
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20031007
 Time 16.54
 INSTRUM drx400
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 404
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 1149.4
 OW 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
 SF01 100.6232933 MHz

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

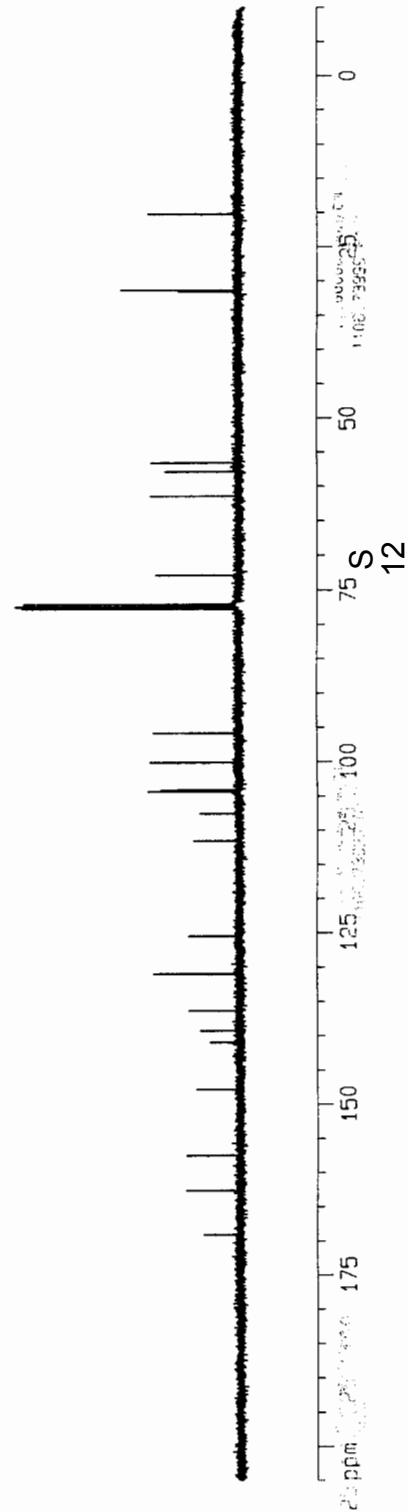
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SF02 400.1316005 MHz

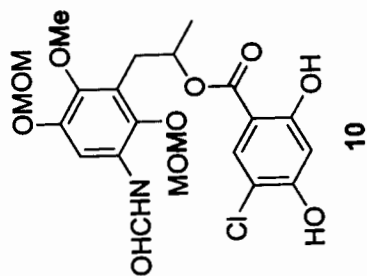
F2 - Processing parameters

SI 32768
 SF 100.6127290 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 19.55 cm
 CY 3.00 cm
 F1P 205.000 ppm
 F1 20625.61 Hz
 F2P -10.036 ppm
 F2 -1009.74 Hz
 PPMCM 11.00000 ppm/cm
 HZCM 1106.73999 Hz/cm





Current Data Parameters
NAME sg423
EXPNO 1
PROCNO 1

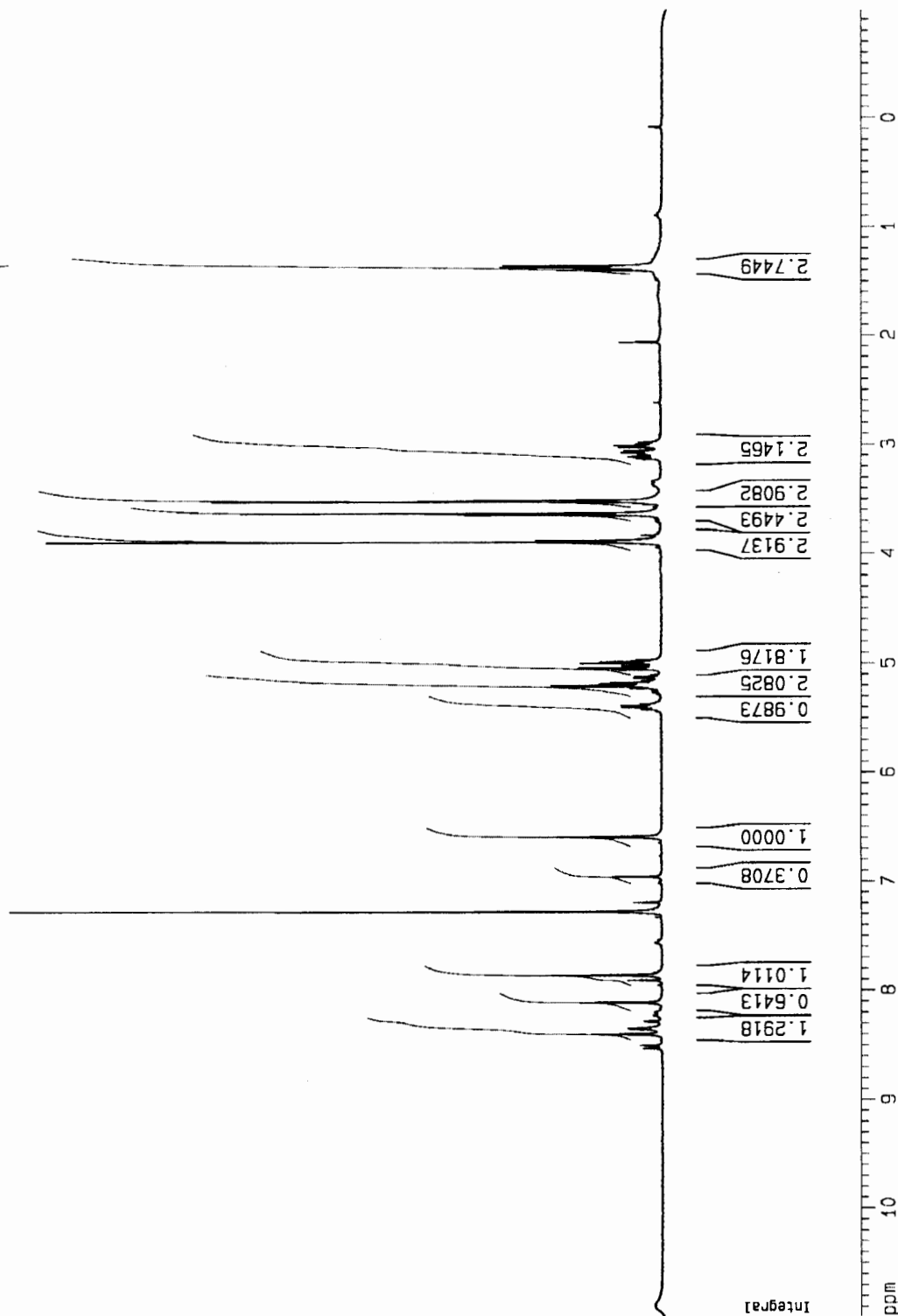
F2 - Acquisition Parameters

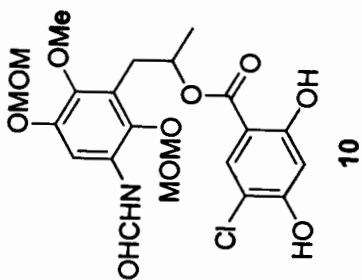
Date_ 20050310
Time 12.34
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 512
DM 104.400 usec
DE 5.50 usec
TE 293.2 K
D1 1.0000000 sec
MCREST 0.0000000 sec
MCWPK 0.0150000 sec

===== 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 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





Current Data Parameters
 NAME sg-166
 EXPNO 2
 PROCNO 1

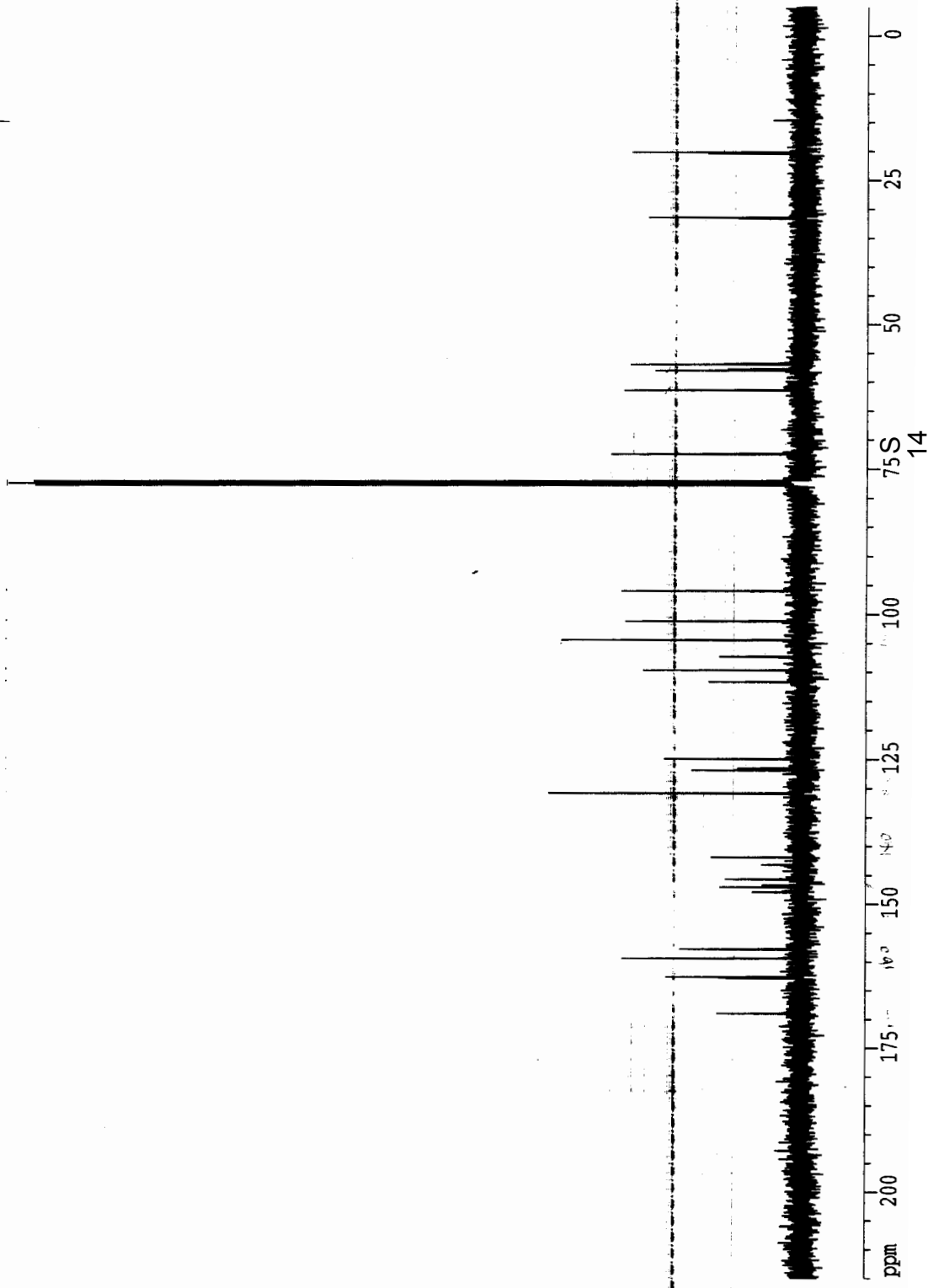
F2 - Acquisition Parameters
 Date_ 20031010
 Time 8.27
 INSTRUM drx400
 PROBD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 459
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQC 1.4156276 sec
 RG 114
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

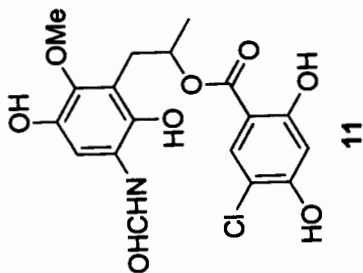
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 2.00 dB
 SF01 100.6232933 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 18.00 dB
 PL13 18.00 dB
 SF02 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

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 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 gs-574 isopro hydro
 EXPNO 1
 PROCNO 1

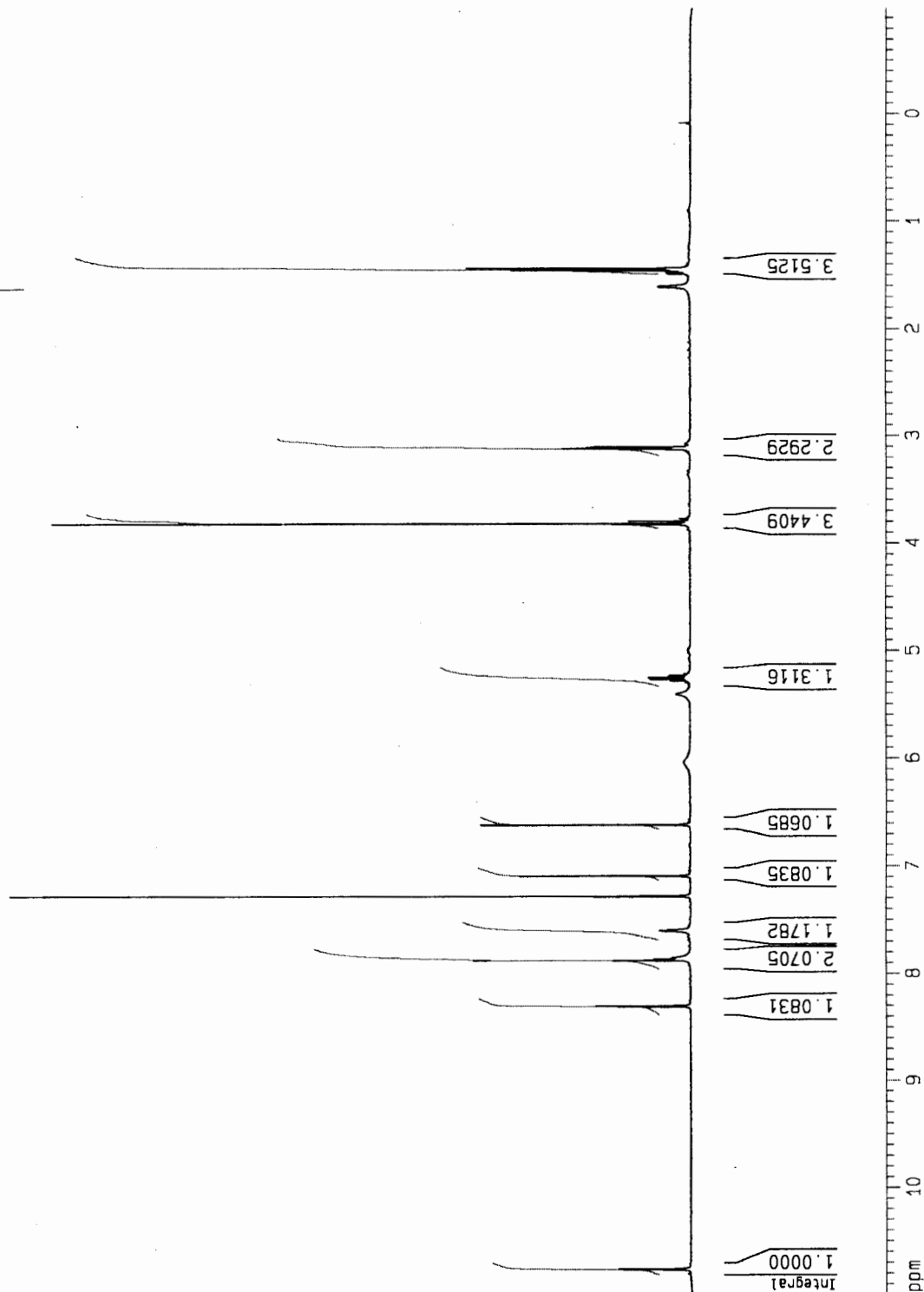
F2 - Acquisition Parameters

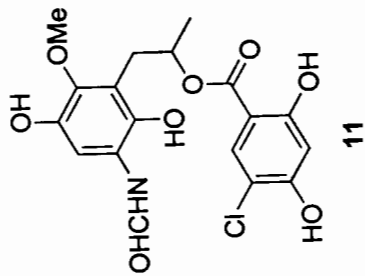
Date_ 20050308
 Time 9.43
 INSTRUM drx400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 512
 DM 104.400 usec
 DE 5.50 usec
 TE 292.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCRRK 0.01500000 sec

===== 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

1D NMR plot parameters
 CX 20.00 cm
 CY 12.00 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 sg422
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050308
Time 22.07
INSTRUM dr400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 28670
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
OM 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
MCMRK 0.01500000 sec

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

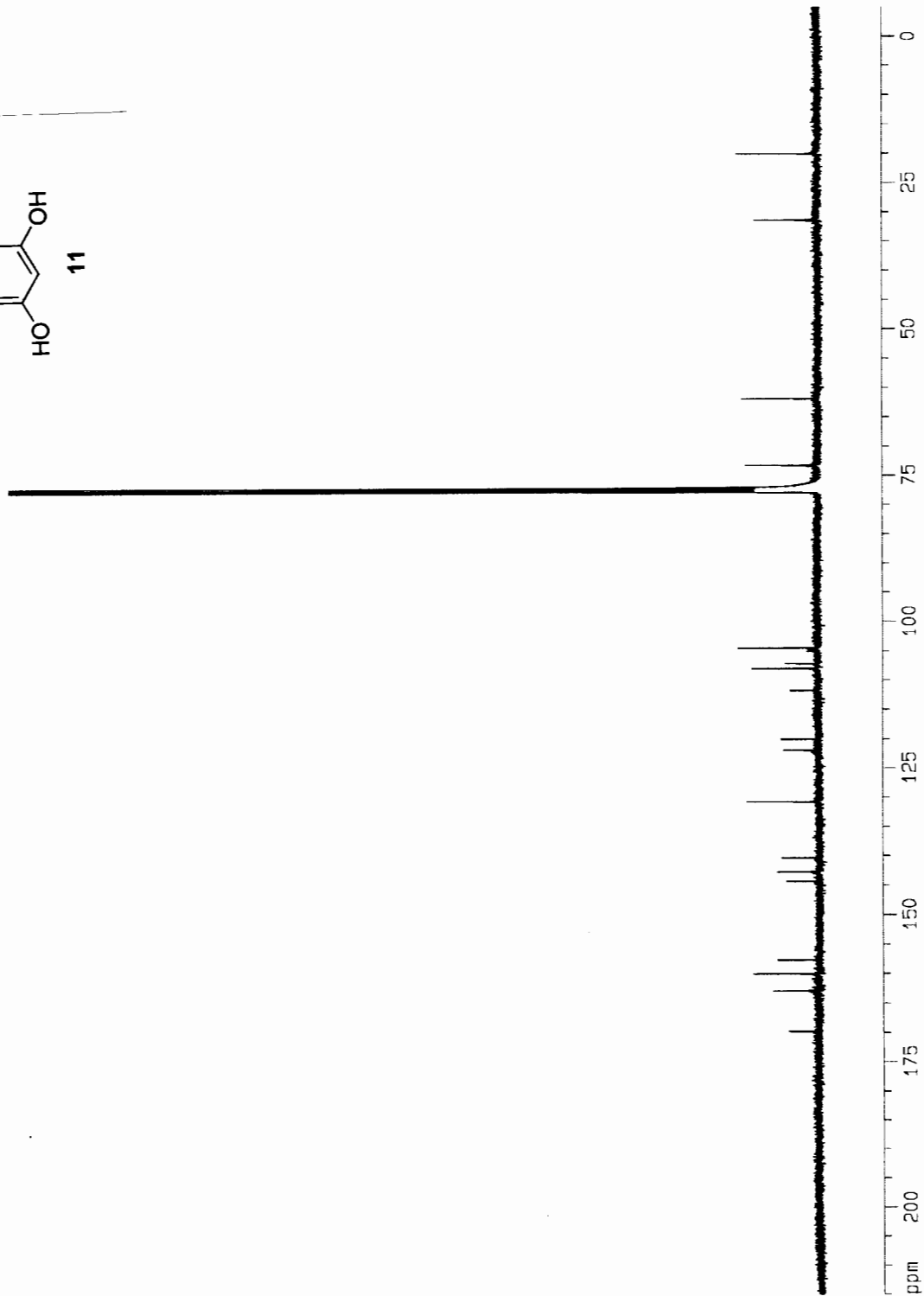
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 16.58 dB
PL13 17.00 dB
SF02 400.1316005 MHz

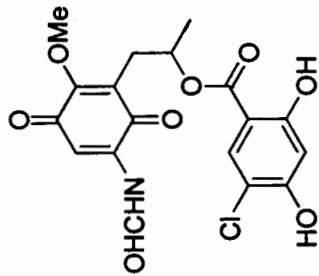
F2 - Processing parameters

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 1105.73999 Hz/cm





Current Data Parameters

NAME sg-172
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

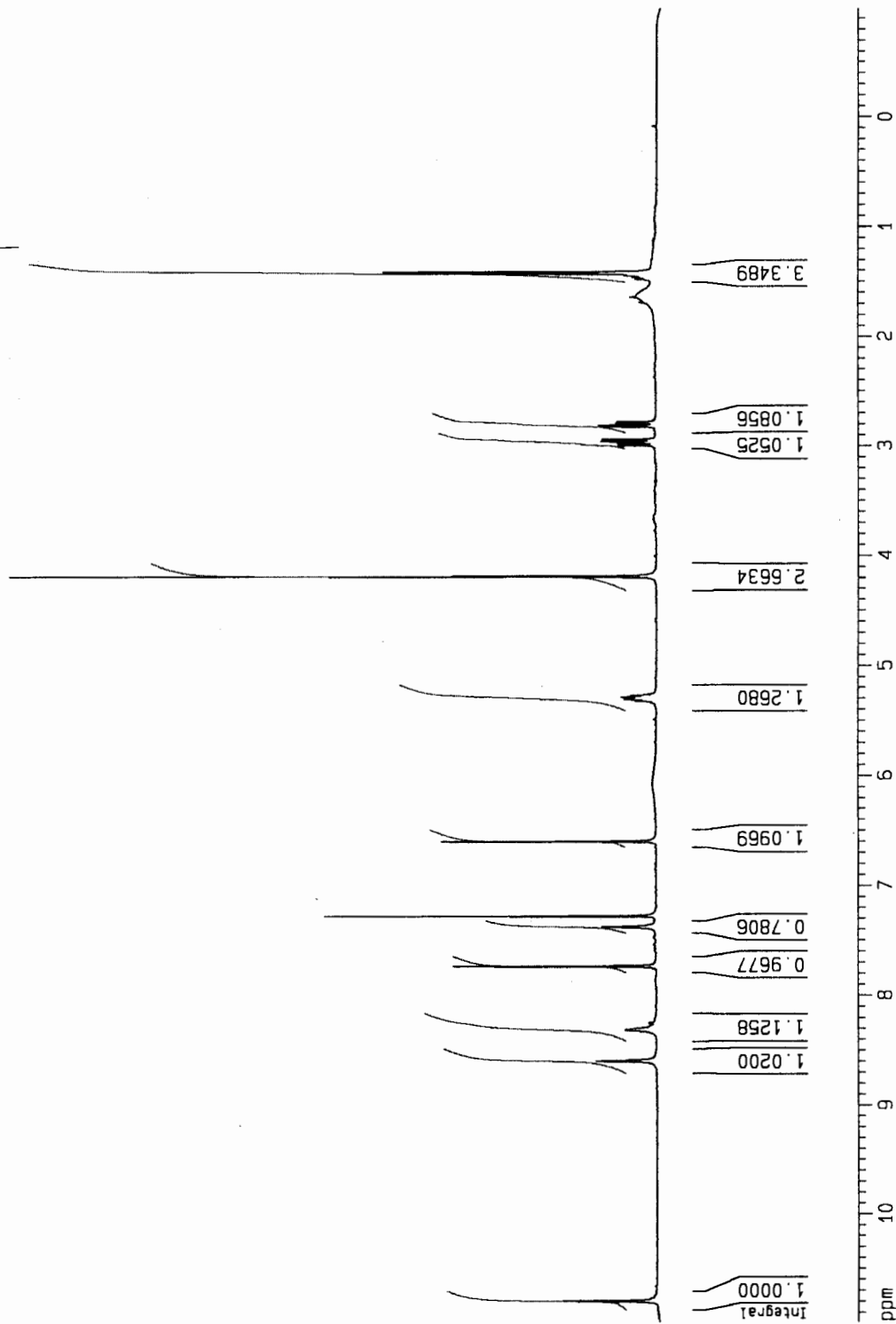
Date_ 20031019
Time 17.41
INSTRUM drx400
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 181
DM 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

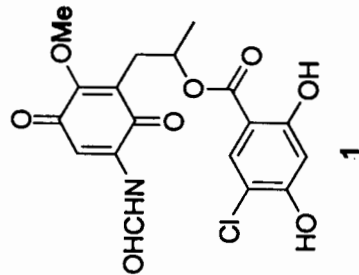
===== CHANNEL f1 =====

NUC1 1H
P1 7.70 usec
PL1 -6.00 dB
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
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
PPMCH 0.60000 ppm/cm
HZCM 240.07800 Hz/cm





Current Data Parameters
 NAME sg-173
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20031019
 Time 19.00
 INSTRUM drx400
 PROHD 5 mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 7000
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 0.05000000 sec
 d11 0.03000000 sec
 d12 0.0002000 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

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

