

Electronic Supplementary Information

Conversion of lapachol to lomatiol: synthesis of novel naphthoquinone derivatives

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General Information:

General Methods: All the solvents were distilled prior to use. Dry solvents were prepared according to the standard procedures. All other reagents were used as received from either Aldrich or Lancaster chemical companies. Reactions requiring inert atmosphere were carried out under argon atmosphere. Infrared (IR) spectra were recorded on a JASCO 4100 FT-IR spectrometer. ^1H NMR spectra were measured on Bruker AVANCE 400 MHz and 500 MHz spectrometers. Chemical shifts were reported in ppm from tetramethylsilane in the case of CDCl_3 as an internal standard. ^{13}C NMR spectra were recorded on Bruker 100 MHz and 125 MHz spectrometers with complete proton decoupling. Chemical shifts were reported in ppm from the residual solvent as an internal standard. The high-resolution mass spectra (HRMS) were performed on Micromass QTOF micro mass spectrometer equipped with a Harvard apparatus syringe pump. Optical rotations were measured on a JASCO P-2000 polarimeter. X-ray crystallographic data were recorded using Bruker-AXS Kappa CCD-Diffractometer with graphite monochromator $\text{MoK}\alpha$ radiation ($\lambda=0.7107 \text{ \AA}$). The structures were solved by direct methods (SHELXS-97) and refined by full-matrix least squares techniques against F^2 (SHELXL-97). Hydrogen atoms were inserted from geometry consideration using the HFIX option of the program. For thin layer chromatography (TLC) analysis throughout this work, E-merck precoated TLC plates (silica gel 60 F254 grade, 0.25 mm) were used. Acme (India) silica gel (100-200 mesh) was used for column chromatography. The enantiomeric excess was determined by chiral HPLC analyses using DAICEL's CHIRALPAK ADH column with hexanes/isopropyl alcohol mixtures as eluent.

Current Data Parameters

NAME sb41013
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131002
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INSTRUM spect
PROBHD 5 mm PABO BB-
PULPROG zg30
TD 65536

SOLVENT CDCl3

NS 16

DS 2

SWH 8012.820 Hz

FIDRES 0.122266 Hz

AQ 4.0894966 sec

RG 200.34

DW 62.400 usec

DE 6.50 usec

TE 303.2 K

D1 0.50000000 sec

TD0 1

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PLW1 7.7500000 W

SFO1 400.1320007 MHz

F2 - Processing parameters

SI 65536

SF 400.130094 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00

1.914

3.671
3.652

6.518

6.521

6.536

6.539

6.555

6.558

7.260

7.523

7.694

7.696

7.712

7.715

7.731

7.734

7.768

7.771

7.787

7.789

7.806

7.808

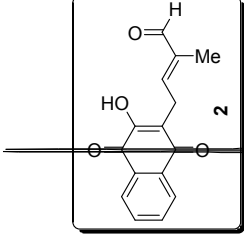
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8.115

8.131

8.150

9.387



S3

ppm

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1.05

0.89

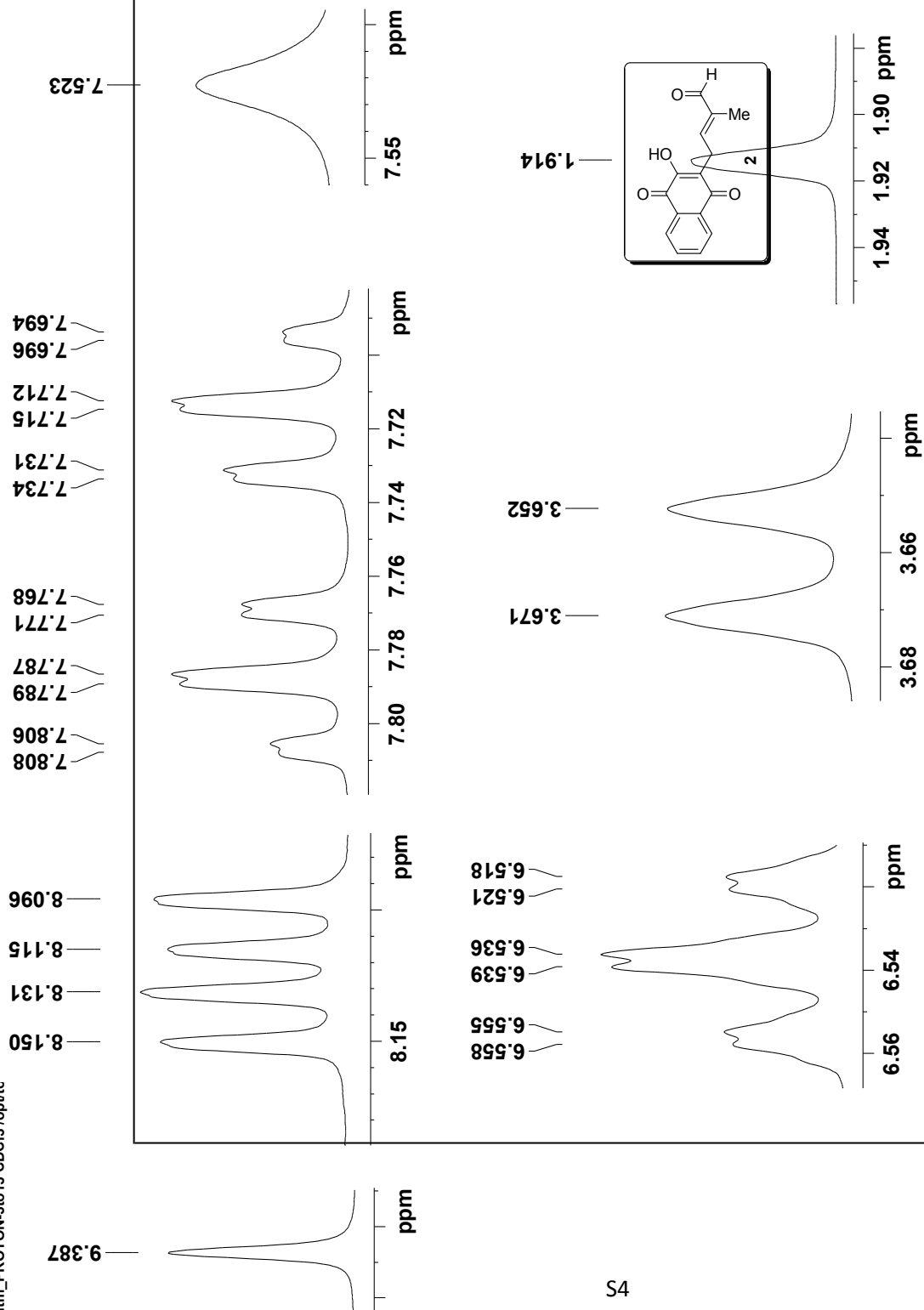
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1.06

2.02

1.00

¹H NMR spectrum of compound 2



¹H NMR expanded spectrum of compound 2

lab sb
sb-ok1
iitm_carbonshort CD

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PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 1000

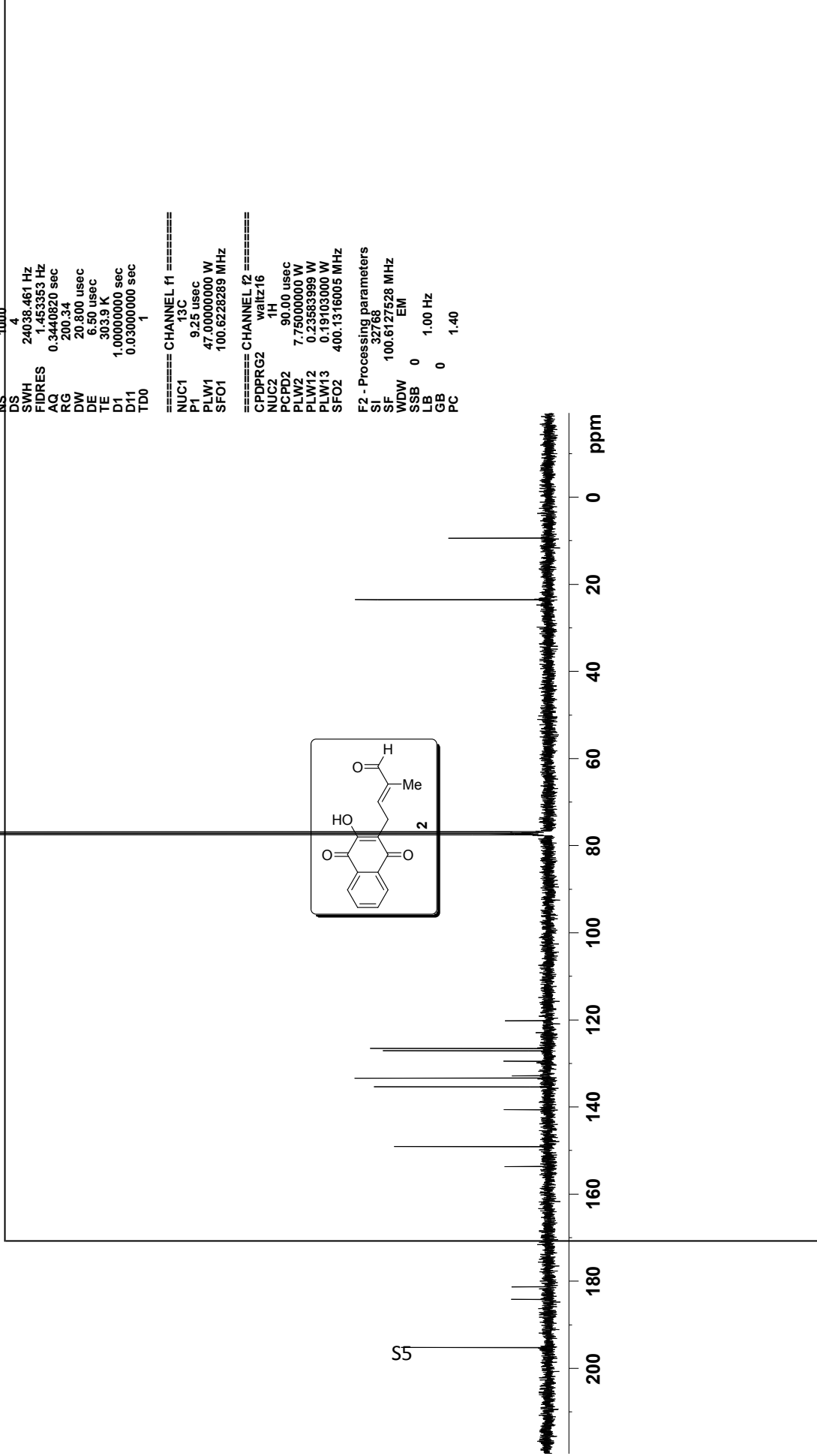
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DE 6.50 usec
TE 303.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

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NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
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SF 100.6127528 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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184.19
181.31
153.74
149.12
140.64
135.39
133.41
132.86
129.49
127.10
126.55
120.22
76.84
77.16
77.48
23.53
9.41



¹³C NMR spectrum of compound 2

lab sb
sb-ok1
itrm_C13DEPT13!

Current Data Parameters
NAME sb41013
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131002
Time 13.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG depts135
TD 32768

SOLVENT CDCl3
NS 105
DS 4
SWH 20161.291 Hz
FIDRES 0.615274 Hz
AQ 0.8126964 sec
RG 200.34
DW 24.800 usec
DE 6.50 usec
TE 303.6 K
CNST2 145.0000000
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D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

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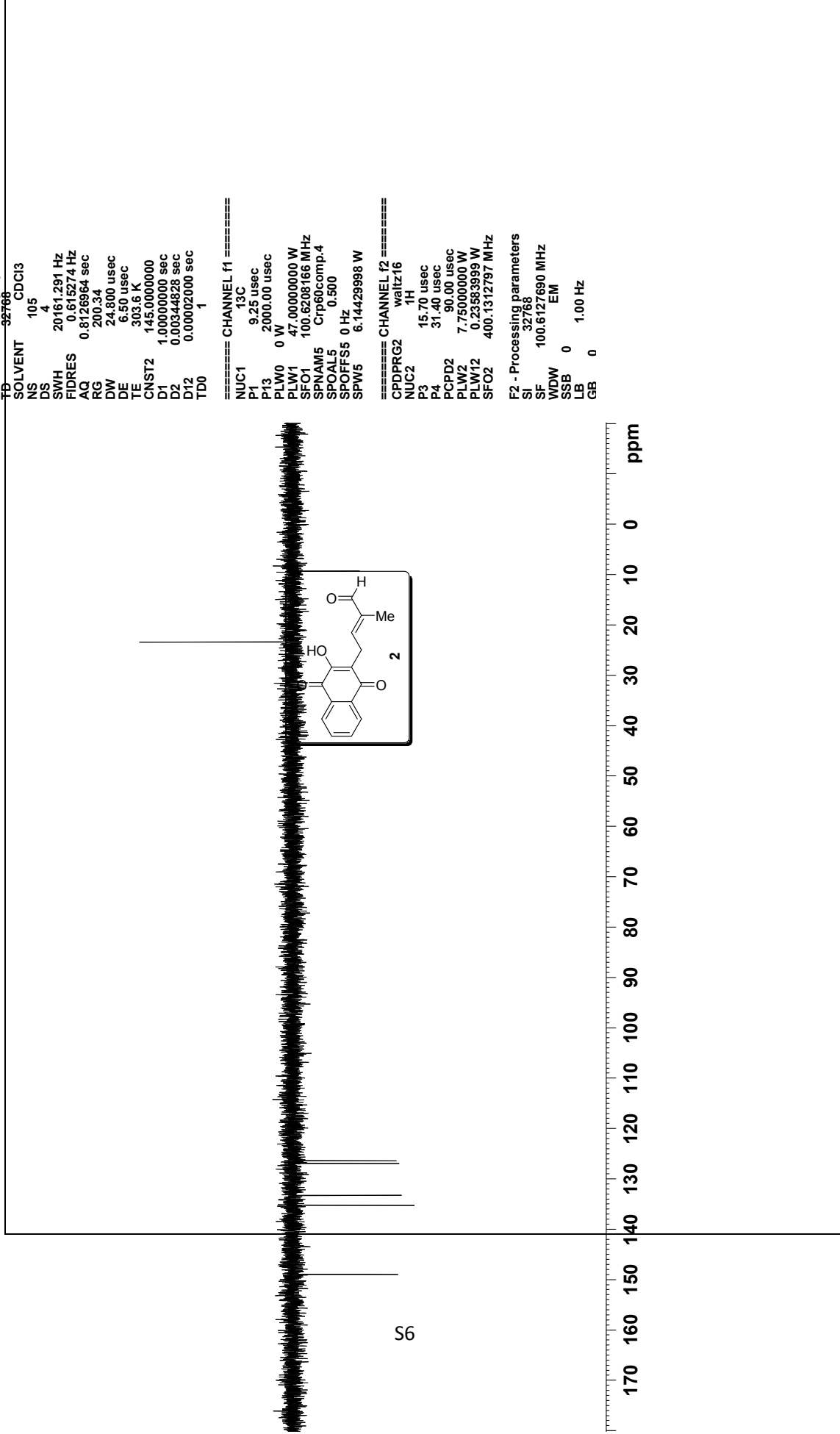
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P1 9.25 usec
P13 2000.00 usec
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PLW1 47.00000000 W
SFO1 100.6208166 MHz
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SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 6.14429998 W

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

CPDPRG2 waltz16
NUC2 1H
P3 15.70 usec
P4 31.40 usec
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
SFO2 400.1312797 MHz

F2 - Processing parameters
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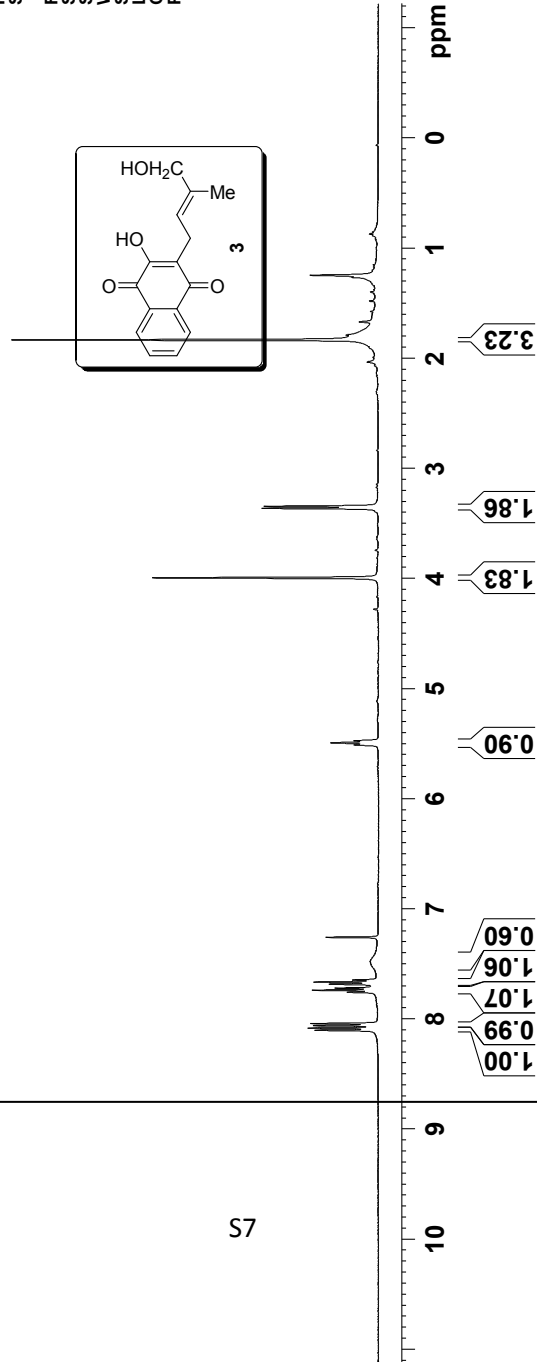
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126.39
23.37
9.26



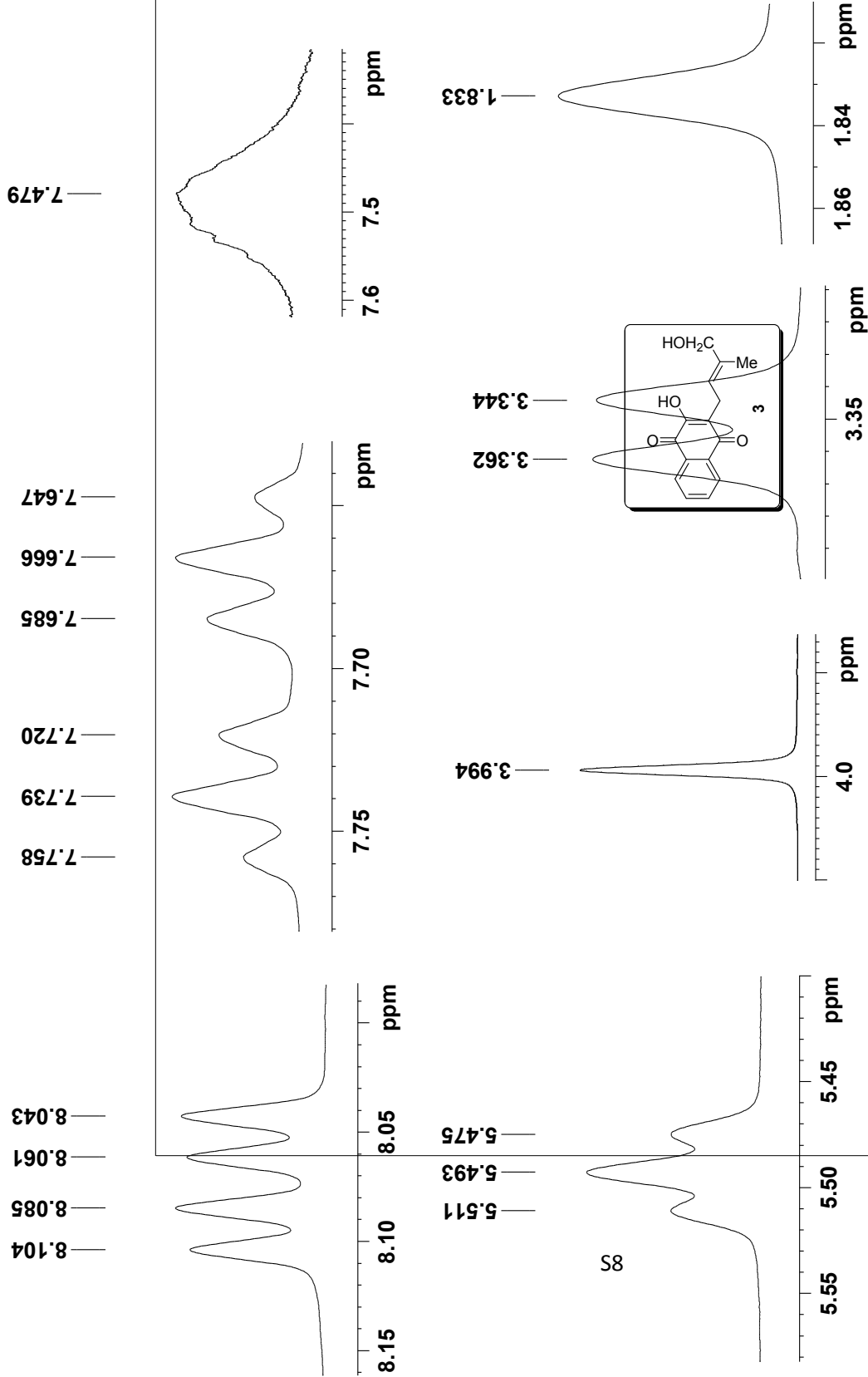
DEPT NMR spectrum of compound 2

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 PROCNO 1
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 169.77
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 0.50000000 sec
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 15.70 usec
 PLW1 7.75000000 W
 SFO1 400.1320007 MHz
 F2 - Processing parameters
 SI 65536
 SF 400.1300094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S7



¹H NMR spectrum of compound 3



^1H NMR expanded spectrum of compound **3**

Current Data Parameters
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EXPNO 83
PROCNO 1

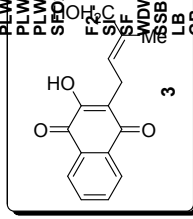
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Time 1.31
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PULPROG zgpg30
TD 16540
SOLVENT CDCl3

NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440820 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

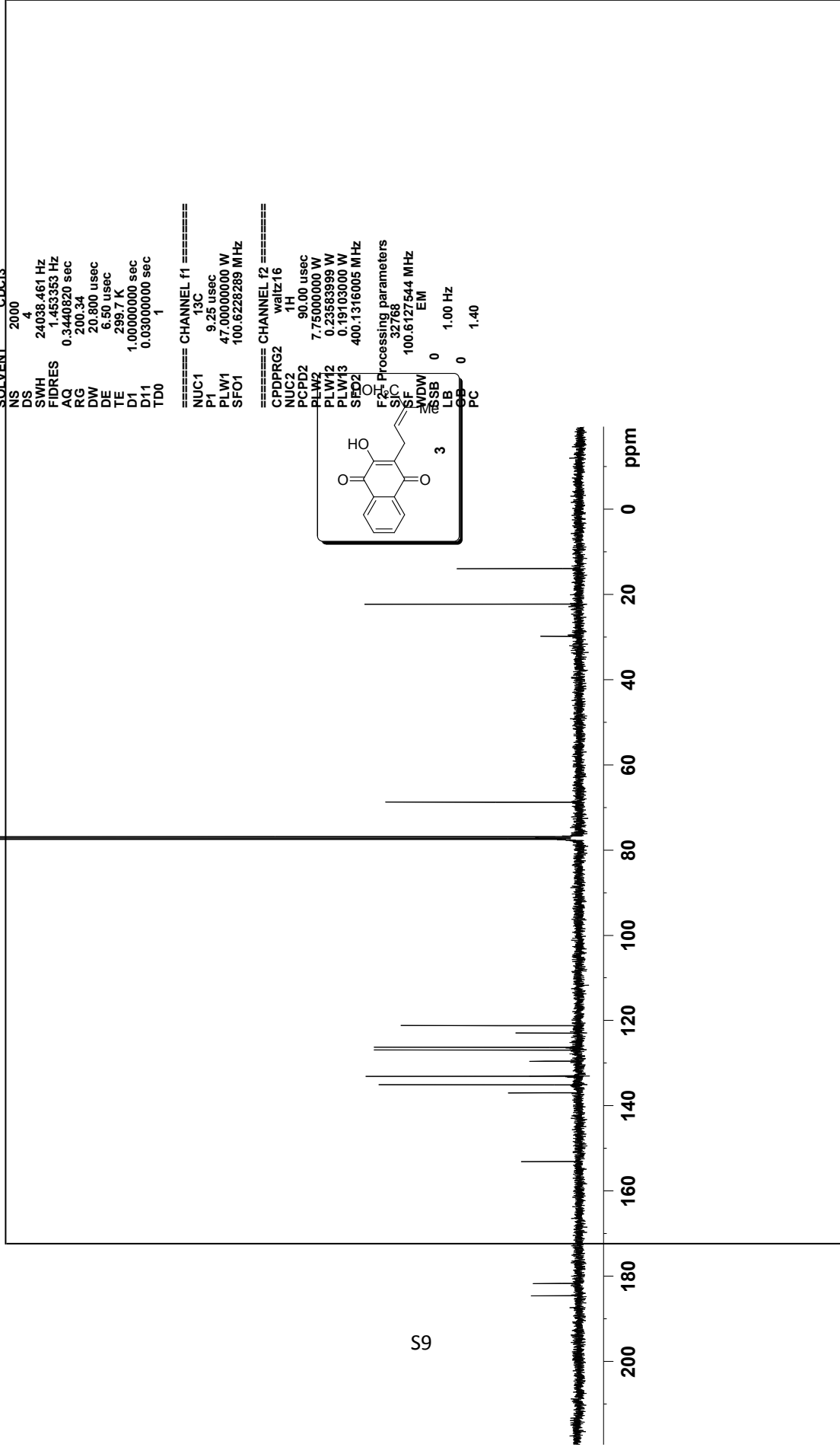
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NUC1 13C
P1 9.25 usec
PLW1 47.0000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SFO 327.68
SF 100.5127544 MHz
WDW EM
SSB 0
LB 0 1.00 Hz
GB 0
PC 1.40



184.61
181.71
153.11
136.96
135.08
133.10
132.99
129.55
126.93
126.28
122.90
121.19
77.48
77.16
76.84
68.75
22.28
13.95



¹³C NMR spectrum of compound 3

Current Data Parameters
NAME sb41013
EXPNO 47
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131004
Time 12.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 128

DS 4
SWH 20161.291 Hz
FIDRES 0.615274 Hz
AQ 0.8126964 sec
RG 200.34
DW 24.800 usec
DE 6.50 usec
TE 298.5 K
CNST2 145.000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW0 2000.00 usec
PLW1 0 W
SFO1 47.00000000 W
SPNAM5 100.6208166 MHz
SFOALS Crip60comp.4
SFOFFS5 0 Hz
SPW5 6.14429998 W

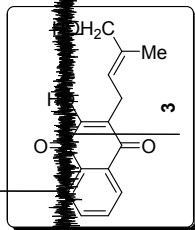
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P4 31.40 usec
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
SFO2 400.1312797 MHz

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SF 100.6127690 MHz
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LB 1.00 Hz
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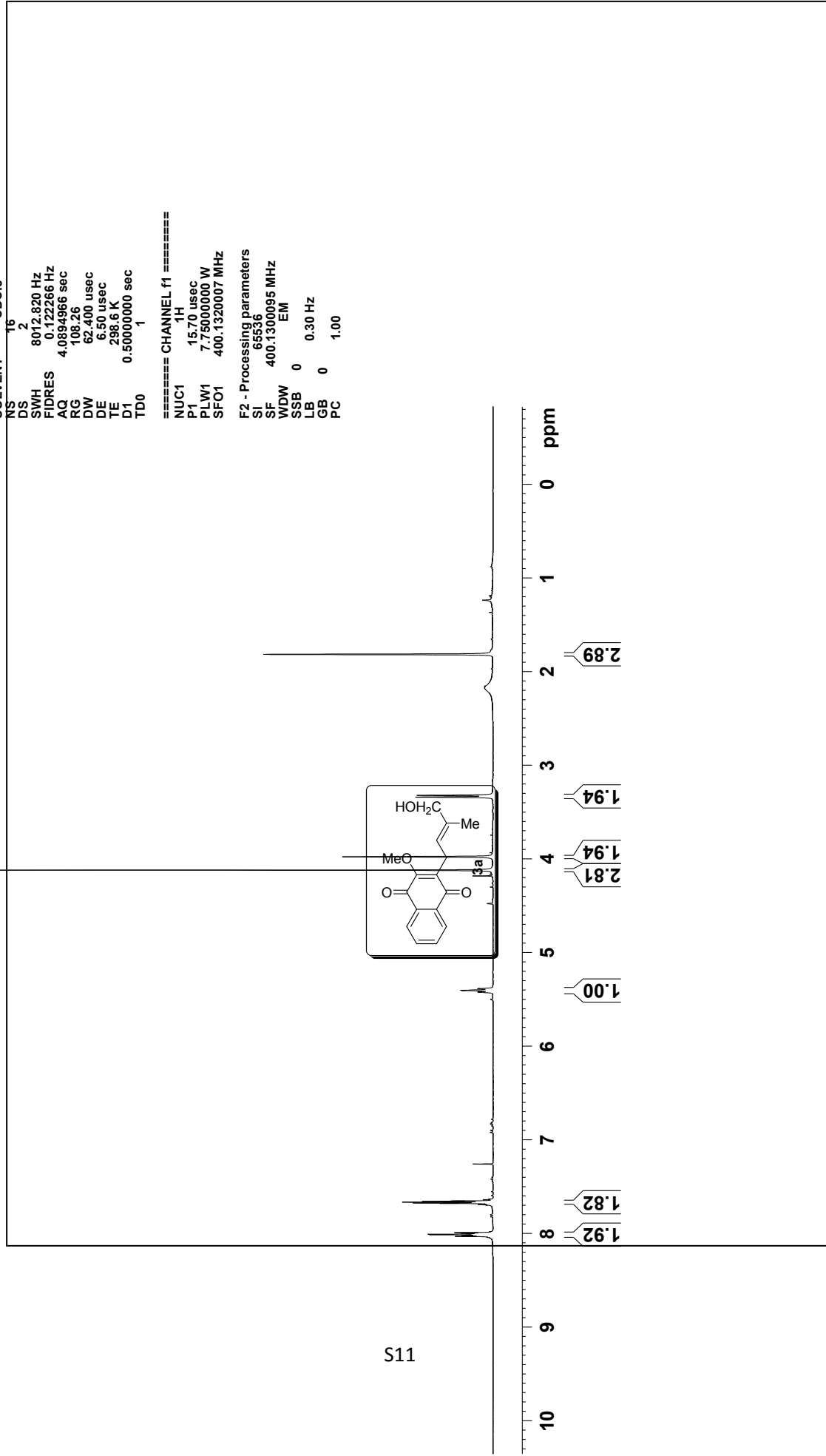
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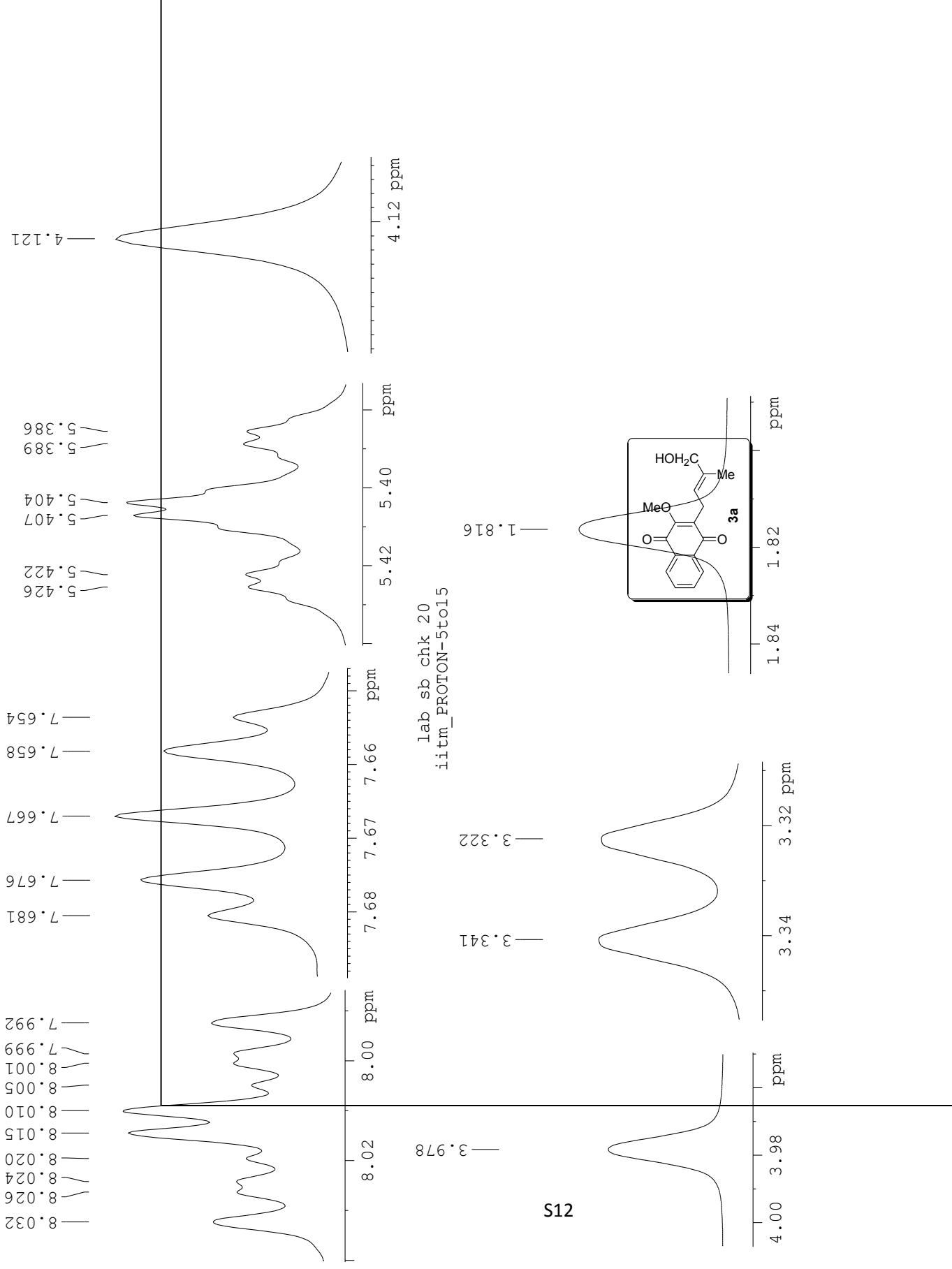
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PROCNO 1
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 108.26
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 0.50000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.7500000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.032
8.026
8.024
8.020
8.015
8.010
8.005
8.001
7.999
7.992
7.681
7.676
7.667
7.658
7.654
7.260
5.426
5.422
5.407
5.404
5.389
5.386
4.121
3.978
3.341
3.322
1.816



¹H NMR spectrum of compound 3a



¹H NMR expanded spectrum of compound **3a**

Current Data Parameters
NAME sb41113
EXPNO 398
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131129
Time 16:39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540

SOLVENT CDCl3
NS 187
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440820 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.0000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

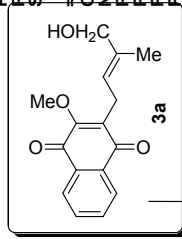
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SSB 0 1.00 Hz
LB 0
GB 0
PC 1.40

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61.34
68.66
76.84
77.16
77.47

121.51
126.22
126.29
131.57
131.98
133.37
133.77
133.93
136.78
157.69

181.74
185.29



ppm

¹³C NMR spectrum of compound 3a

Current Data Parameters
NAME sb41113
EXPNO 399
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131129
Time 16.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135
TD 32768

SOLVENT CDCl3
NS 64
DS 4
SWH 20161.291 Hz
FIDRES 0.615274 Hz
AQ 0.8126964 sec
RG 200.34
DW 24.800 usec
DE 6.50 usec
TE 298.8 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

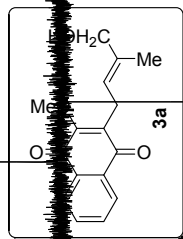
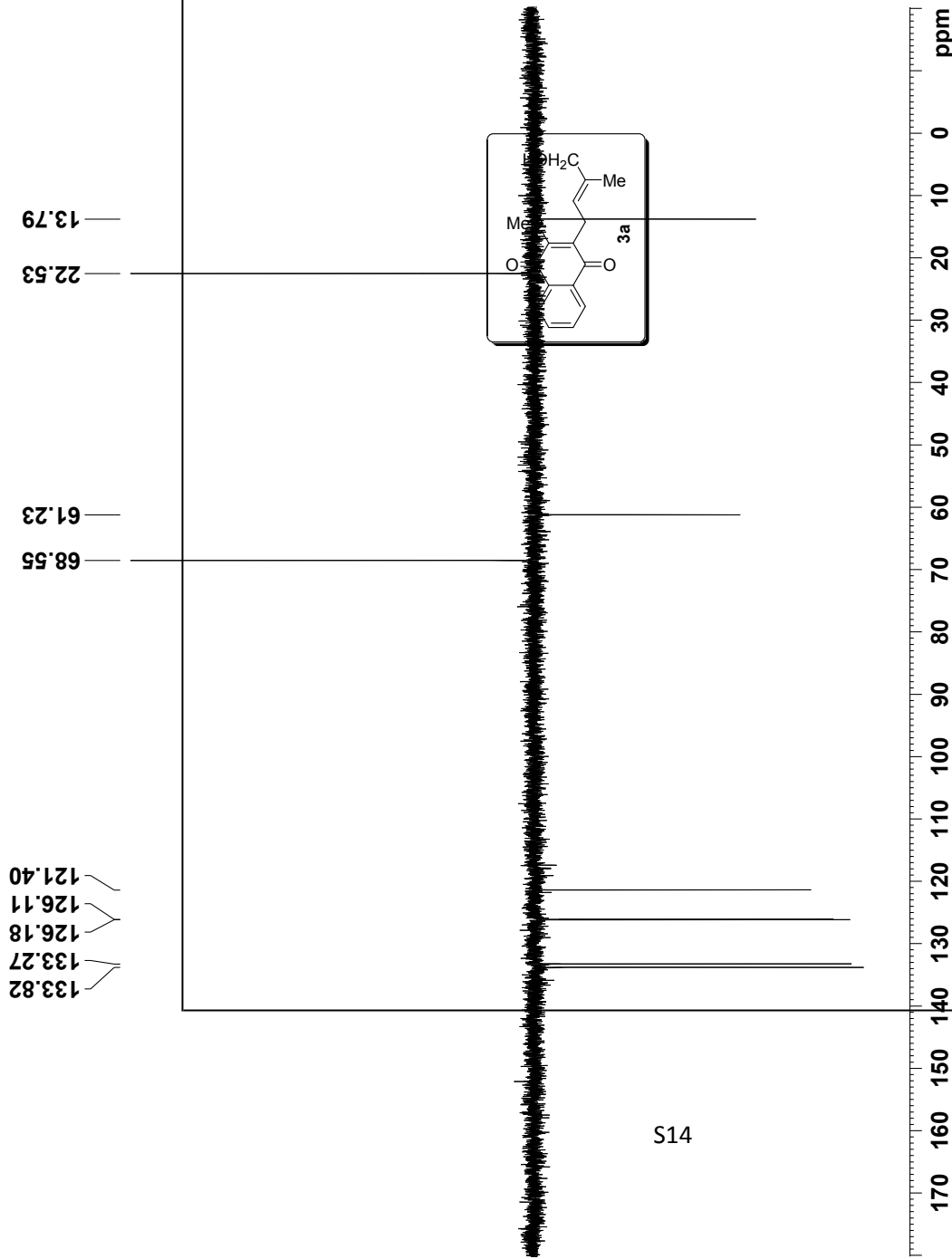
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P1 9.25 usec
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PLW1 47.00000000 W
SFO1 100.6208166 MHz
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SFOAL5 0 Hz
SPOFFS5 0 Hz
SPW5 6.14429998 W

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

CPDPRG2 waltz16
NUC2 ¹H
P3 15.70 usec
P4 31.40 usec
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.2358399 W
SFO2 400.1312797 MHz

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



Current Data Parameters

NAME sb41113
EXPNO 136
PROCNO 1

F2 - Acquisition Parameters

Date_ 20131106
Time_ 22.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCI3
NS 16
DS 2

SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 108.26
DW 62.400 usec
DE 6.50 usec
TE 297.1 K
D1 0.5000000 sec
TD0 1

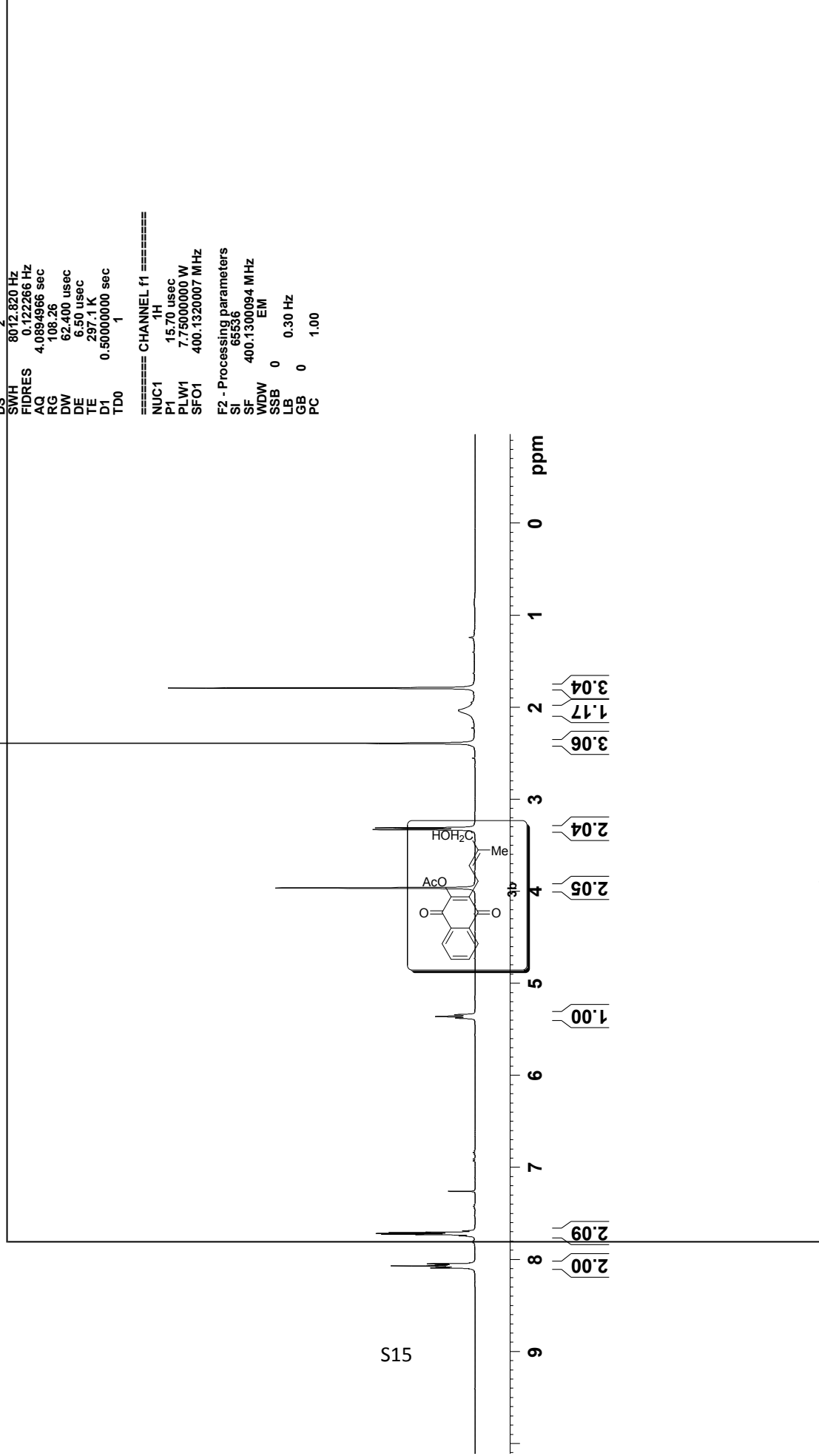
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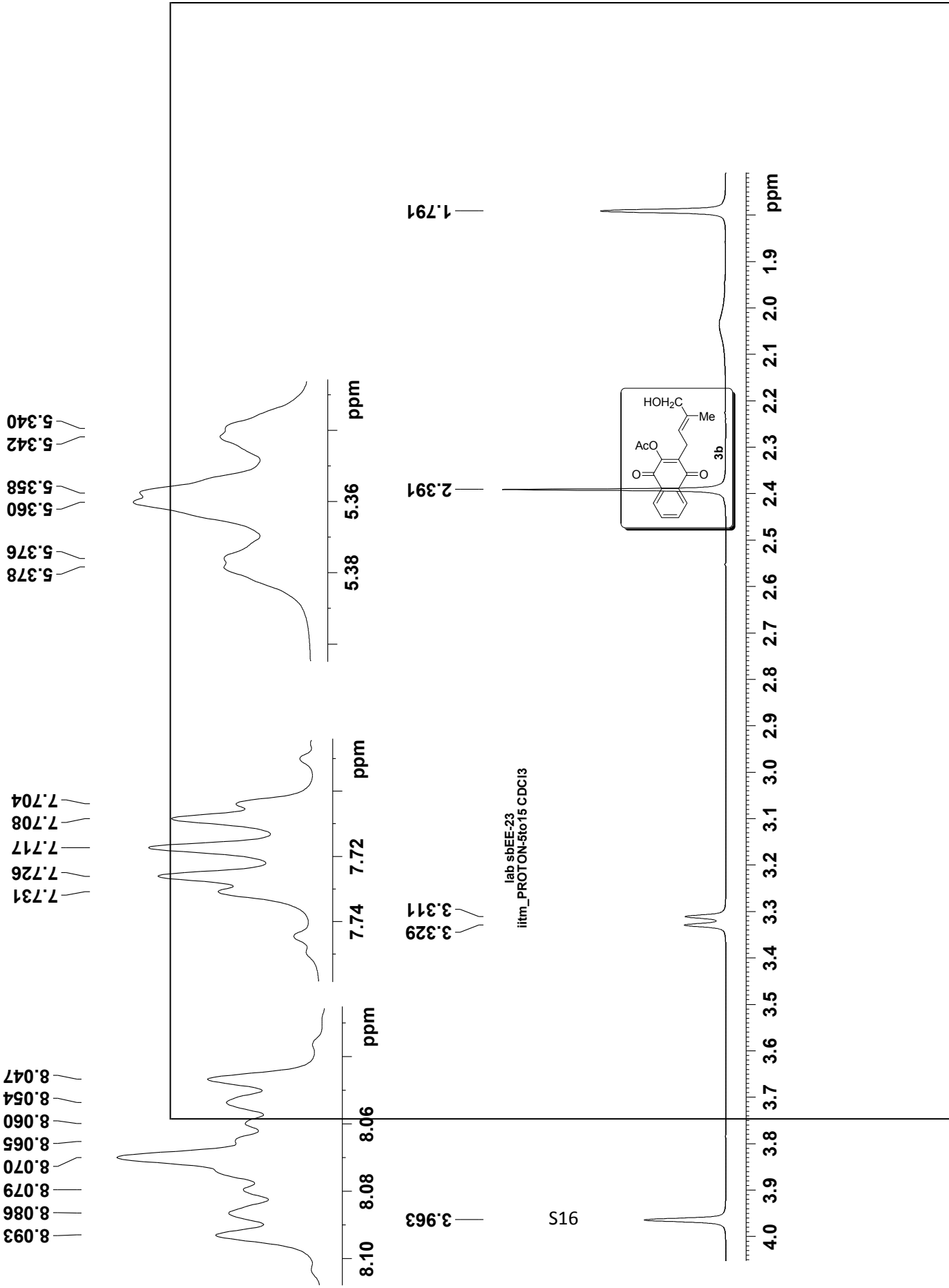
F2 - Processing parameters

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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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8.070
8.065
8.060
8.054
8.047
7.731
7.726
7.717
7.708
7.704
7.260
5.378
5.376
5.360
5.358
5.342
5.340
3.963
3.329
3.311
2.391
1.791



¹H NMR spectrum of compound 3b



¹H NMR expanded spectrum of compound **3b**

Current Data Parameters
NAME sb41113
EXPNO 137
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131106
Time 22.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
DS 4

SWH 24038.461 Hz
FIDRES 1.45353 Hz
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RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

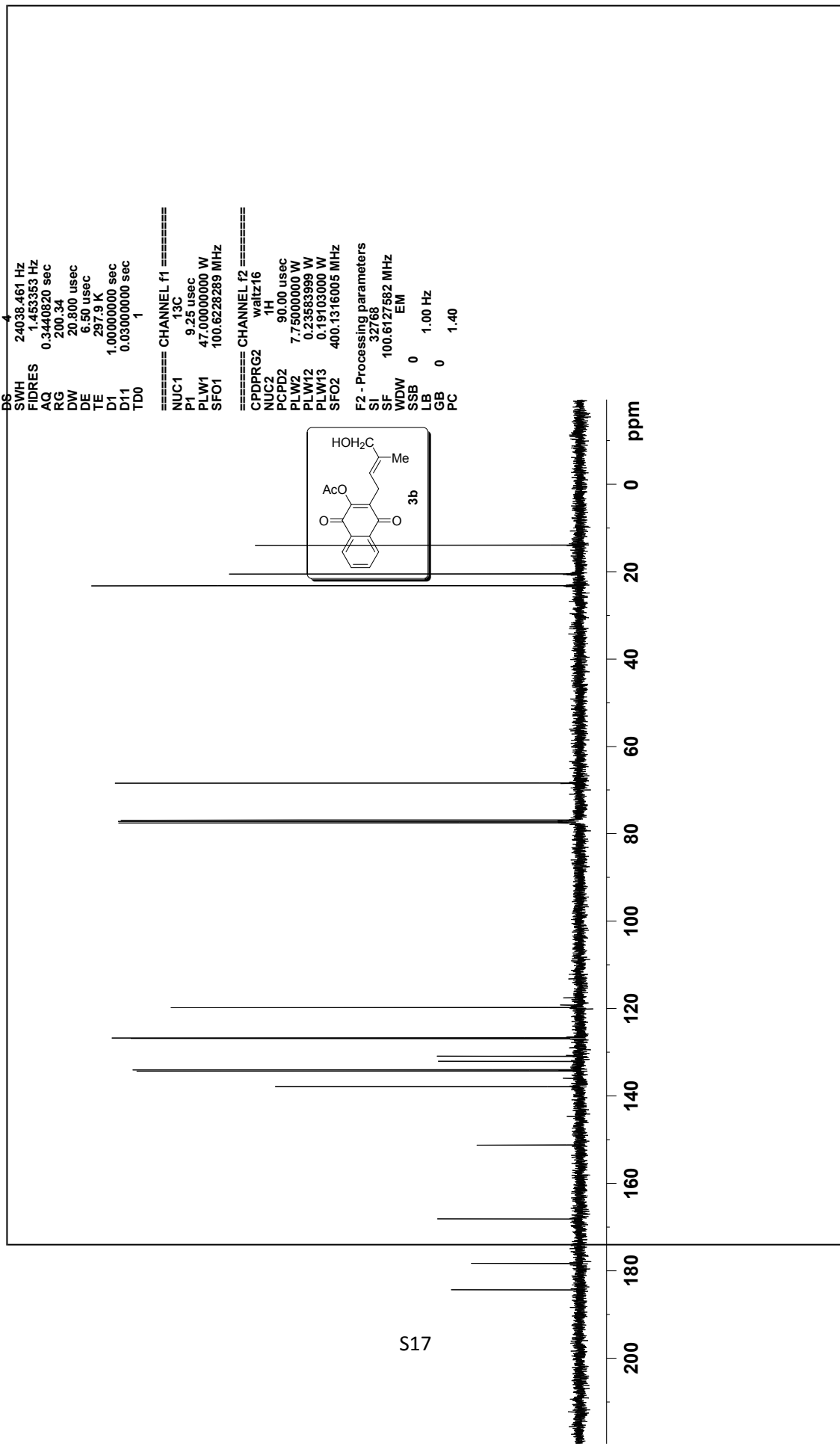
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NUC1 ¹³C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
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NUC2 ¹H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127582 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

184.38
178.32
168.13
151.24
137.85
134.28
134.25
134.04
134.01
132.07
130.90
126.88
126.85
126.81
126.72
126.69
119.79

77.48
77.16
76.84
68.39



¹³C NMR spectrum of compound 3b

Current Data Parameters
NAME sb41113
EXPNO 138
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131106
Time 23.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135
TD 32768
SOLVENT CDC13
NS 128
DS 4

SWH 20161.291 Hz
FIDRES 0.615274 Hz
AQ 0.8126964 sec
RG 200.34
DW 24.800 usec
DE 6.50 usec
TE 297.5 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

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

NUC1 13C
P1 9.25 usec
PLW0 2000.00 usec
PLW1 0 W
SFO1 47.00000000 W
SFO1 100.6208166 MHz
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SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 6.14429998 W

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

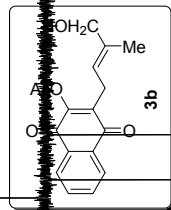
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NUC2 1H
P3 15.70 usec
P4 31.40 usec
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
SFO2 400.1312797 MHz

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

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13.83

134.18
133.90
126.74
126.62
119.68

68.28



DEPT NMR spectrum of compound 3b

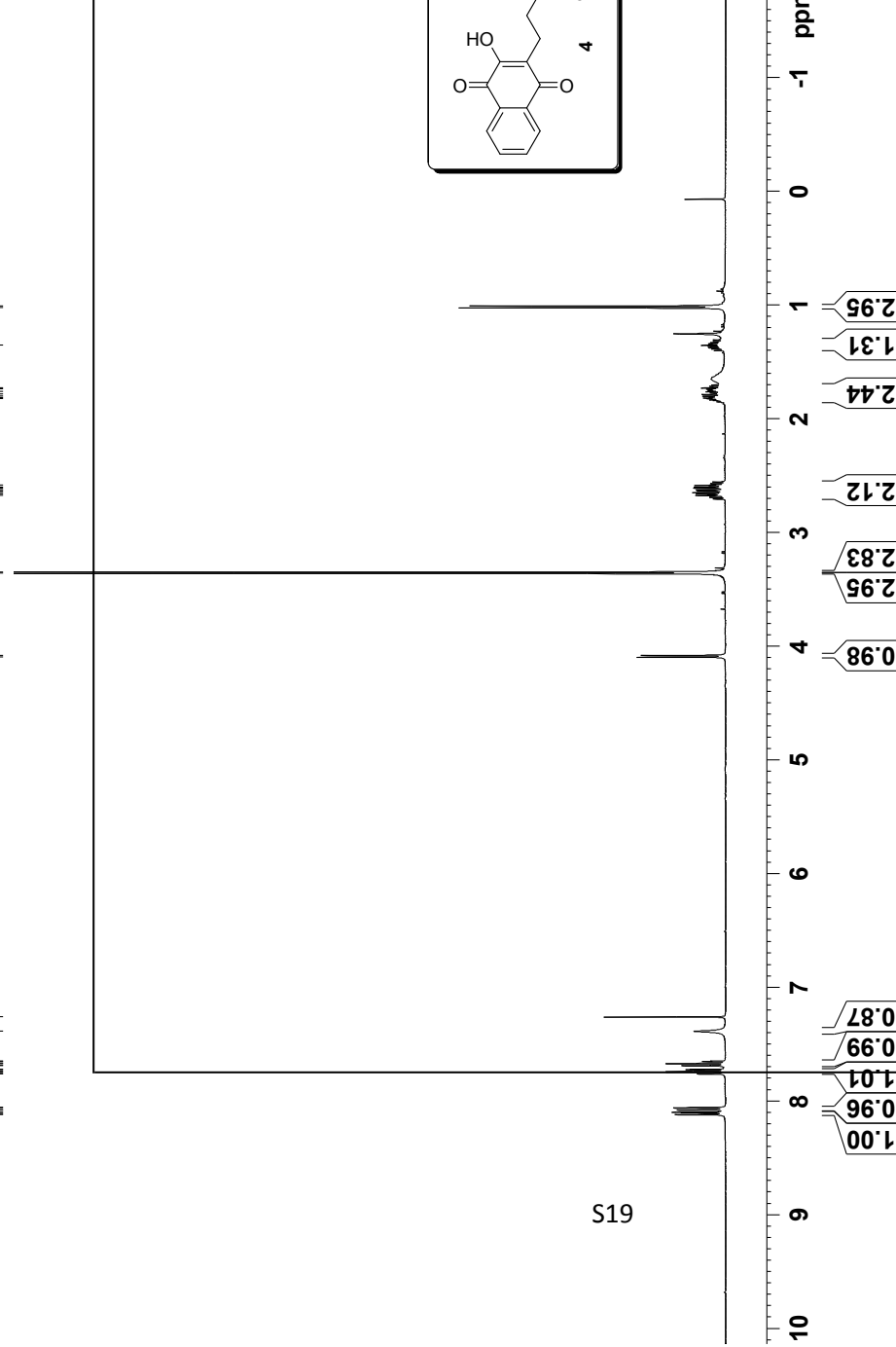
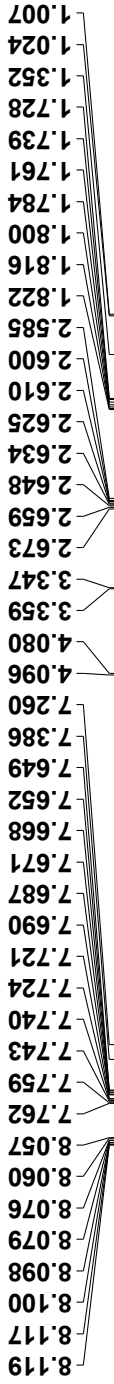
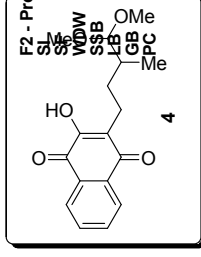
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EXPNO 271
PROCNO 1

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INSTRUM spect
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PULPROG zg30

TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 302.0 K
D1 0.5000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.7500000 W
SFO1 400.1320007 MHz

F2 - Processing parameters
SL 65536
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



S19

H NMR spectrum of compound 4

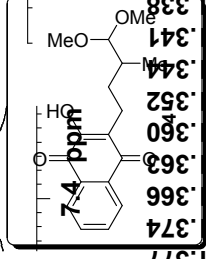
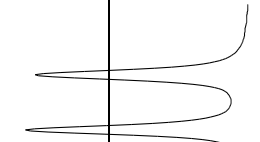
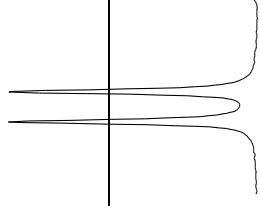
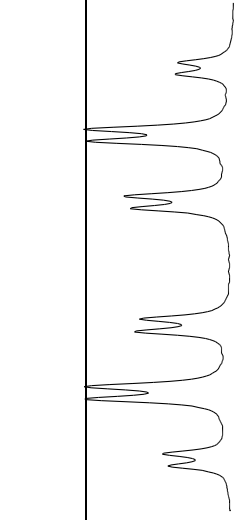
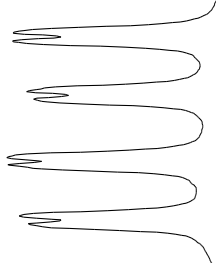
8.119
8.117
8.100
8.098
8.079
8.076
8.060
8.057

7.762
7.759
7.743
7.740
7.724
7.721
7.690
7.687
7.671
7.668
7.652
7.649

3.359
3.347

4.096
4.080

7.386



8.10 ppm

7.75 ppm

4.10 ppm

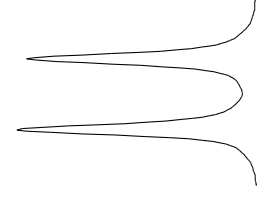
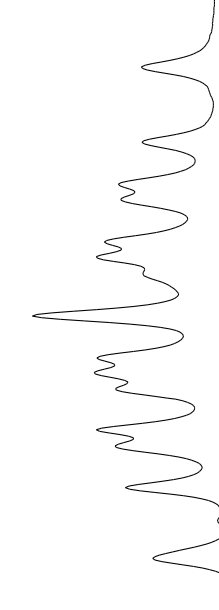
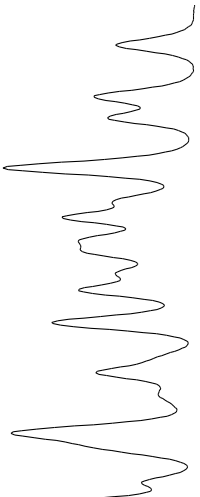
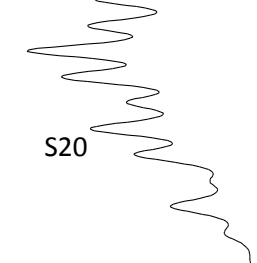
3.35 ppm

1.849
1.838
1.833
1.827
1.822
1.816
1.811
1.805

1.800
1.795
1.784
1.776
1.772
1.761
1.754
1.751
1.744
1.739
1.736
1.728
1.718
1.713
1.702

1.398
1.385
1.377
1.374
1.366
1.363
1.360
1.352
1.344
1.341
1.338
1.330
1.327
1.319
1.305

1.024
1.007



1.84 ppm

1.80 ppm

1.40 ppm

1.02 ppm

¹H NMR expanded spectrum of compound 4

lab sb
SB-EE-12
iitm_carbonshort

Current Data Parameters
NAME sb40913
EXPNO 272
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130930
Time_ 9.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540

SOLVENT CDC13

NS 1000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440820 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 302.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

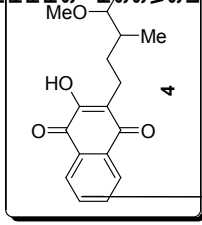
===== CHANNEL f1 =====

NUC1 ¹³C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

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

CPDPRG2 waltz16
NUC2 ¹H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SD 32768
SI 100.6127530 MHz
WDW EM
SSB 0 1.00 Hz
GB 0 1.40
PC



184.73
181.57
153.25
134.96
133.13
133.00
129.66
126.90
126.22
124.87
108.89
77.48
77.16
76.84
54.41
54.28
36.15
30.51
21.08
14.36

S21

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

¹³C NMR spectrum of compound 4

134.81
132.85
126.74
126.06
108.72
54.25
54.13
35.99
30.35
20.92
14.20

Current Data Parameters
NAME sb40913
EXPNO 273
PROCNO 1

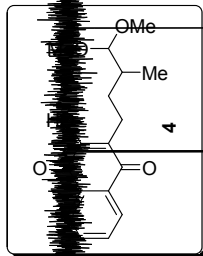
F2 - Acquisition Parameters
Date_ 20130930
Time 9.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135

TD 32768
SOLVENT CDCl3
NS 128
DS 4
SWH 20161.291 Hz
FIDRES 0.615274 Hz
AQ 0.8126964 sec
RG 200.34
DW 24.800 usec
DE 6.50 usec
TE 302.4 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW0 2000.00 usec
PLW1 0 W
SFO1 47.00000000 W
SPNAM5 Cnp60comp.4
SFO1 100.6208166 MHz
SPOALS Cnp60comp.4
SPOFFS5 0 Hz
SPW5 6.14429998 W

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 15.70 usec
PLW2 31.40 usec
PCPD2 90.00 usec
PLW2 7.75000000 W
SFO2 400.1312797 MHz
SFO2 0.23583999 W

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

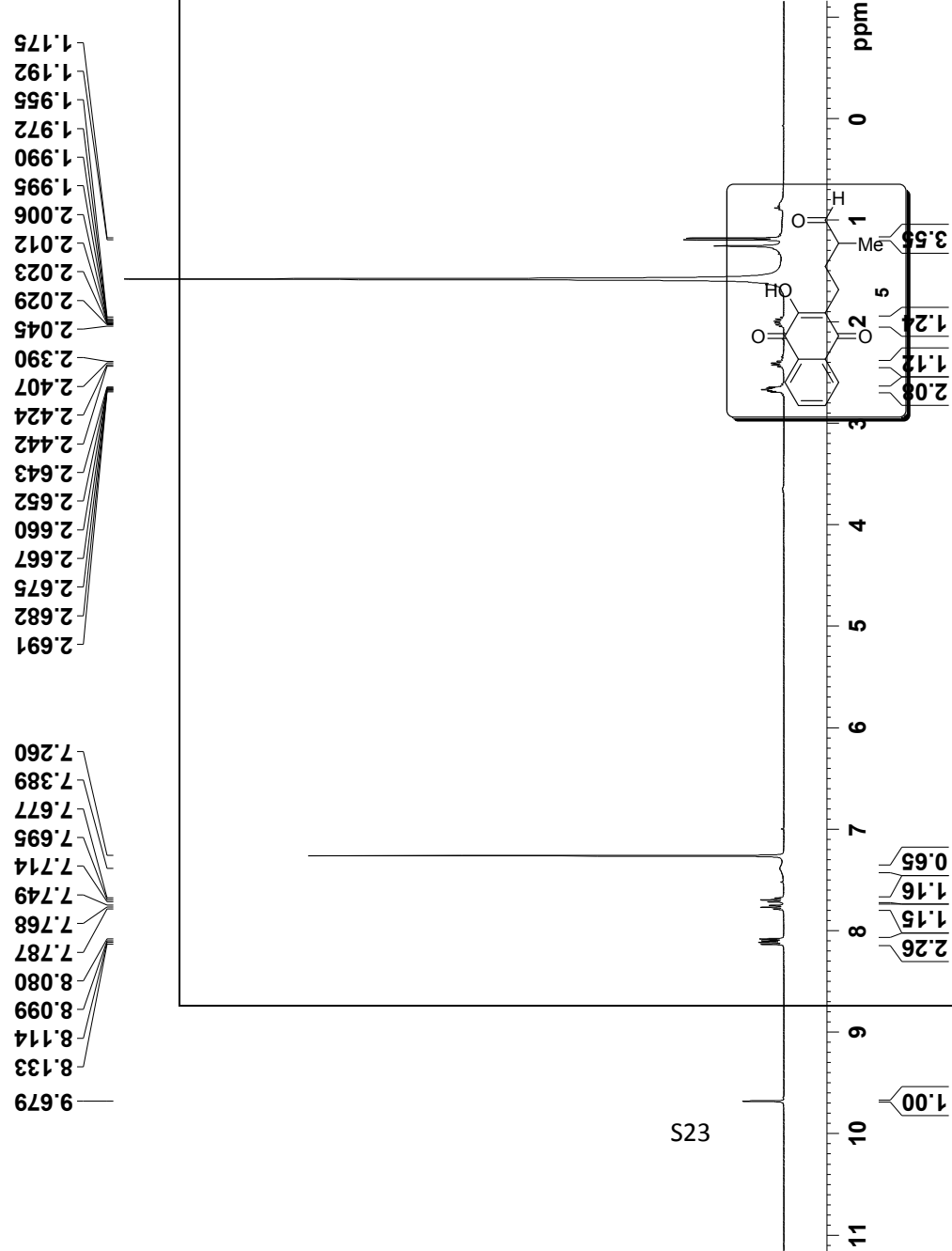


S22

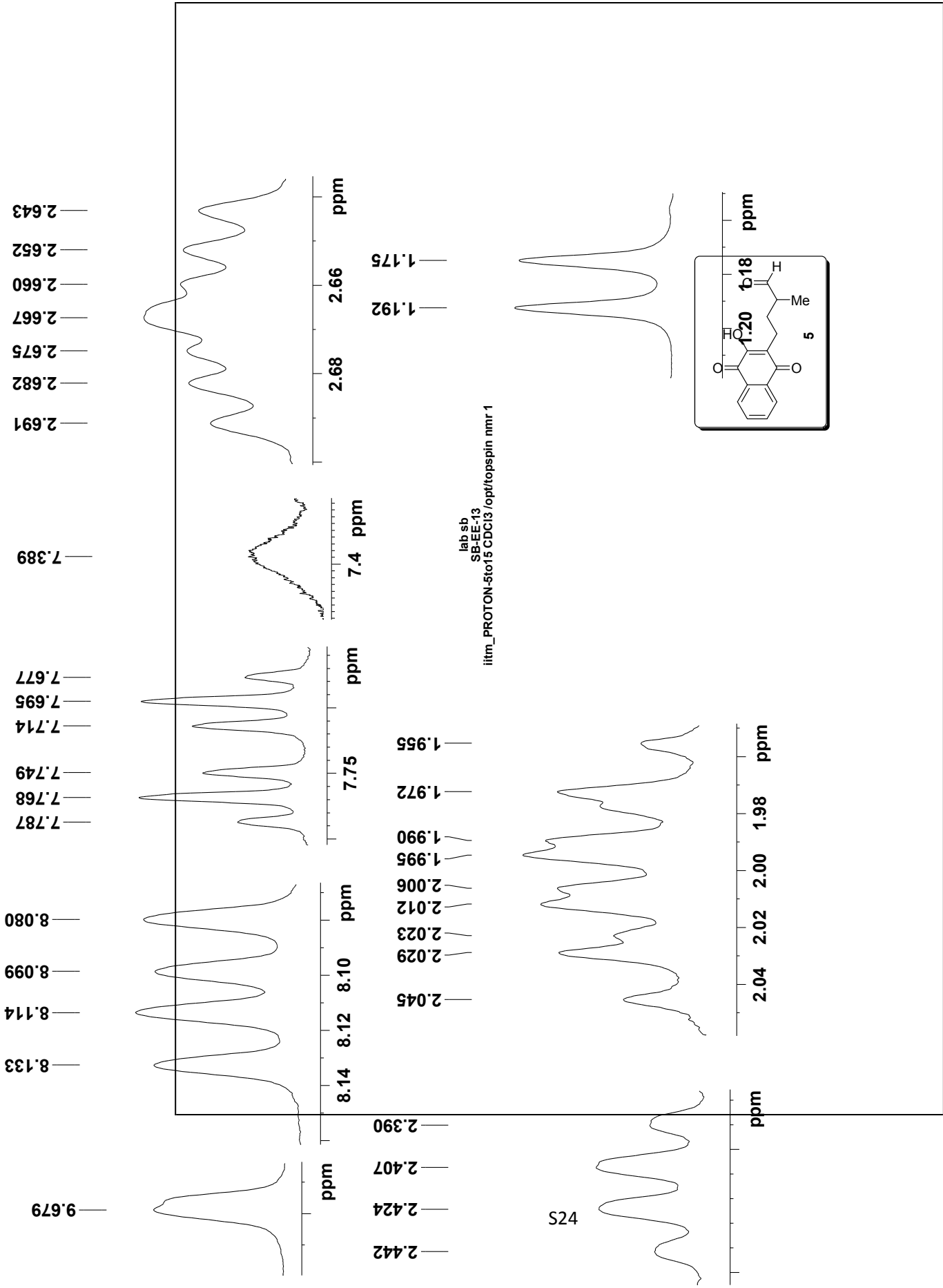
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

DEPT NMR spectrum of compound 4

Current Data Parameters
NAME sb41013
EXPNO 233
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131016
Time 8.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 488
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 297.7 K
D1 0.50000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR spectrum of compound 5



¹H NMR expanded spectrum of compound 5

Current Data Parameters
NAME sb51013
EXPNO 56
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131012
Time_ 10:18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 32

DS 2

SWH 10000.000 Hz

FIDRES 0.305176 Hz

AQ 1.6384500 sec

RG 202.34

DW 50.000 usec

DE 6.50 usec

TE 298.2 K

D1 0.5000000 sec

TD0 1

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

SFO1 500.1525008 MHz

NUC1 1H

P1 11.75 usec

PLW1 15.30000019 W

F2 - Processing parameters

SI 65536

SF 500.1500229 MHz

WDW EIM

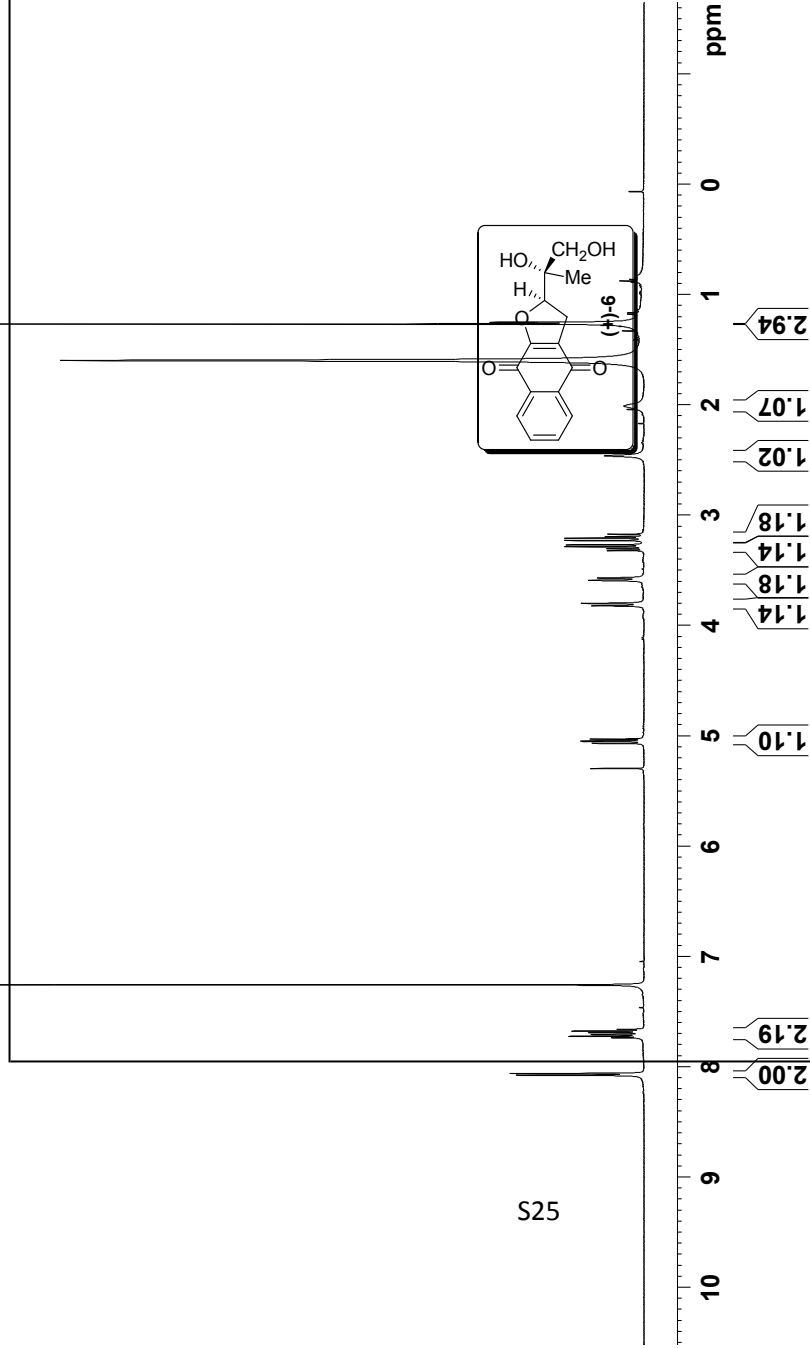
SSB 0

LB 0.30 Hz

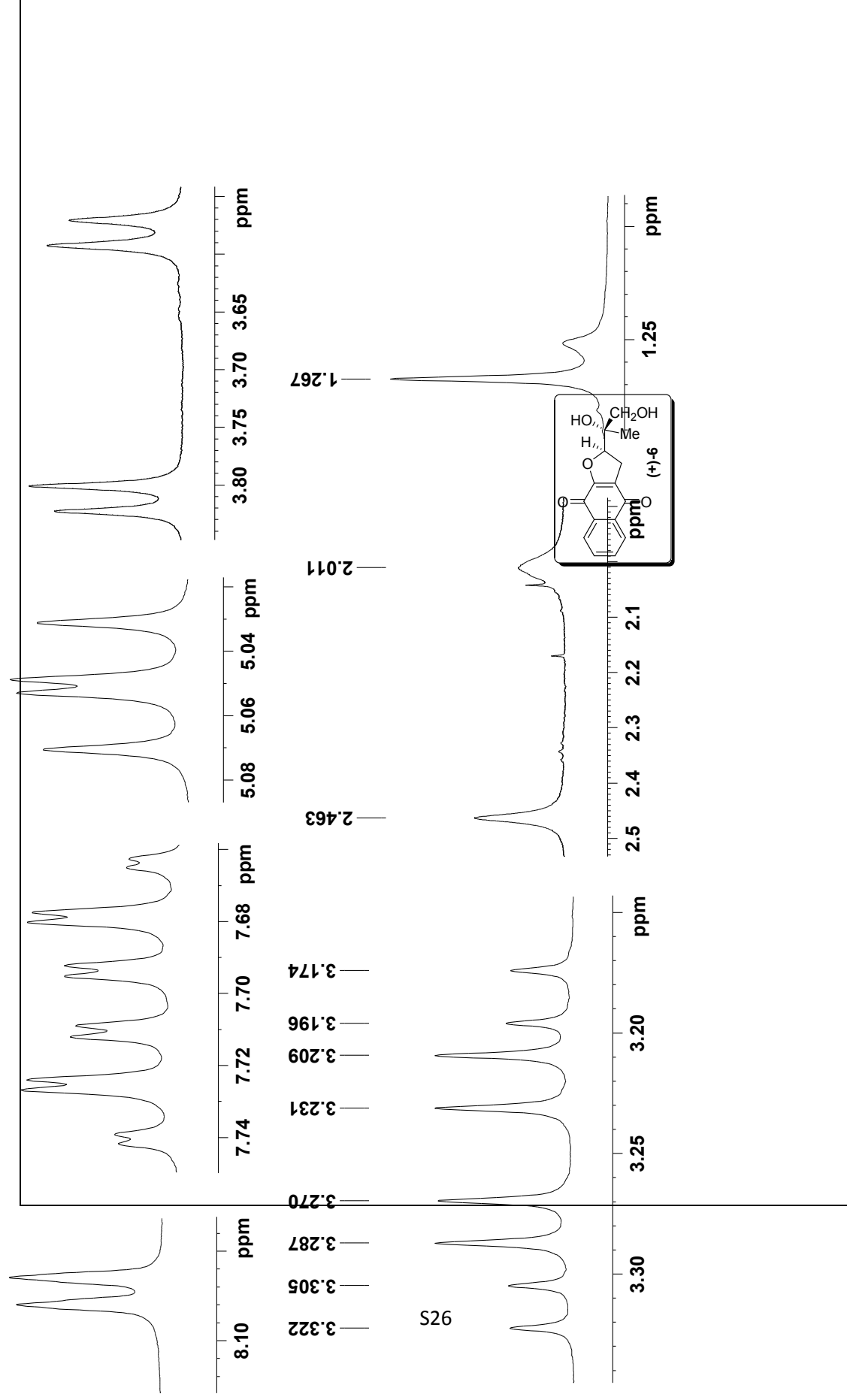
GB 0

PC 1.00

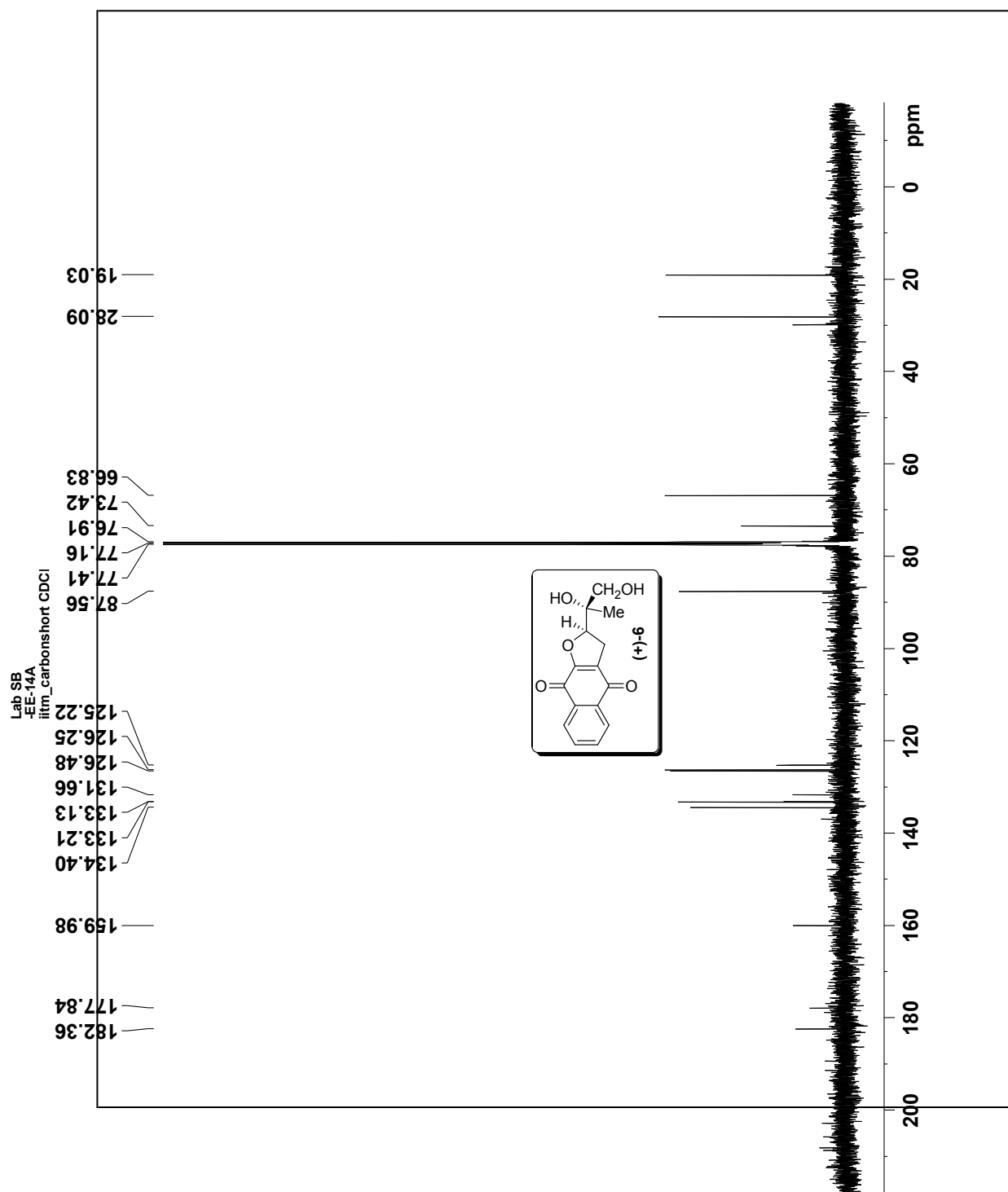
8.080
8.065
7.742
7.739
7.727
7.724
7.712
7.709
7.695
7.692
7.680
7.677
7.665
7.662
7.260
5.071
5.053
5.049
5.031
3.823
3.801
3.592
3.571
3.322
3.305
3.287
3.270
3.231
3.209
3.196
3.174
2.463
2.011
1.267



1H NMR spectrum of compound (+)-6

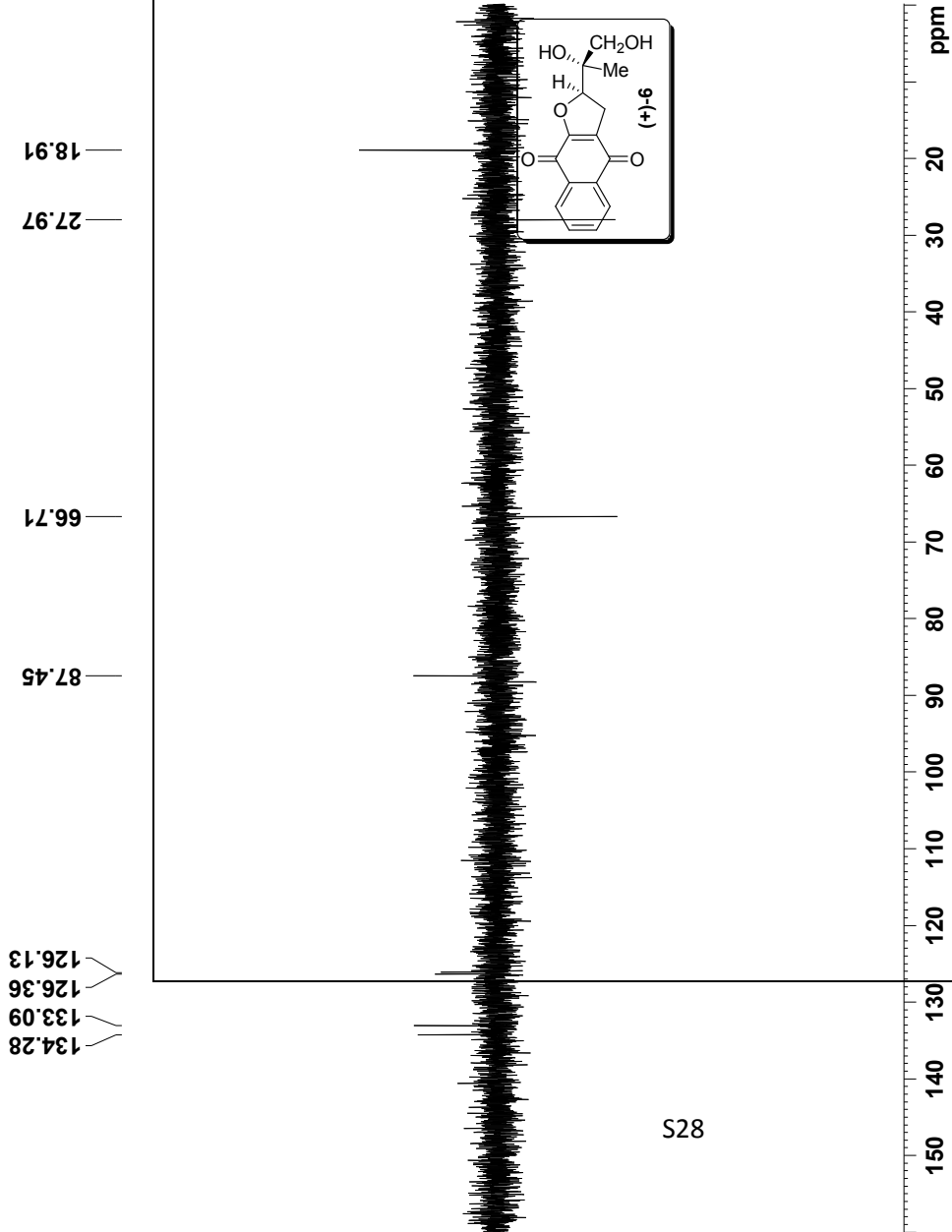


^1H NMR expanded spectrum of compound (+)-6



^{13}C NMR spectrum of compound (+)-6

Current Data Parameters
NAME sb51013
EXPNO 58
PROCNO 1



DEPT NMR spectrum of compound (+)-6

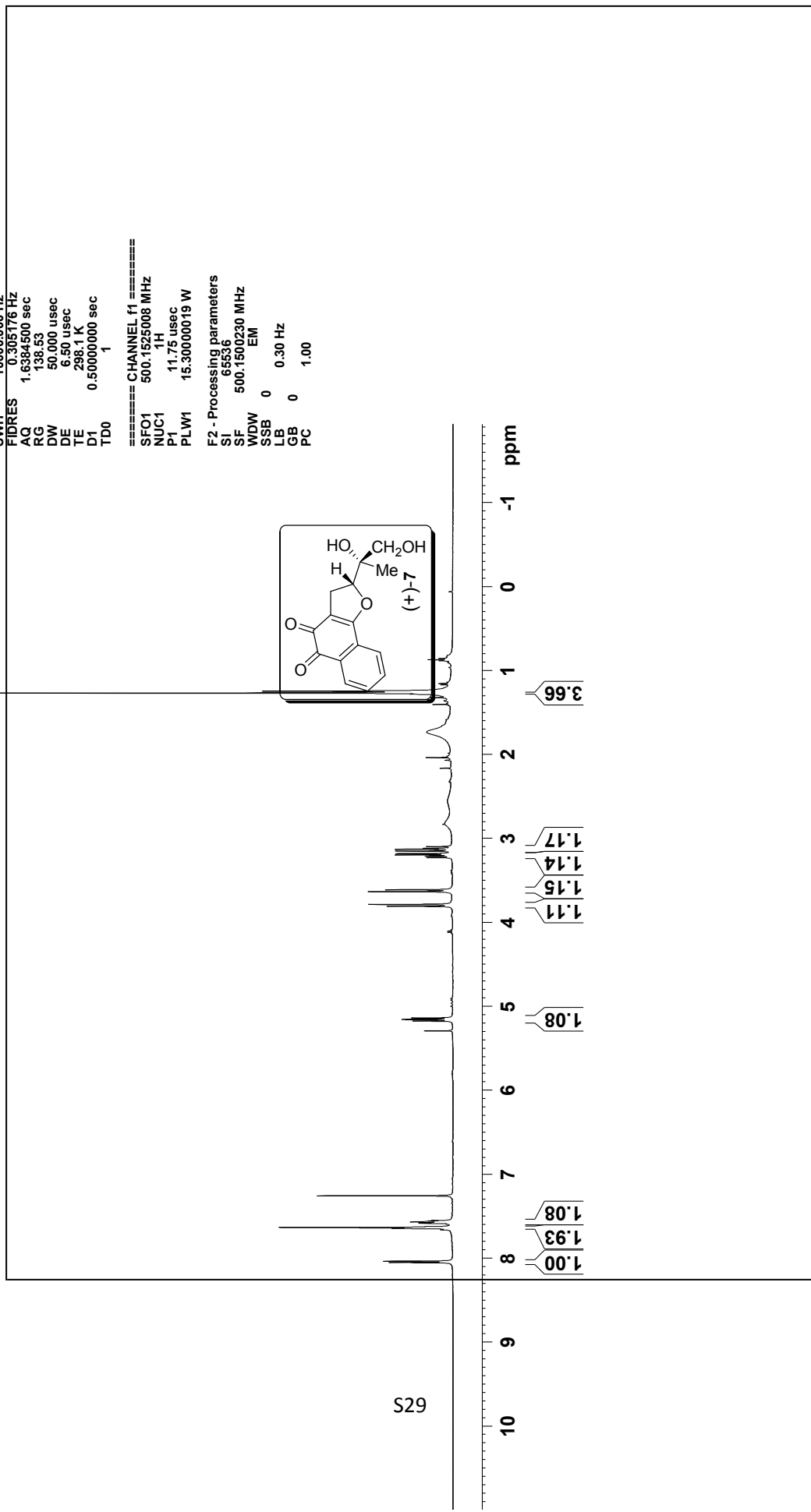
Current Data Parameters
NAME sb51013
EXPNO 49
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131012
Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6384500 sec
RG 138.53
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 0.50000000 sec
TD0 1

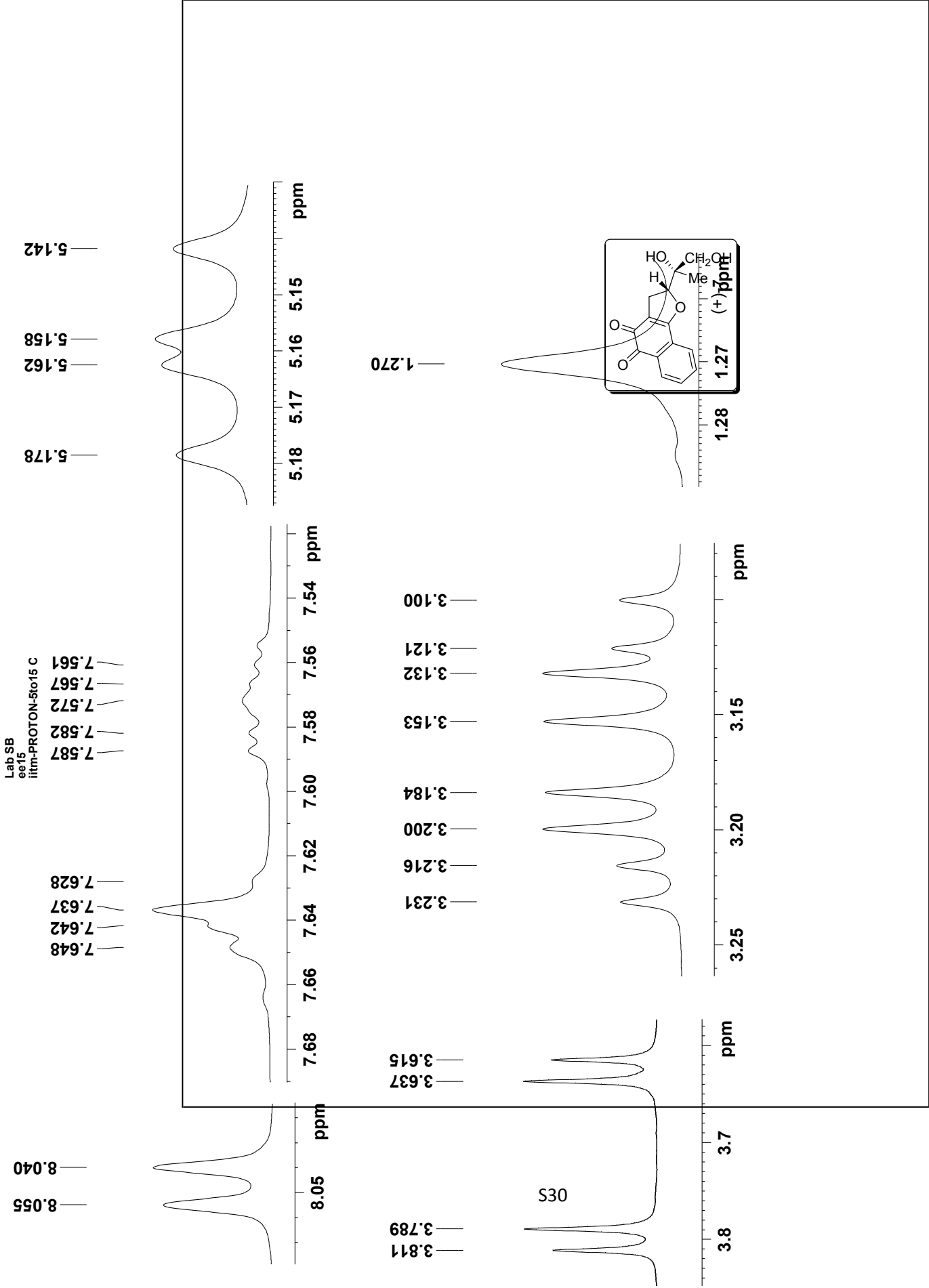
===== CHANNEL f1 =====
SFO1 500.1525008 MHz
NUC1 1H
P1 11.75 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 500.1500230 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.055
8.040
7.648
7.642
7.637
7.628
7.587
7.582
7.572
7.567
7.561
7.260
5.178
5.162
5.158
5.142
3.811
3.789
3.637
3.615
3.231
3.216
3.200
3.184
3.153
3.132
3.121
3.100
1.270

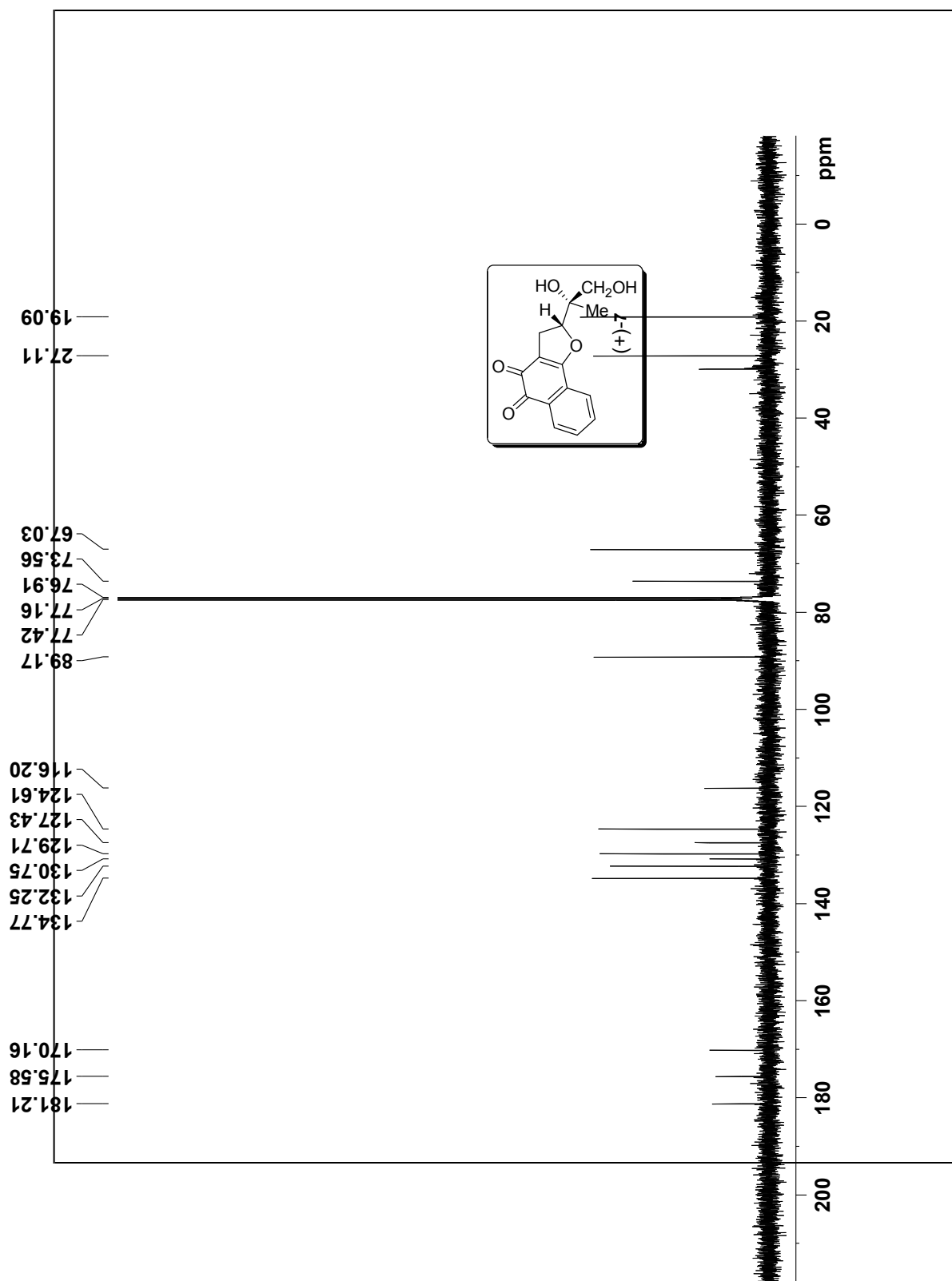


¹H NMR spectrum of compound (+)-7



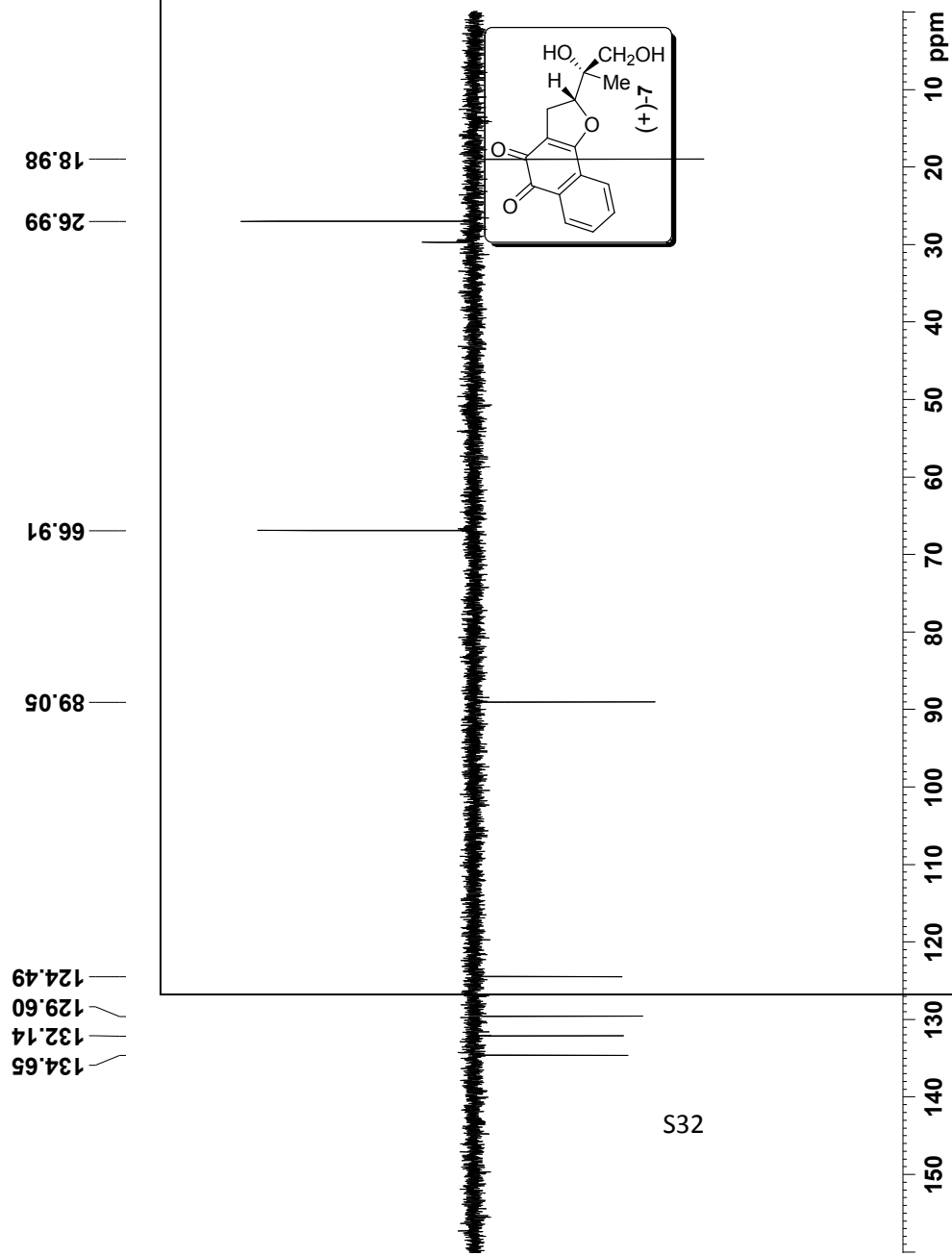
¹H NMR expanded spectrum of compound (+)-7

Lab SB
ee15
itm_carbonshort CDCl₃



¹³C NMR spectrum of compound (+)-7

Current Data Parameters
NAME sb51013
EXPNO 51
PROCNO 1

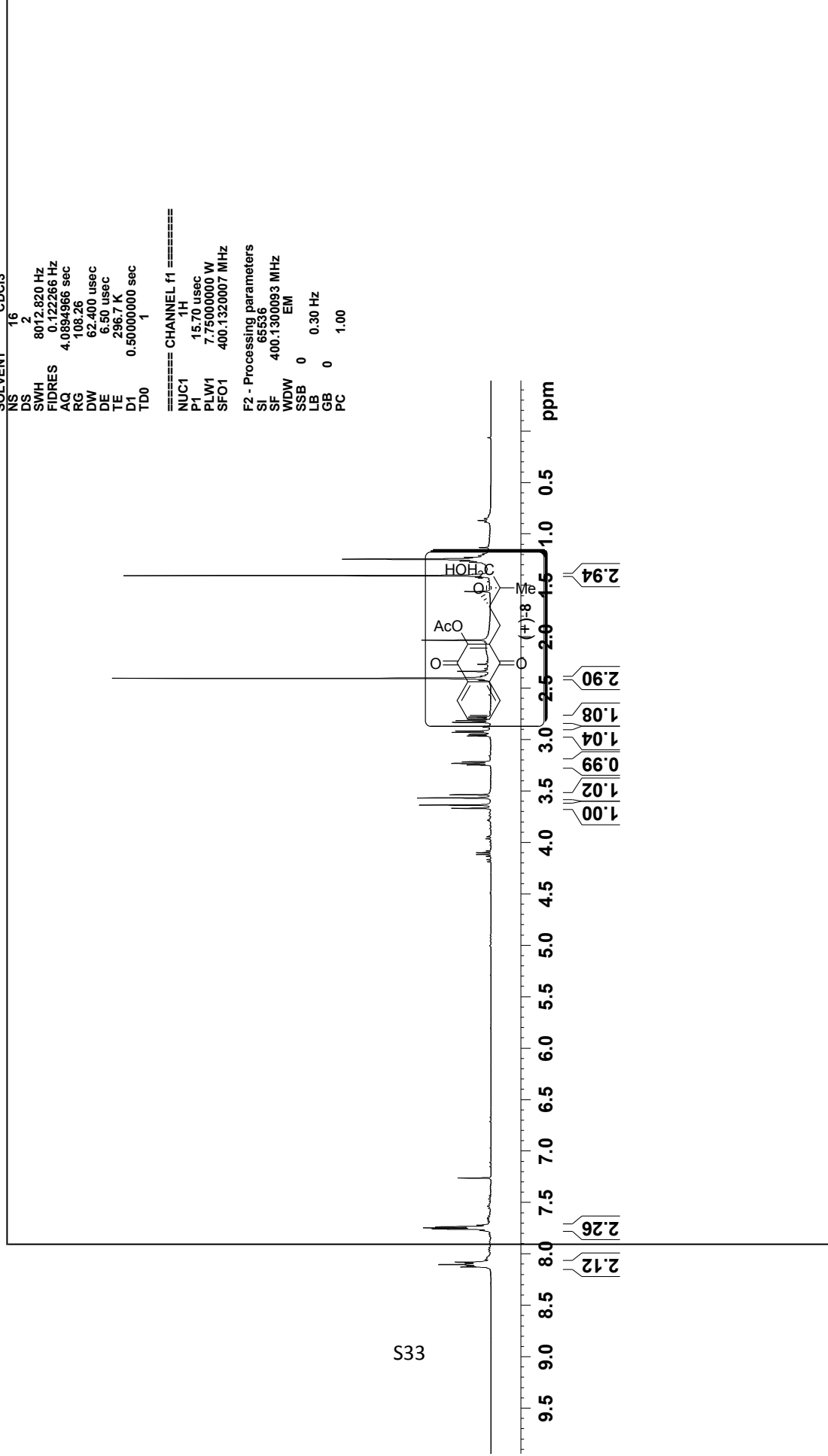


Current Data Parameters

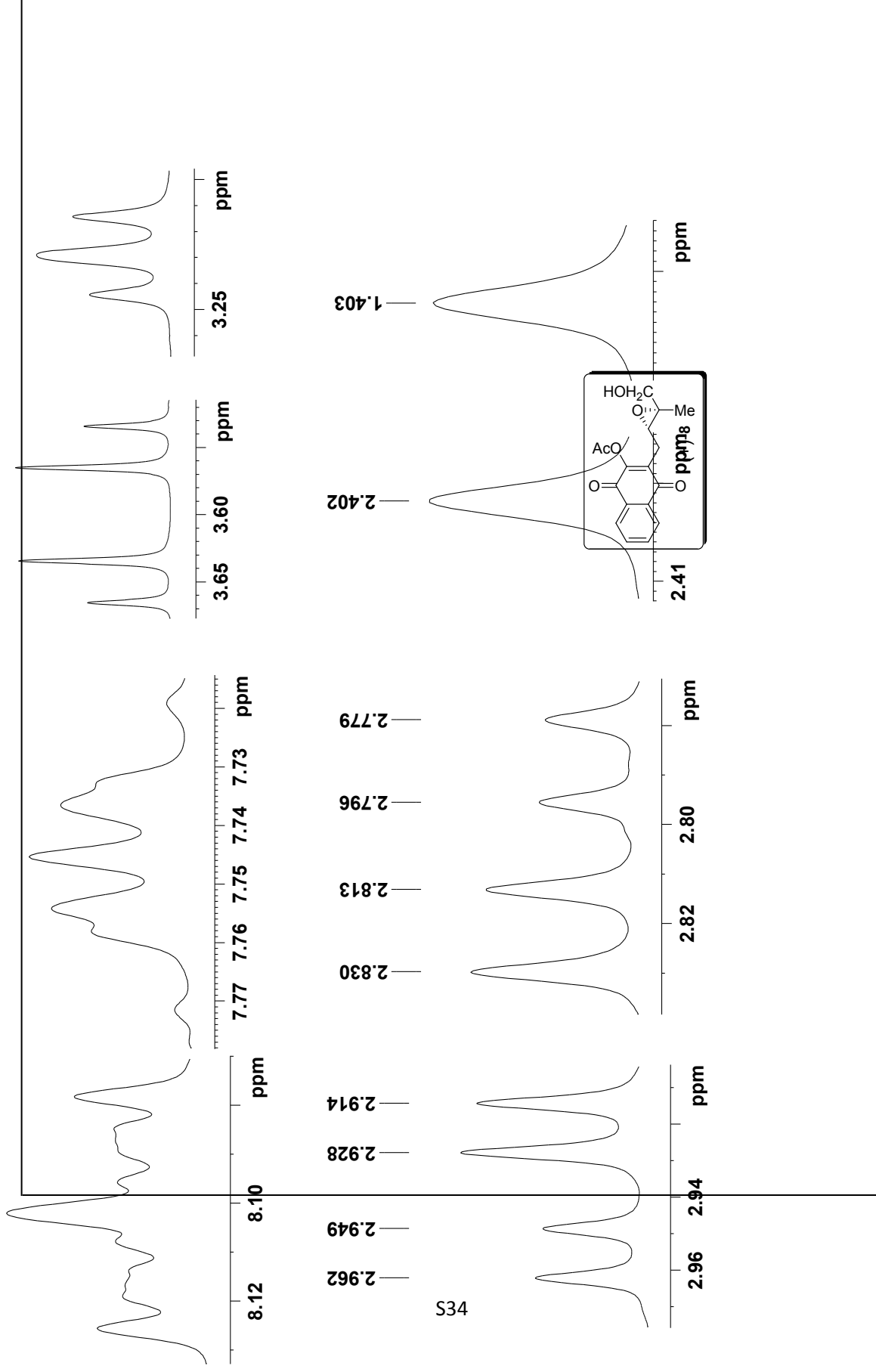
NAME sd41113
EXPNO 235
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131113
Time 0.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 108.26
DW 62.400 usec
DE 6.50 usec
TE 296.7 K
D1 0.50000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.7500000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.130093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3.665
3.635
3.565
3.534
3.244
3.229
3.214
2.962
2.949
2.928
2.914
2.830
2.813
2.796
2.779
2.402
1.403

8.126
8.119
8.117
8.114
8.108
8.102
8.096
8.087
8.085
8.078
7.771
7.758
7.754
7.745
7.737
7.719
7.260



1H NMR spectrum of compound (+)-8



^1H NMR expanded spectrum of compound (+)-8

Current Data Parameters
NAME sb41113
EXPNO 236
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131113
Time 1.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCI3
NS 376
DS 4

SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440820 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

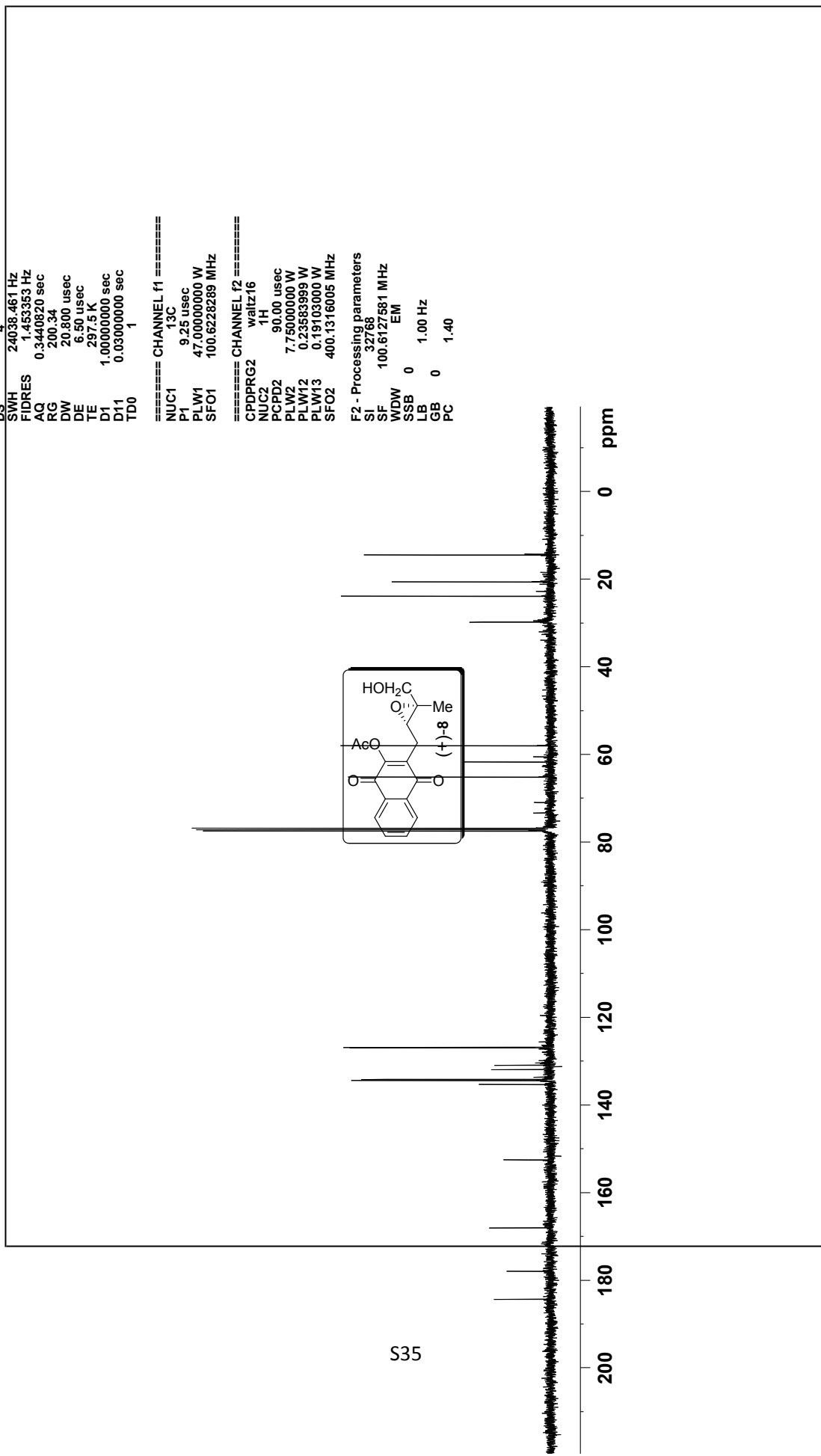
F2 - Processing parameters
SI 32768
SF 100.6127581 MHz
WDW EM
SSB 0 1.00 Hz
LB 0
GB 0
PC 1.40

23.89
20.60
14.48

77.48
77.16
76.84
65.16
61.72
58.00

152.55
135.33
134.42
134.18
131.96
130.94
126.96
126.88

184.37
177.98
168.06



¹³C NMR spectrum of compound (+)-8

Current Data Parameters
NAME sb41113
EXPNO 237
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131113
Time_ 1.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG depts135
TD 32768
SOLVENT CDC13
NS 110

DS 4
SWH 20161.291 Hz
FIDRES 0.615274 Hz
AQ 0.8126964 sec
RG 200.34
DW 24.800 usec
DE 6.50 usec
TE 297.1 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

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

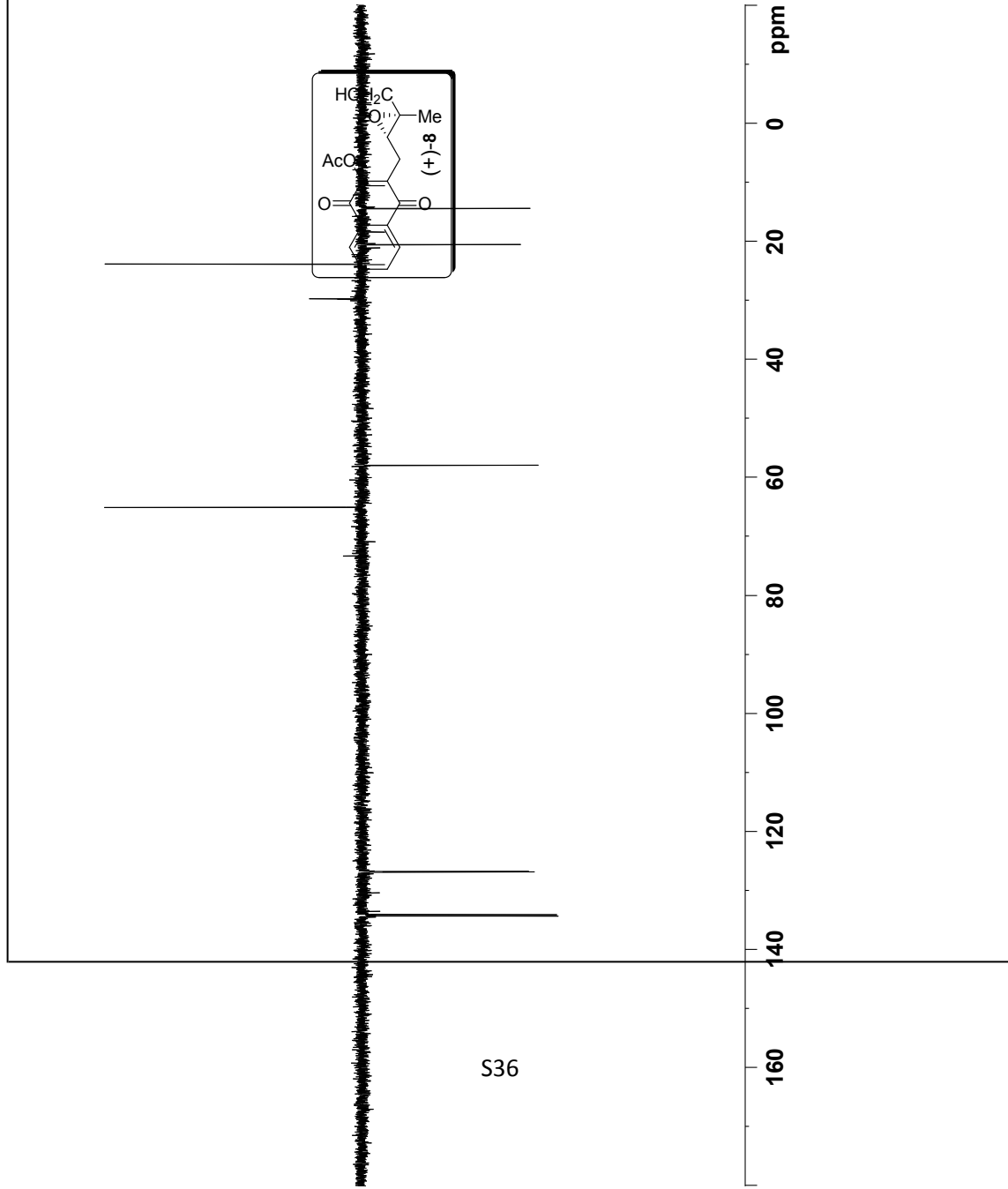
NUC1 13C
P1 9.25 usec
PLW0 2000.00 usec
PLW1 0 W
SFO1 47.00000000 W
SPNAM5 C1p60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 6.14429998 W

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

CPDPRG2 waltz16
NUC2 1H
P3 15.70 usec
P4 31.40 usec
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
SFO2 400.1312797 MHz

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

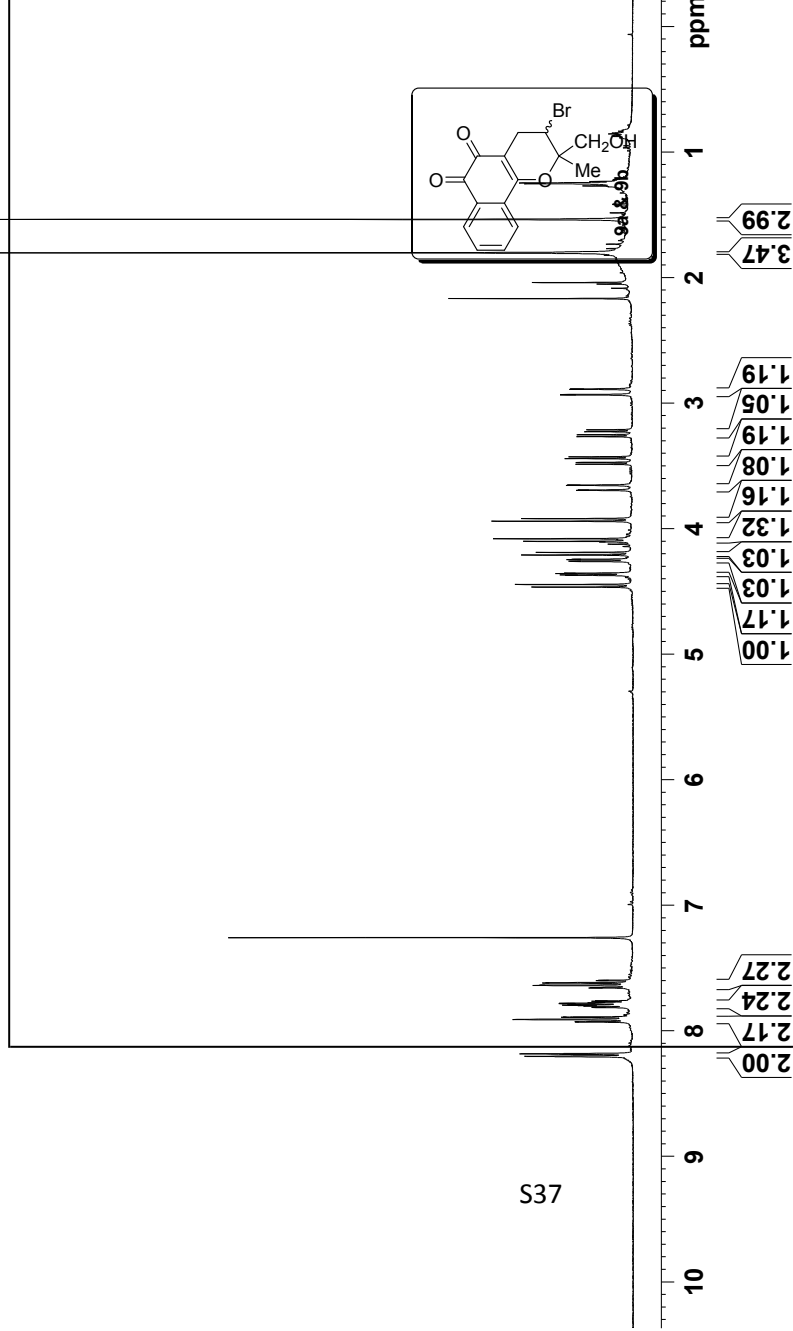
126.77
126.85
134.08
134.31
57.89
65.05
23.78
20.49
14.37



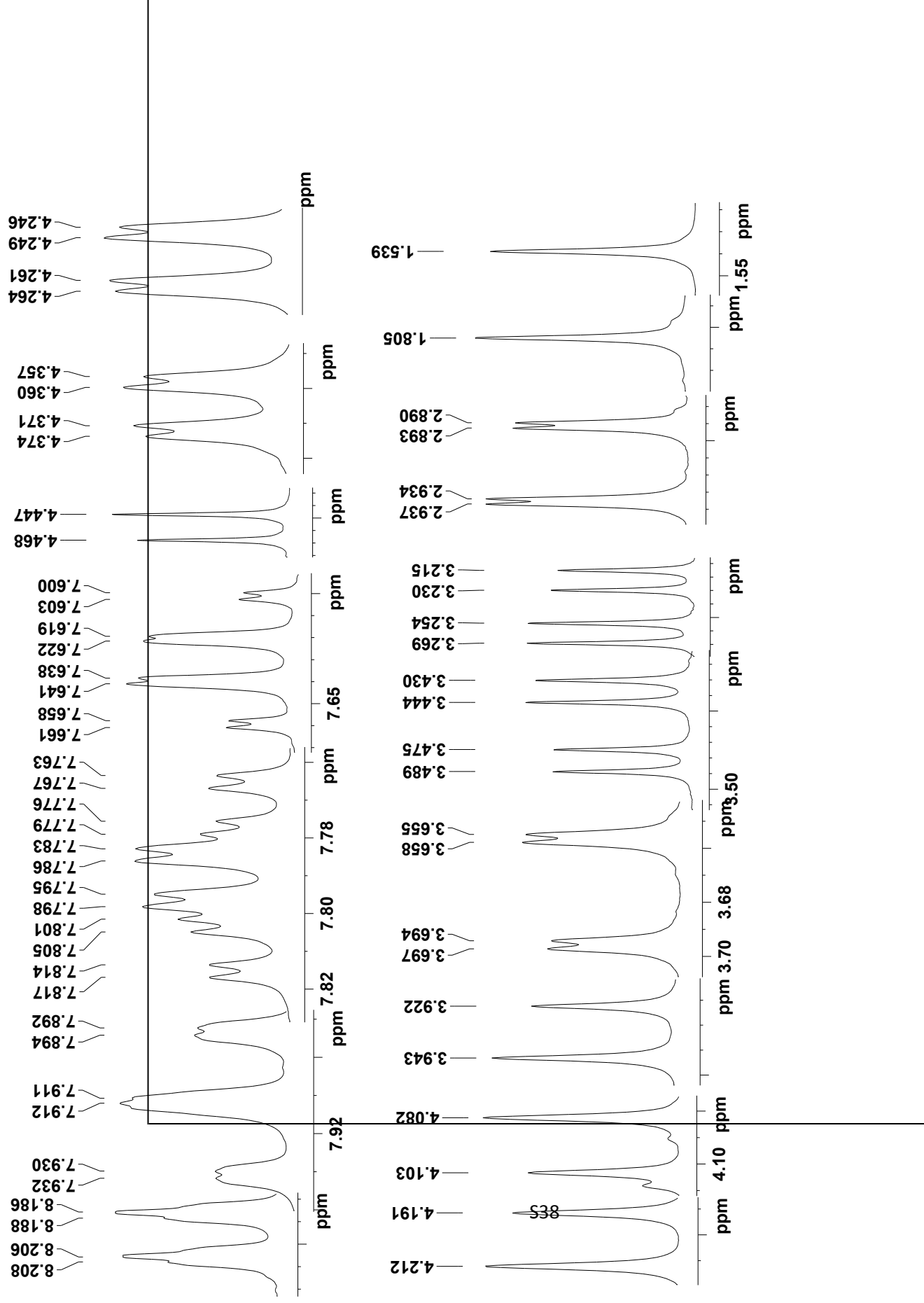
DEPT NMR spectrum of compound (+)-8

Current Data Parameters
 NAME sb41113
 EXPNO 304
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131118
 Time_ 17:27
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 200.34
 DW 62.400 usec
 DE 6.50 usec
 TE 296.0 K
 D1 0.5000000 sec
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 15.70 usec
 PLW1 7.7500000 W
 SFO1 400.1320007 MHz
 F2 - Processing parameters
 SI 65536
 SF 400.1300094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.208
8.206
8.188
8.186
7.912
7.911
7.894
7.892
7.798
7.795
7.786
7.783
7.641
7.638
7.622
7.619
7.260
4.468
4.447
4.374
4.371
4.360
4.357
4.264
4.261
4.249
4.246
4.212
4.191
4.103
4.082
3.943
3.922
3.658
3.655
3.444
3.430
2.937
2.934
2.893
2.890
1.805
1.539



¹H NMR spectrum of compound 9a & 9b



¹H NMR expanded spectrum of compound 9a & 9b

Current Data Parameters
 NAME sb41113
 EXPNO 305
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131118
 Time 18.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 16540

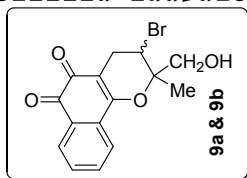
SOLVENT CDC13

NS 2500
 DS 4
 SWH 24038.461 Hz
 FIDRES 1.453353 Hz
 AQ 0.3440820 sec
 RG 200.34
 DW 20.800 usec
 DE 6.50 usec
 TE 296.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

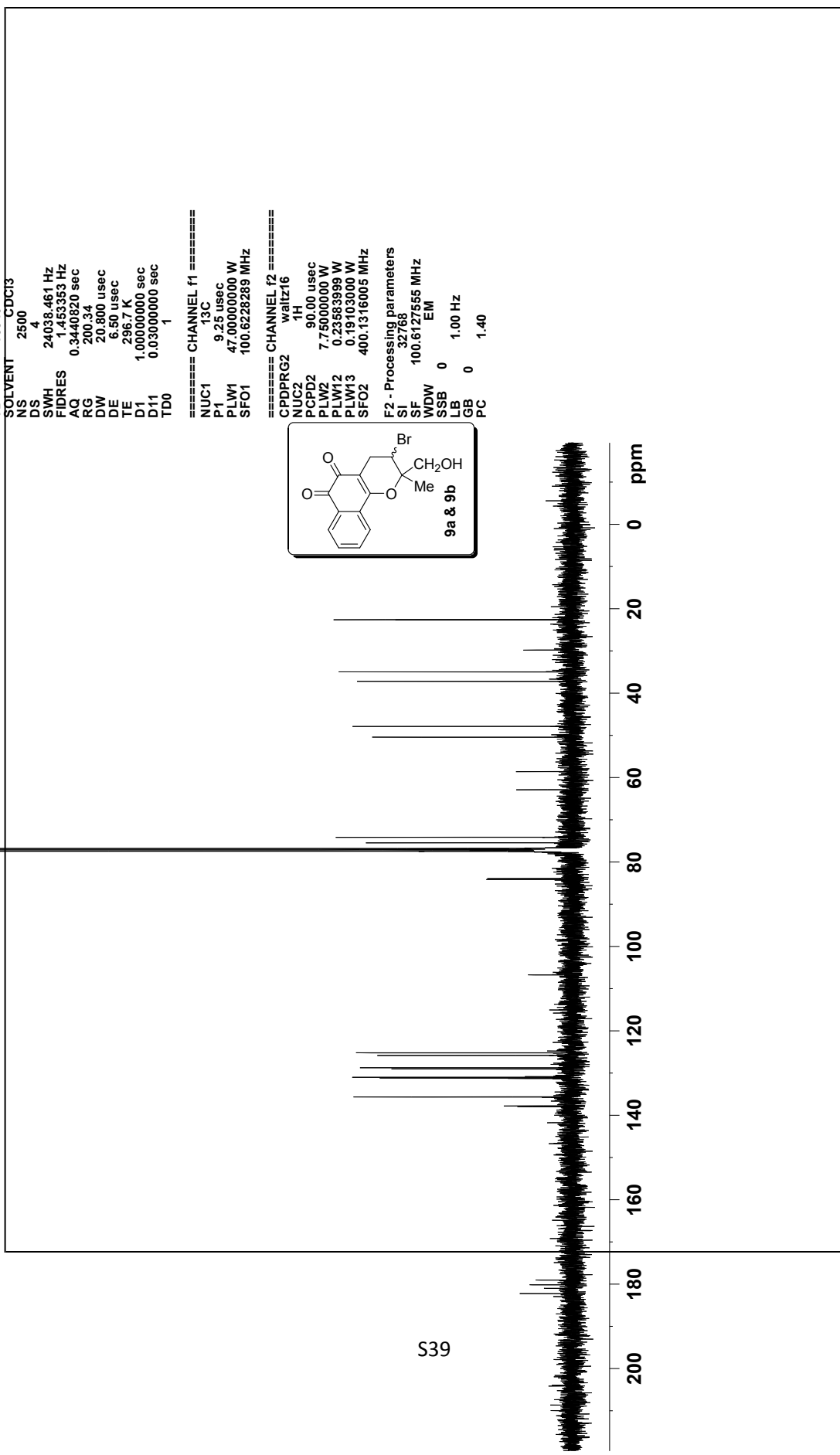
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.25 usec
 PLW1 47.00000000 W
 SFO1 100.6228289 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 7.75000000 W
 PLW12 0.23583999 W
 PLW13 0.19103000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127555 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



182.31
 180.23
 179.10
 138.01
 137.85
 135.70
 131.33
 131.24
 131.06
 130.90
 129.08
 128.79
 125.88
 125.26
 106.80
 84.20
 83.96
 77.48
 77.36
 77.16
 76.84
 75.49
 74.19
 62.92
 58.62
 50.48
 47.93
 37.24
 34.99
 22.67
 22.62



¹³C NMR spectrum of compound 9a & 9b

Current Data Parameters
 NAME sb41113
 EXPNO 306
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131118
 Time 18.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG deptsp135
 TD 32768
 SOLVENT CDCl3
 NS 256
 DS 4

SWH 20161.291 Hz
 FIDRES 0.615274 Hz
 AQ 0.8126964 sec
 RG 200.34
 DW 24.800 usec
 DE 6.50 usec
 TE 296.3 K
 CNST2 145.0000000
 D1 1.000000000 sec
 D2 0.00344828 sec
 D12 0.0002000 sec
 TD0 1

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

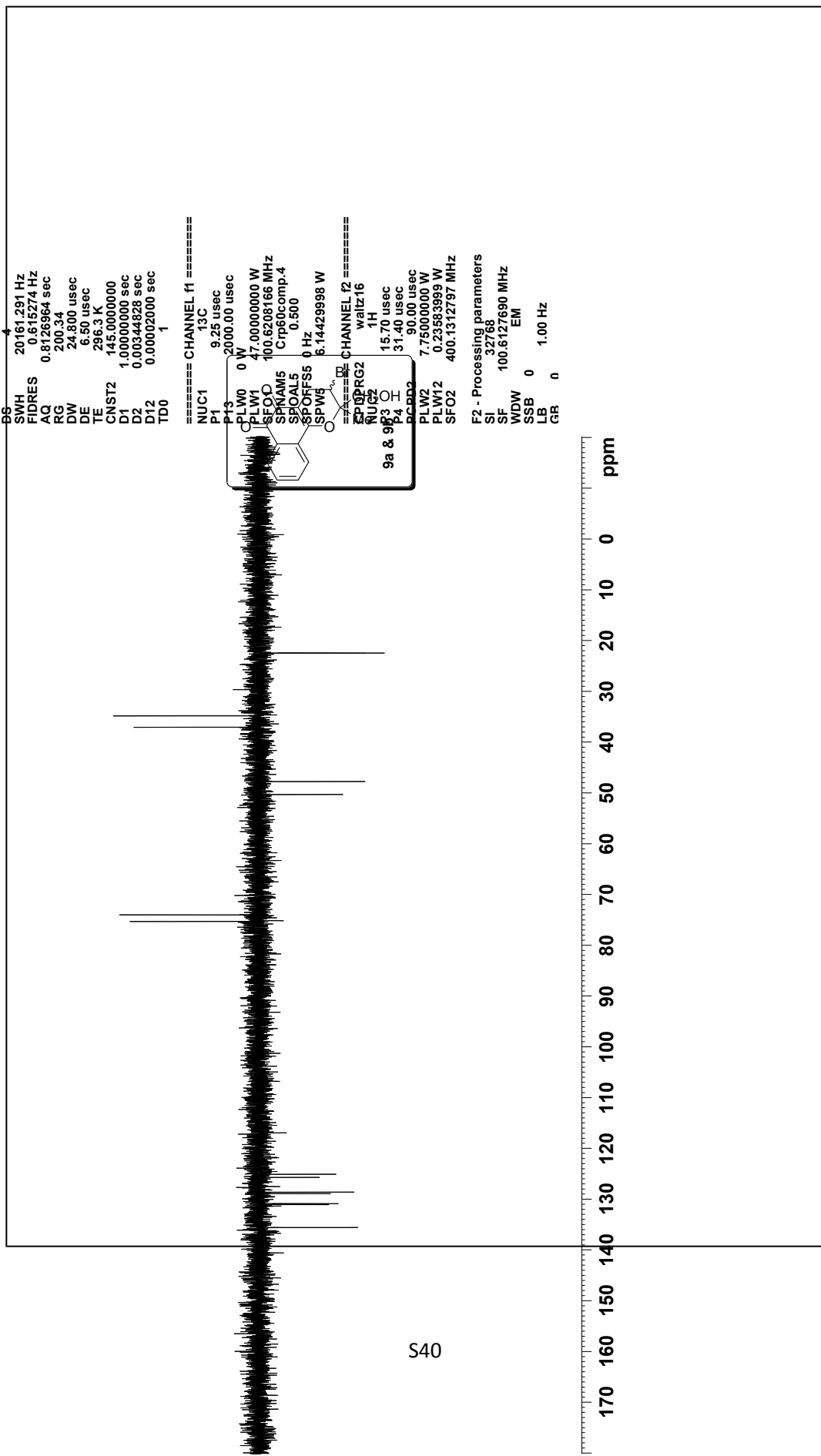
NUC1 13C
 P1 9.25 usec
 PL13 2000.00 usec
 PLW0 0 W
 PLW1 47.00000000 W
 SFO1 100.6208166 MHz
 SPNAM5 Crp50comp.4
 SFOALS 0.500
 SPOF5 0 Hz
 SPW5 6.14429998 W

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

CPDPRG2 waltz16
 NUC2 1H
 P2 15.70 usec
 PL2 31.40 usec
 PLW2 7.75000000 W
 PLW12 0.23583999 W
 SFO2 400.1312797 MHz

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

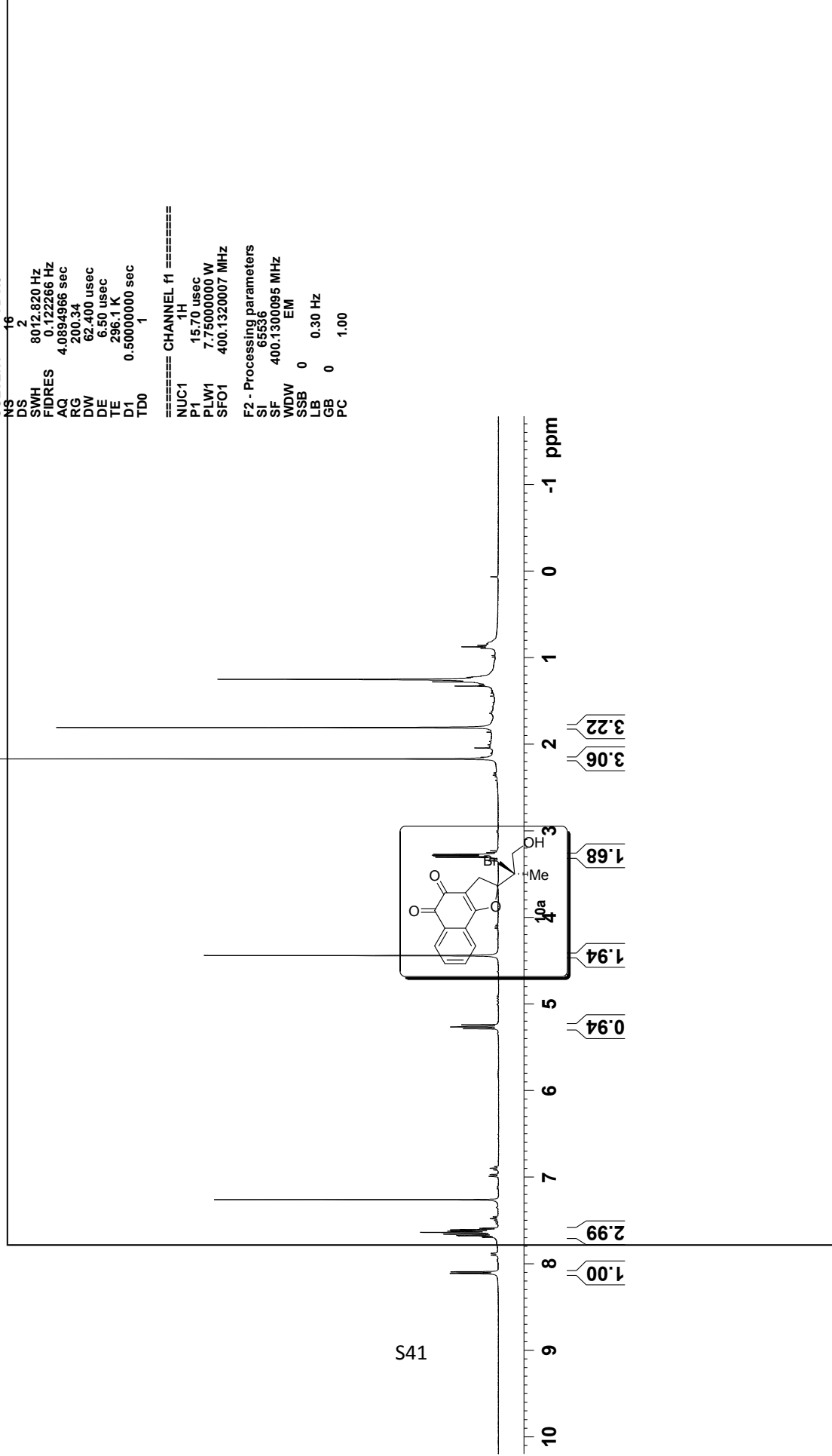
135.59
 135.57
 131.11
 130.93
 128.95
 128.66
 125.75
 125.13
 75.36
 74.05
 50.34
 47.80
 37.11
 34.86
 22.54
 22.49



DEPT NMR spectrum of compound 9a & 9b

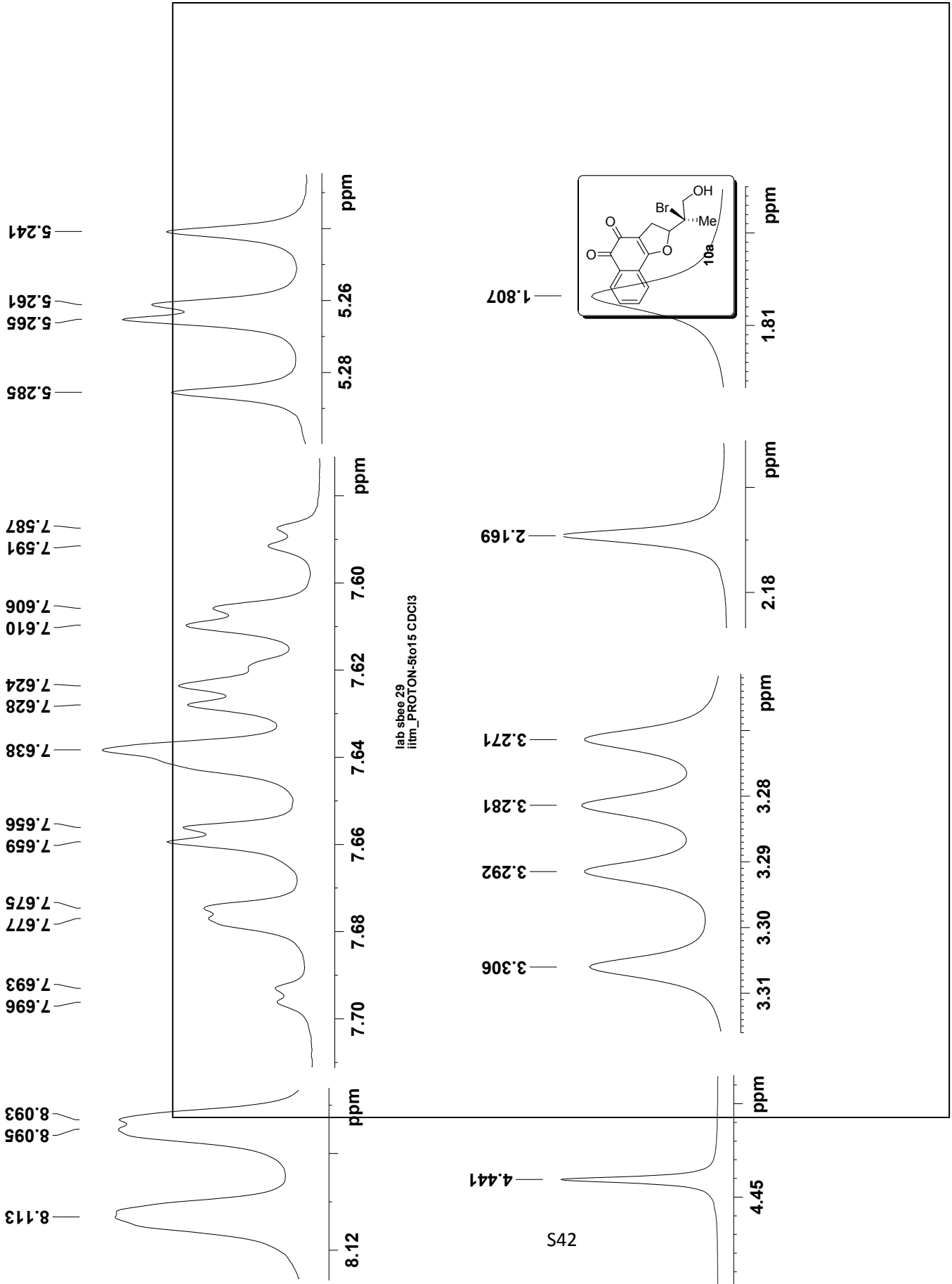
Current Data Parameters
 NAME sb41113
 EXPNO 298
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20131118
 Time_ 15:13
 INSTRUM spect
 PROBHHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 200.34
 DW 62.400 usec
 DE 6.50 usec
 TE 296.1 K
 D1 0.50000000 sec
 TD0 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 15.70 usec
 PLW1 7.75000000 W
 SFO1 400.1320007 MHz
 F2 - Processing parameters
 SI 65536
 SF 400.1300095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.113
8.095
8.093
7.966
7.693
7.677
7.675
7.659
7.656
7.638
7.628
7.624
7.610
7.606
7.591
7.587
7.260
5.285
5.265
5.261
5.241
4.441
3.306
3.292
3.281
3.271
2.169
1.807



¹H NMR spectrum of compound 10a

¹H NMR expanded spectrum of compound **10a**



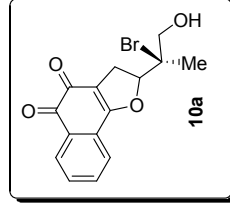
Current Data Parameters
NAME sb41113
EXPNO 299
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131118
Time 16.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 165440
SOLVENT CDCl3
NS 2000
DS 4
SWH 24035.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440820 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

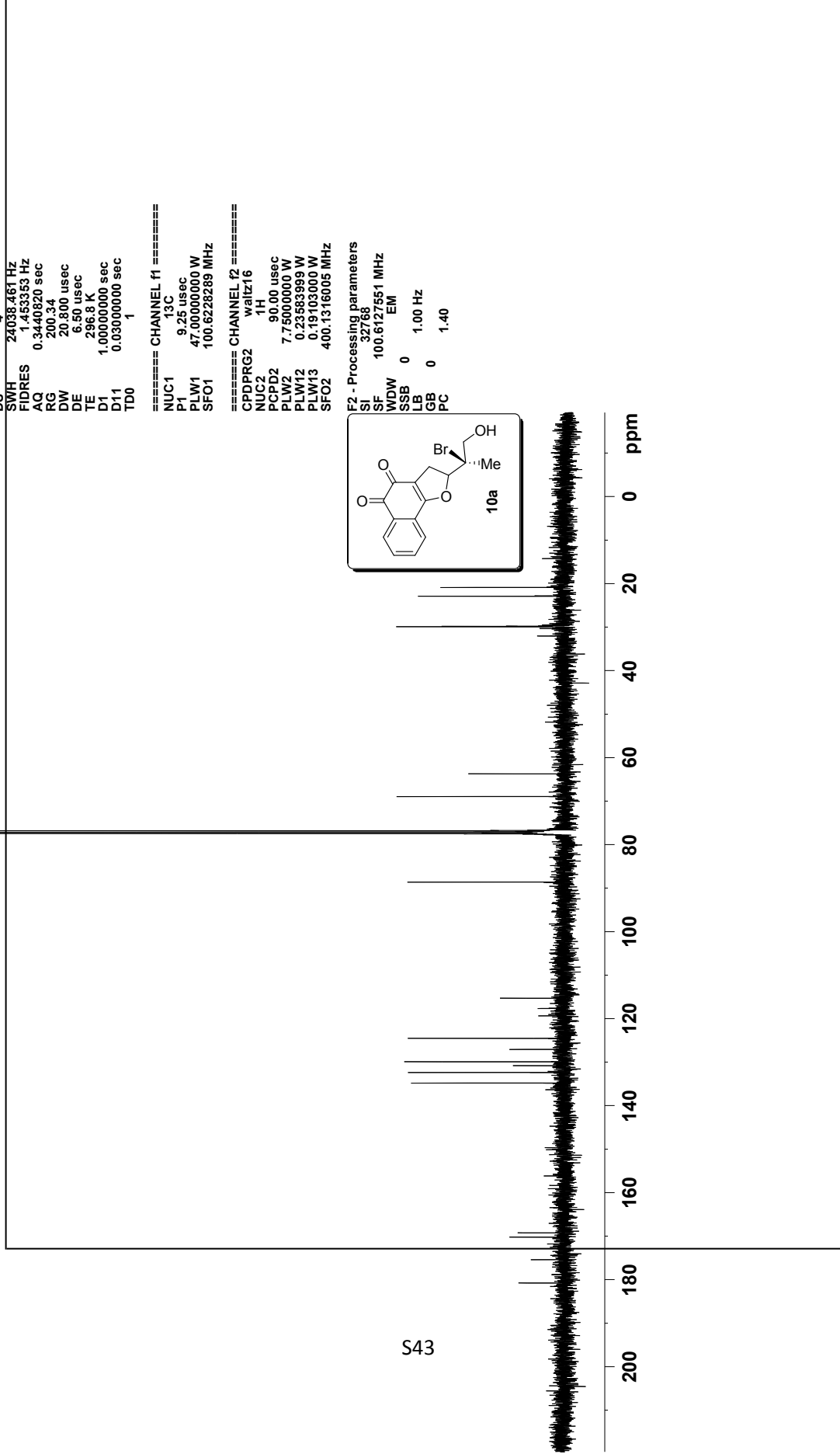
===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.0000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127551 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



180.79
175.43
170.24
169.27
134.83
132.40
130.82
129.93
127.09
124.53
115.33
88.63
77.48
77.16
76.84
68.96
63.75
29.92
29.84
22.91
20.90



¹³C NMR spectrum of compound **10a**

Current Data Parameters
NAME sb41113
EXPNO 300
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131118
Time_ 16.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptspl35
TD 32768

SOLVENT CDC13

NS 256

DS 4

SWH 20161.291 Hz

FIDRES 0.615274 Hz

AQ 0.8126964 sec

RG 200.34

DW 24.800 usec

DE 6.50 usec

TE 296.4 K

CNST2 145.000000

D1 1.00000000 sec

D2 0.00344828 sec

D12 0.00002000 sec

TD0 1

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

NUC1 13C

P1 9.25 usec

P13 2000.00 usec

PLW0 0 W

PLW1 47.00000000 W

SFO1 100.6208166 MHz

SPNAM5 C13cpcomp.4

SFOALS 0.500

SFOFFS5 0 Hz

SPW5 6.14429998 W

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

CPDPRG2 waitz16

NUC2 1H

P3 15.70 usec

P4 31.40 usec

PCPD2 90.00 usec

PLW2 7.75000000 W

PLW12 0.23583999 W

SFO2 400.1312797 MHz

F2 - Processing parameters

SI 32768

SF 100.6127690 MHz

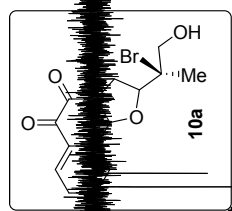
WDW EM

SSB 0

LB 1.00 Hz

GB 0

134.70
132.27
129.80
124.40
88.49
68.83
29.78
22.77
20.77



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

DEPT NMR spectrum of compound 10a

Current Data Parameters
NAME sb41113
EXPNO 223
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131109
Time 10.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122286 Hz
AQ 4.0894966 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 299.2 K
D1 0.50000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz

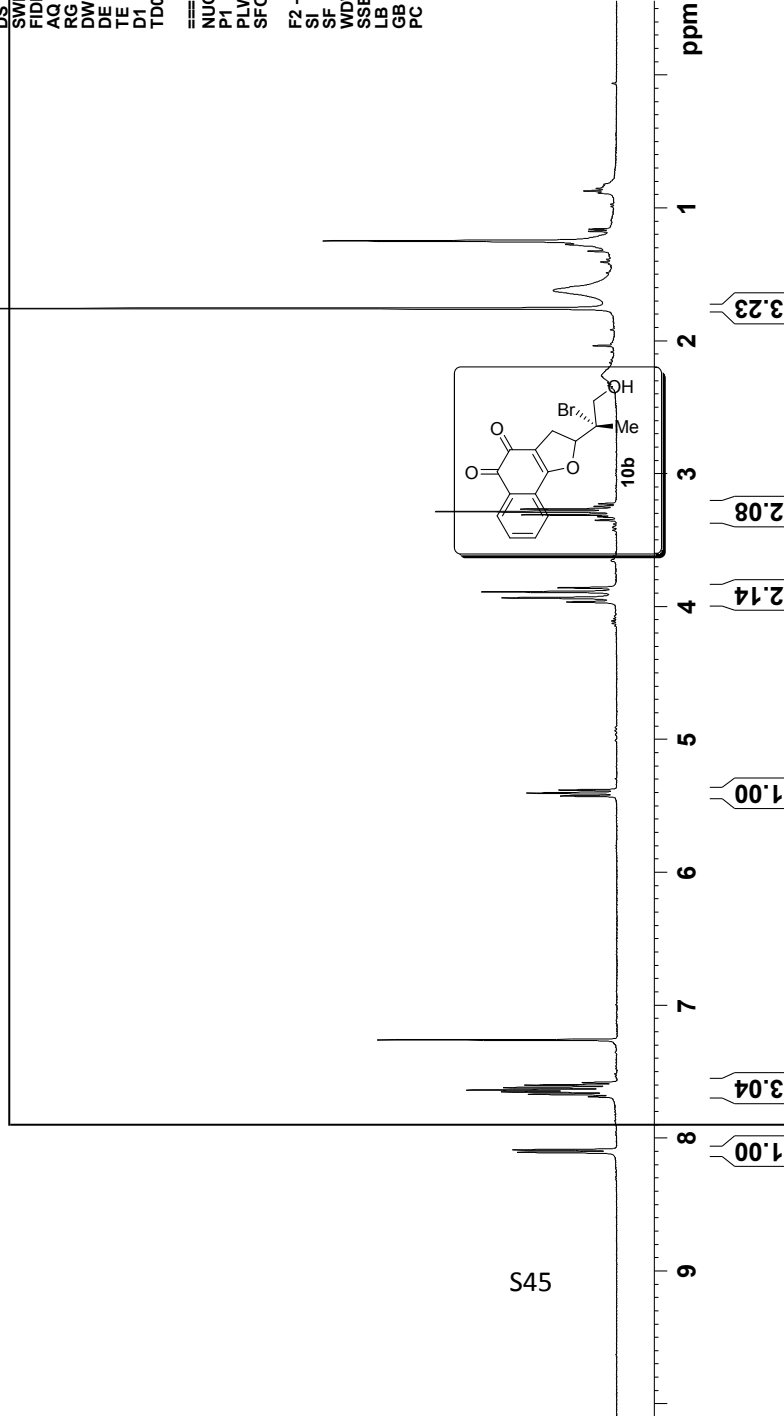
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.106
8.087
7.687
7.669
7.651
7.638
7.619
7.600
7.582
7.260

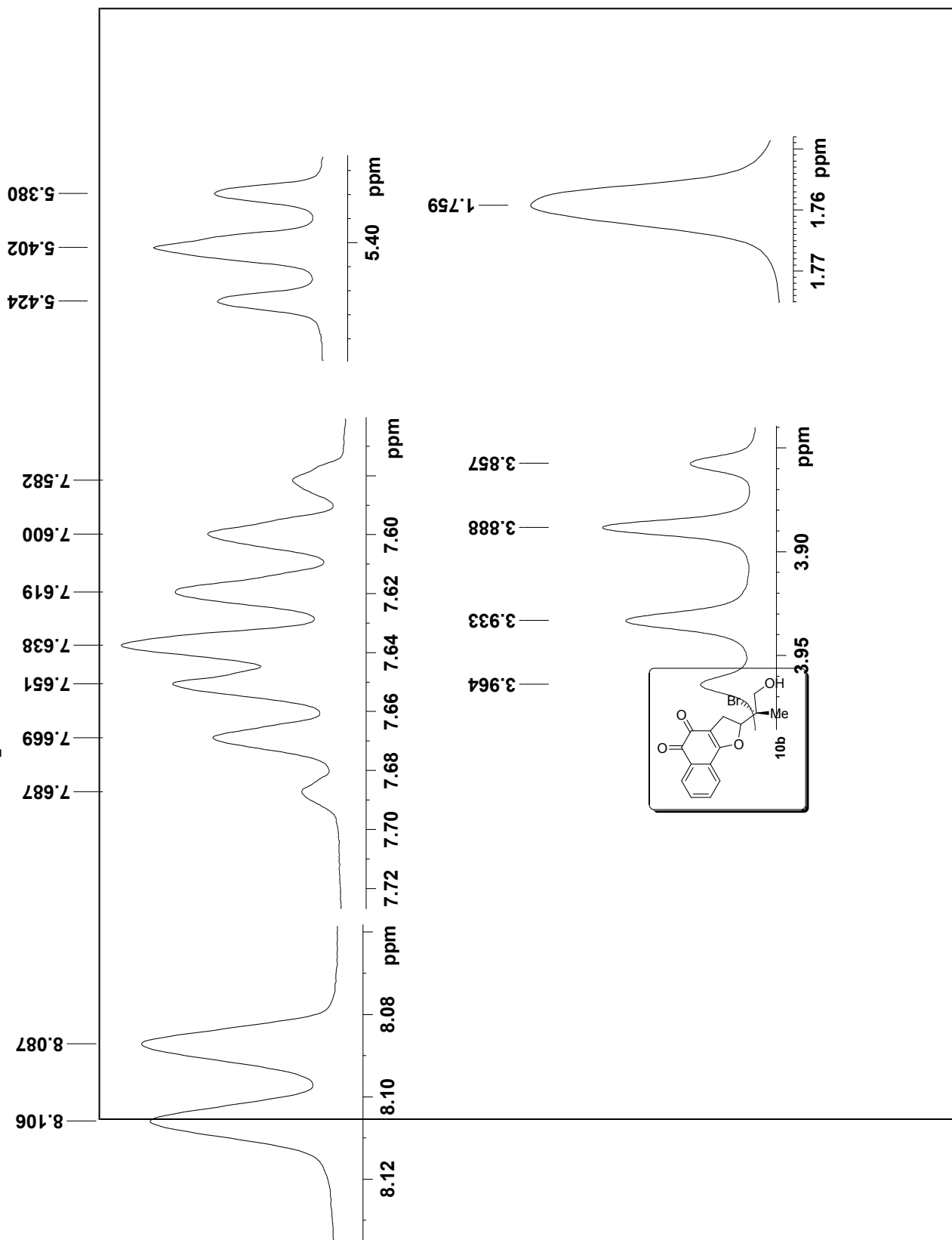
5.424
5.402
5.380

3.964
3.933
3.888
3.857
3.353
3.327
3.312
3.288
3.269
3.249
3.229

1.759



¹H NMR spectrum of compound **10b**



¹H NMR expanded spectrum of compound **10b**

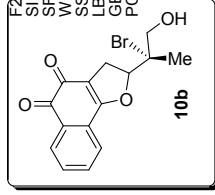
Current Data Parameters
NAME sb41113
EXPNO 224
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131109
Time 10.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440820 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127543 MHz
WDW EM
SSB 0
LB 0 1.00 Hz
GB 0
PC 1.40

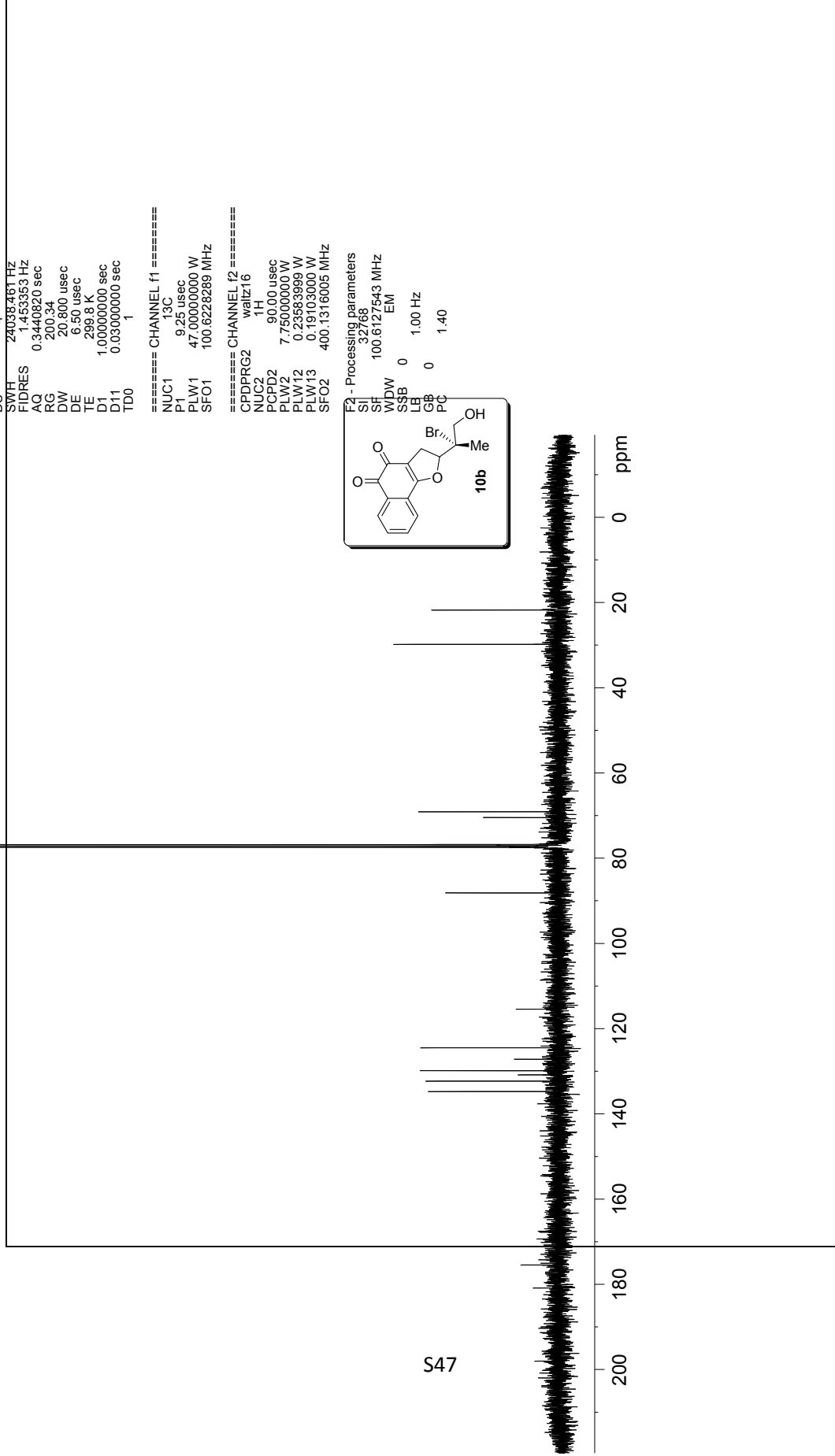


21.79
29.85
69.13
70.49
76.84
77.16
77.48
77.16
88.17

115.45
124.51
127.21
129.89
130.87
132.34
134.78

175.48
180.91

S47



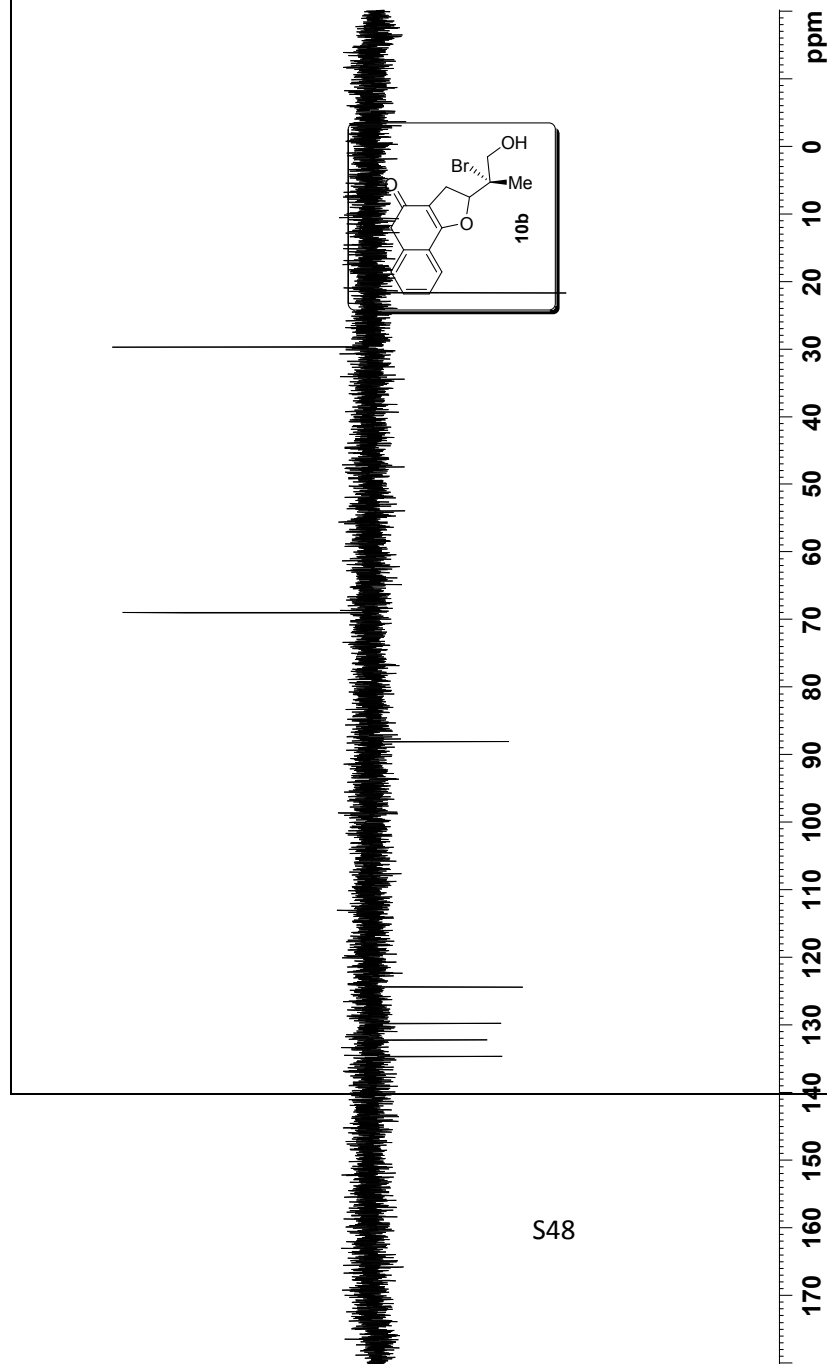
¹³C NMR spectrum of compound 10b

Current Data Parameters
NAME sb41113
EXPNO 225
PROCNO 1

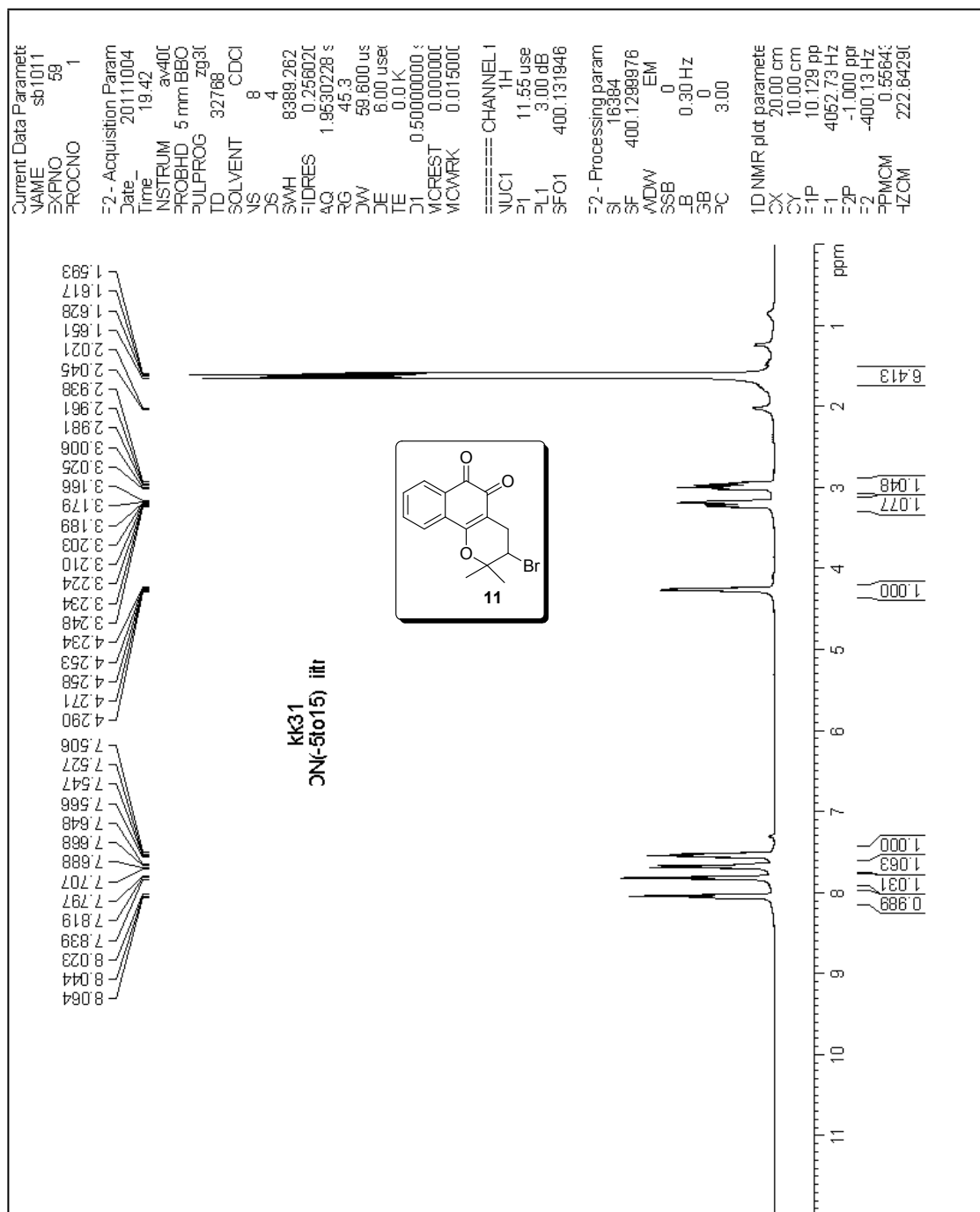
F2 - Acquisition Parameters
Date_ 20131109
Time_ 10.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135
TD 32768
SOLVENT CDCI3

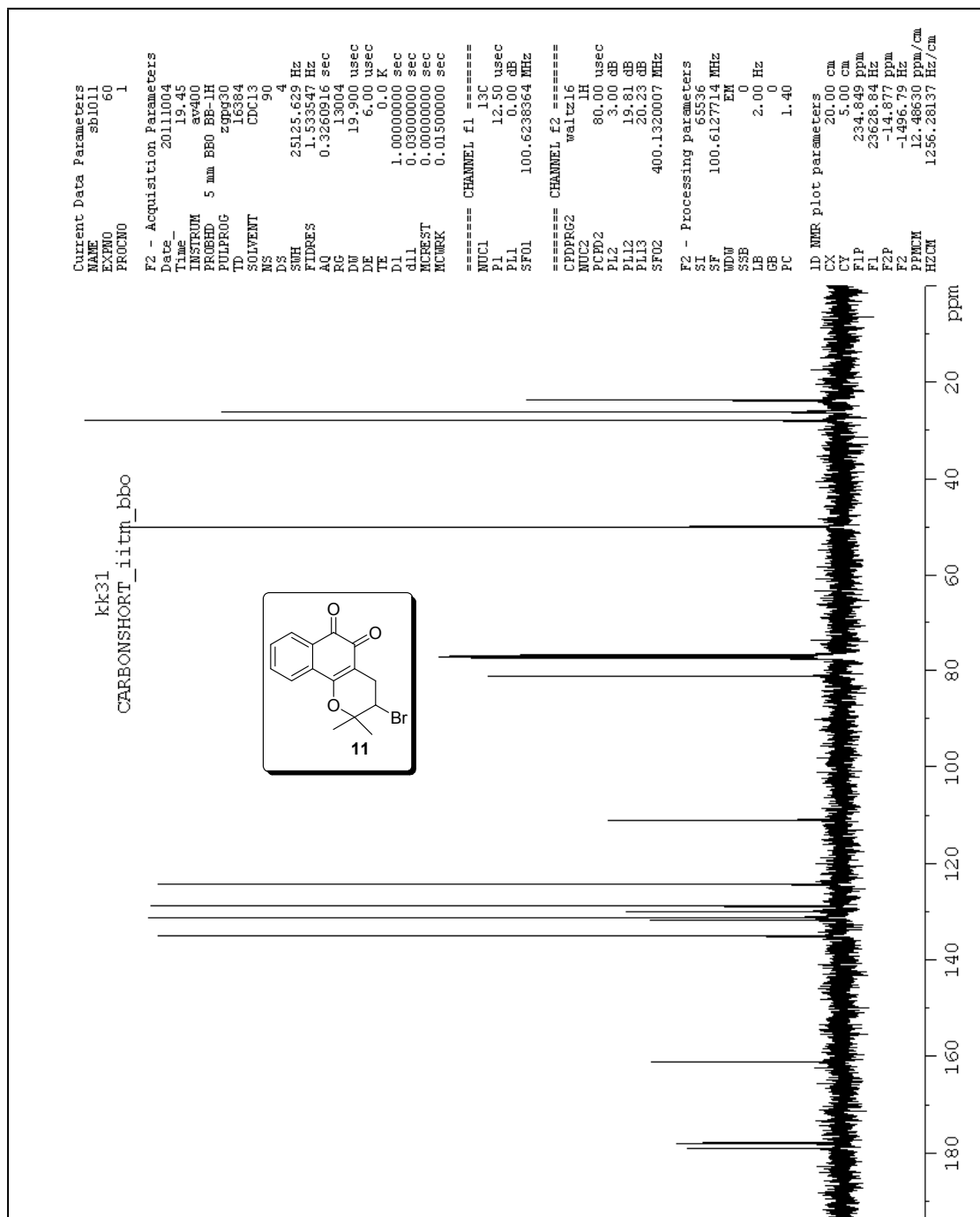
===== CHANNEL f1 =====
NUC1 13C
P1 9.25 usec
PLW0 2000.00 usec
PLW1 0 W
SFO1 47.00000000 W
SPNAM5 100.6208166 MHz
SFOALS Crp60-comp.4
SPOFFS5 0 Hz
SPW5 6.14429998 W
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 15.70 usec
P4 31.40 usec
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
SFO2 400.1312797 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

134.64
132.20
129.74
124.37
88.02
68.98
29.70
21.65

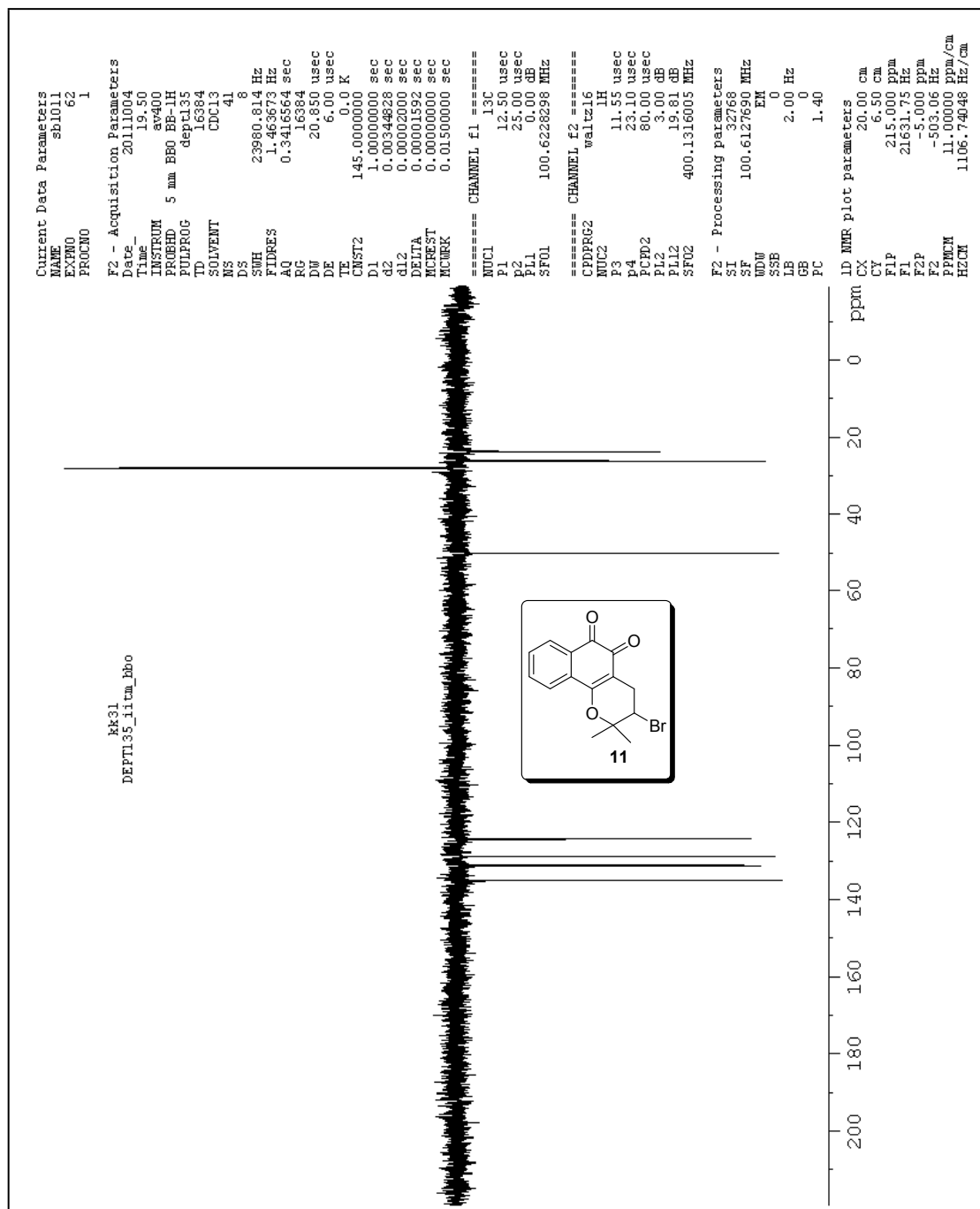


DEPT NMR spectrum of compound 10b

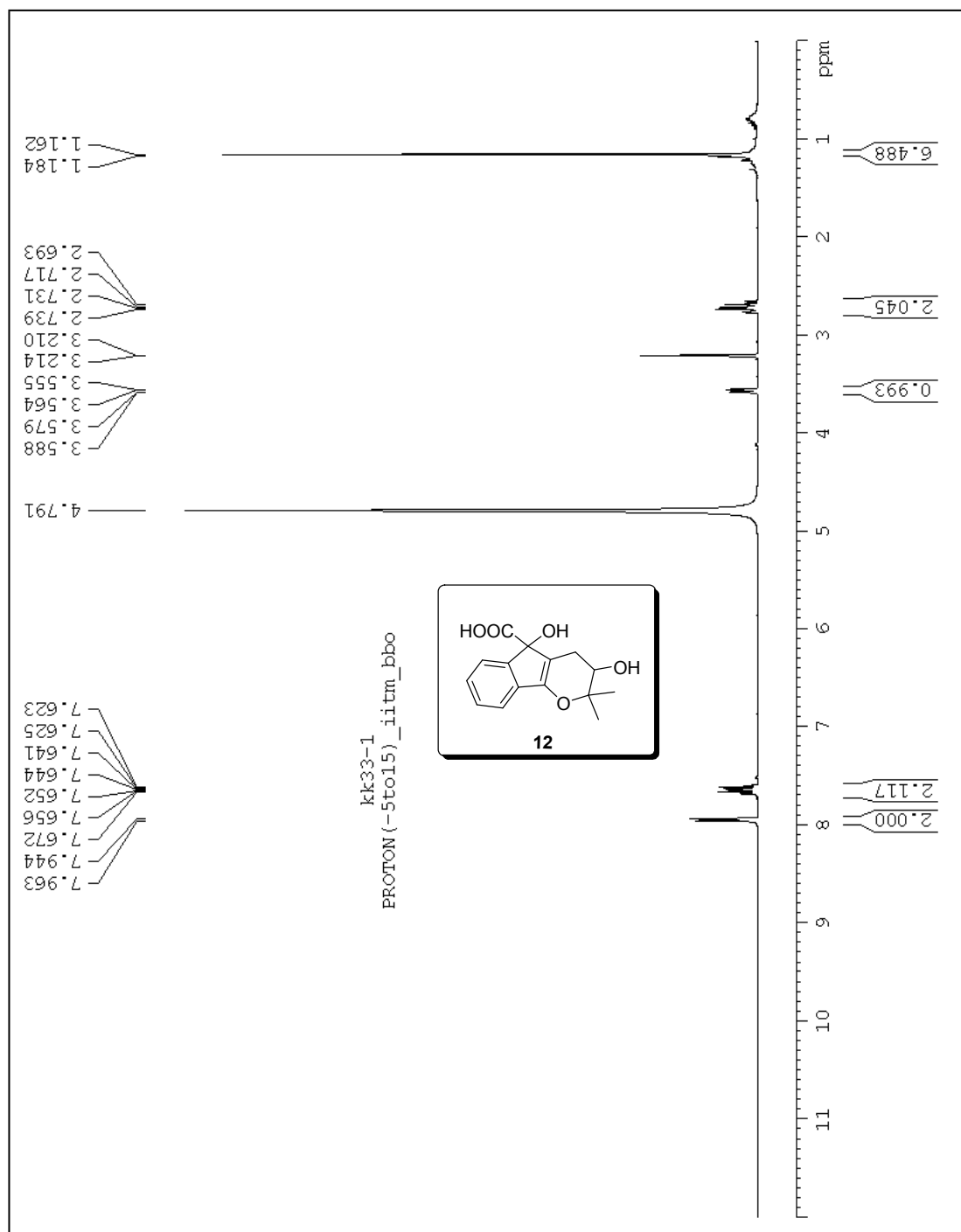




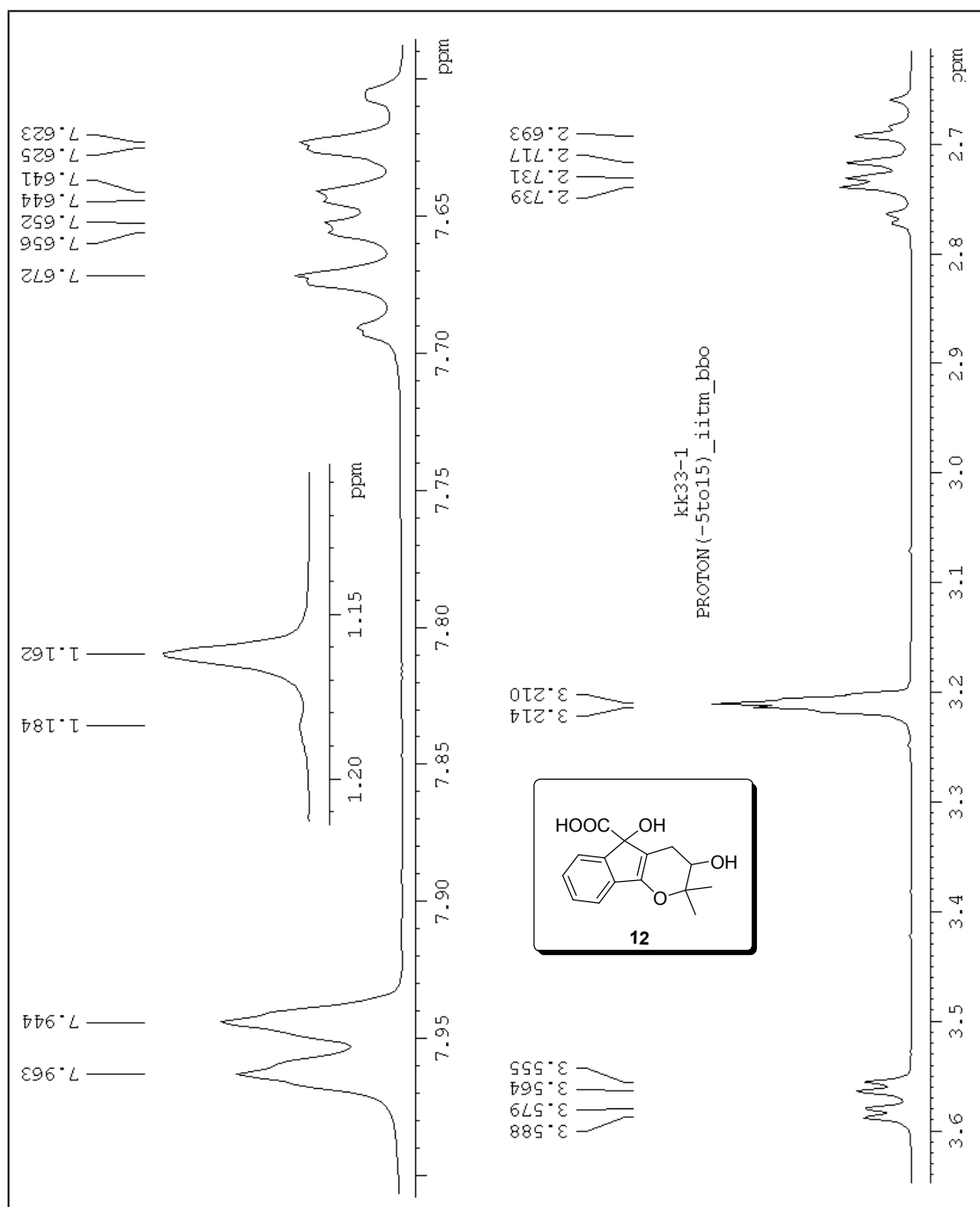
¹³C NMR spectrum of compound **11**



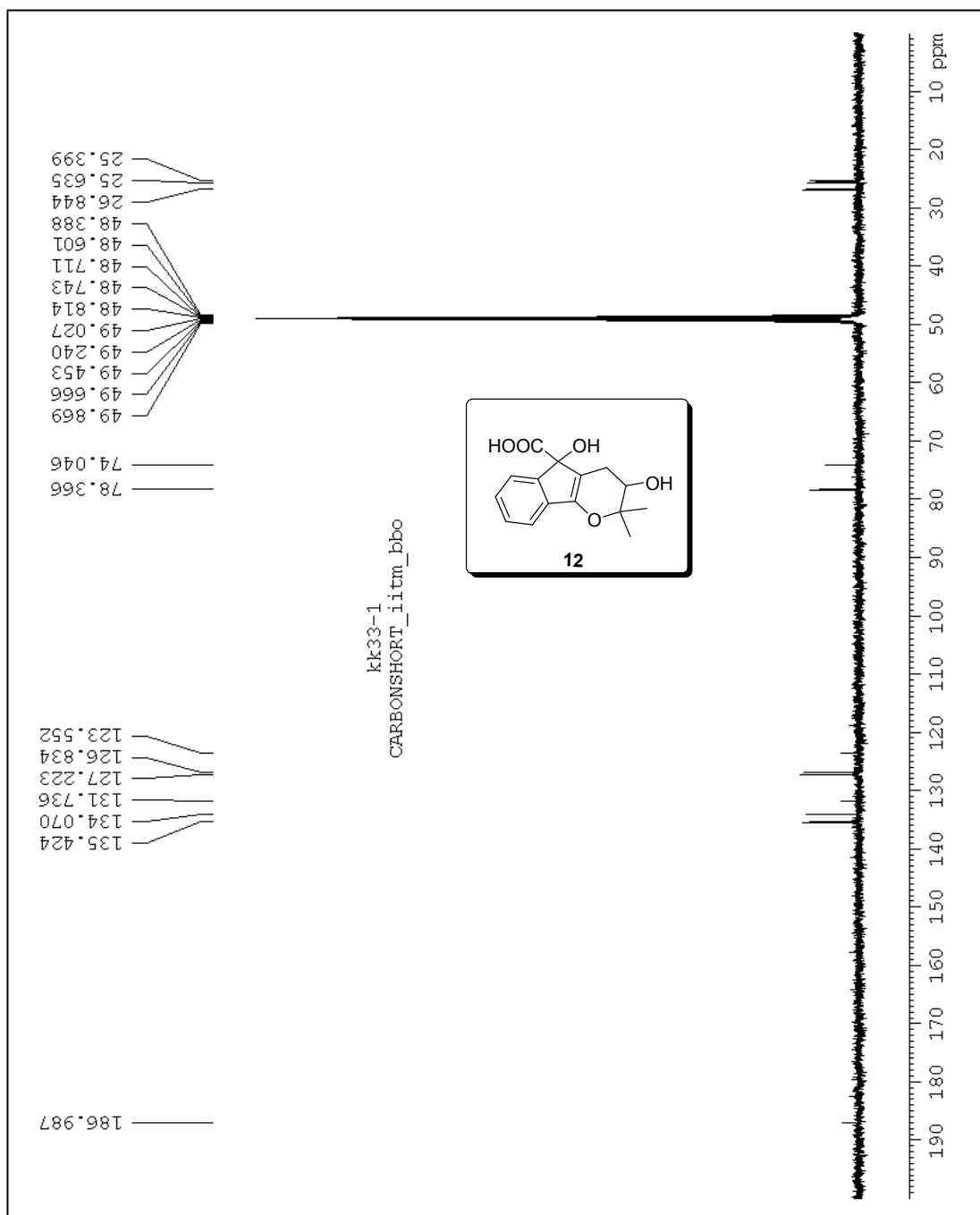
DEPT NMR spectrum of compound 11



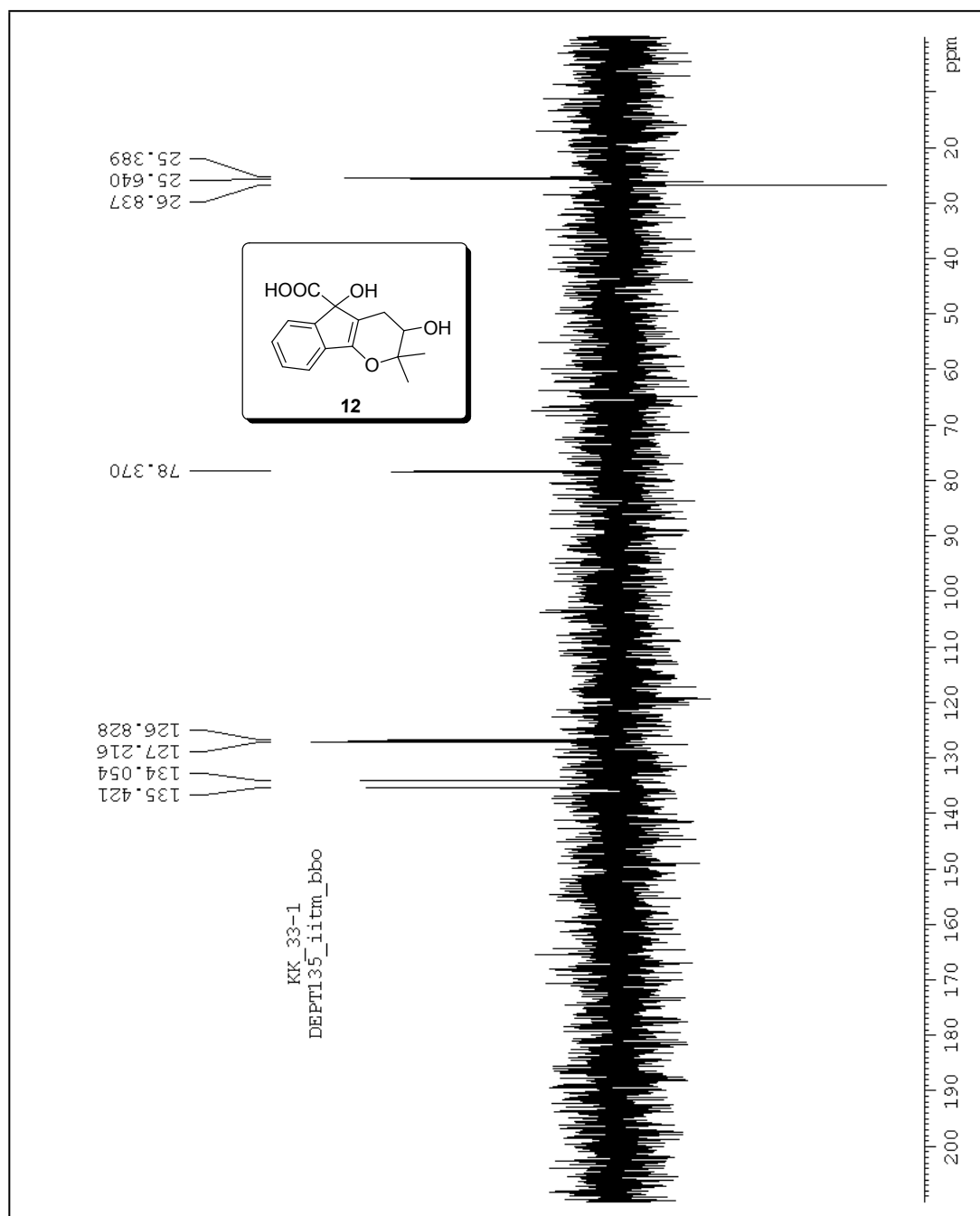
¹H NMR spectrum of compound **12**



¹H NMR expanded spectrum of compound **12**



¹³C NMR spectrum of compound **12**



DEPT NMR spectrum of compound 12

Current Data Parameters

NAME keneth 01
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111015
Time 3.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 2

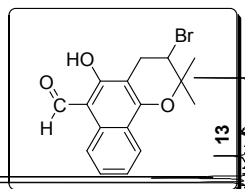
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860212 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.65 usec
PL1 0 dB
PL1W 23.53637505 W
SFO1 500.1330885 MHz

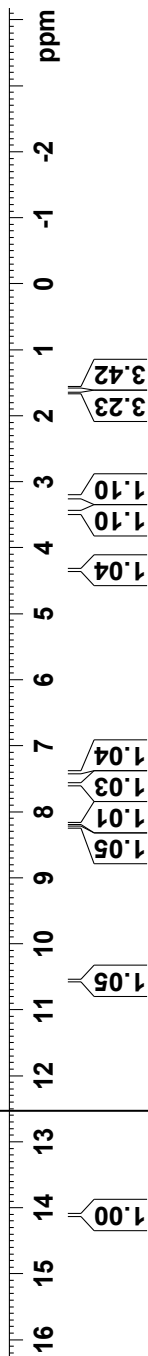
F2 - Processing parameters
SI 32768
SF 500.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

KK33a.

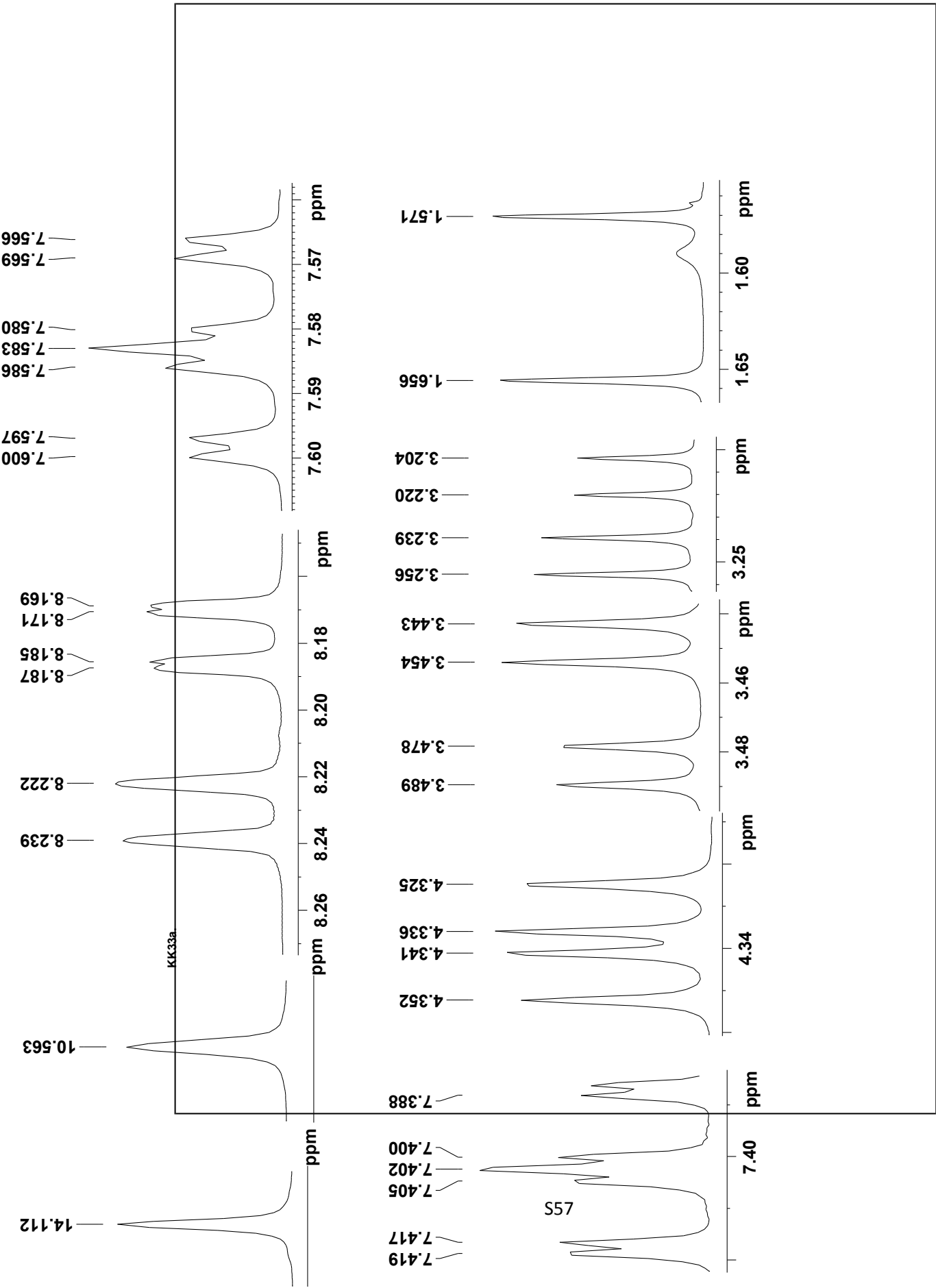
14.112
10.563
8.239
8.222
8.187
8.185
8.171
8.169
7.600
7.597
7.586
7.583
7.580
7.569
7.566
7.419
7.417
7.405
7.402
7.400
7.388
7.386
7.260
4.352
4.341
4.336
4.325
3.489
3.478
3.454
3.443
3.256
3.239
3.220
3.204
1.656
1.571



S56



¹H NMR spectrum of compound 13



¹H NMR expanded spectrum of compound 13

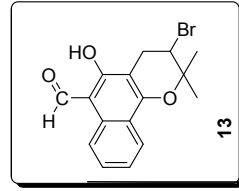
Current Data Parameters
 NAME Kenneth 01
 EXPNO 33
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111015
 Time 3.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 29764.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505524 sec
 RG 203
 DW 16.800 usec
 DE 6.50 usec
 TE 299.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.80 usec
 PL1 0 dB
 PL1W 70.83519745 W
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0 dB
 PL12 17.50 dB
 PL13 17.50 dB
 PL2W 23.53637505 W
 PL12W 0.41864253 W
 PL13W 0.41864253 W
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577720 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



190.95
 165.85
 156.59
 132.88
 129.40
 124.10
 123.09
 120.55
 118.41
 106.37
 105.33
 79.28
 77.41
 77.16
 76.90
 51.07
 28.52
 26.72
 22.95

S58

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

¹³C NMR spectrum of compound 13

Current Data Parameters
 NAME keneth 01
 EXPNO 34
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111015
 Time 4.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG dept135
 TD 32768
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 29761.904 Hz

FIDRES 0.908261 Hz
 AQ 0.5005524 sec
 RG 203
 DW 16.800 usec
 DE 6.50 usec
 TE 297.5 K
 CNST2 145.0000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1

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

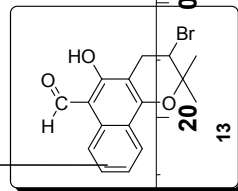
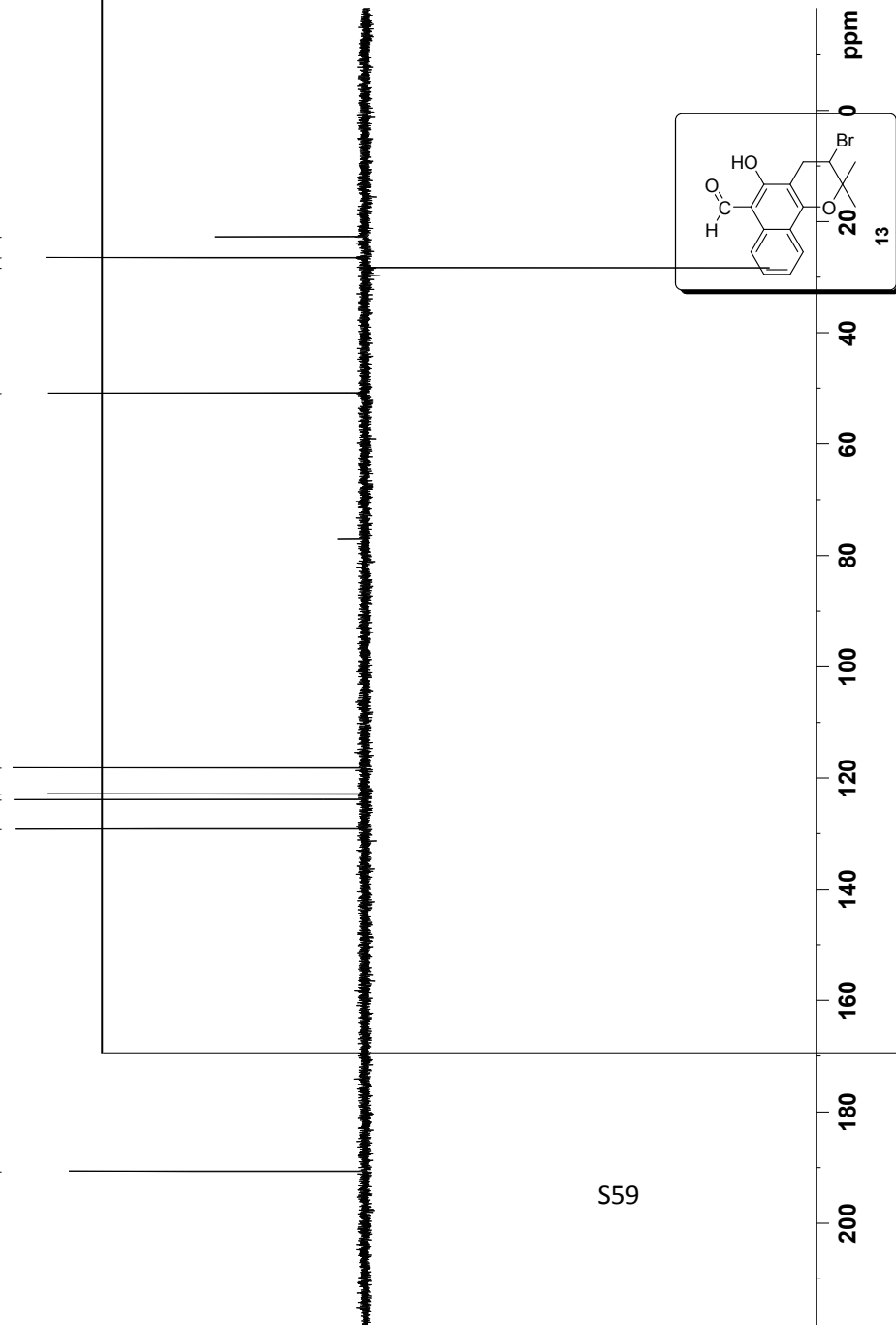
NUC1 13C
 P1 7.80 usec
 F2 15.60 usec
 PL1 0 dB
 PL1W 70.83519745 W
 SFO1 125.7703643 MHz

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

CPDPRG2 waltz16
 NUC2 1H
 P3 10.65 usec
 P4 21.30 usec
 PCPD2 80.00 usec
 PL2 0 dB
 PL12 17.50 dB
 PL2W 23.53637505 W
 PL12W 0.41854253 W
 SFO2 500.1320005 MHz

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

190.82
 129.27
 123.97
 122.96
 118.28
 50.94
 28.39
 26.58
 22.82



DEPT NMR spectrum of compound 13

KK33b

Current Data Parameters
NAME Kenneth 01
EXPNO 44
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111016
Time 9.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30

TD 32768
SOLVENT CDCl3
DS 32
NS 2
SWH 10330.578 Hz
FIDRES 0.316264 Hz
AQ 1.5860212 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.0000000 sec
TD0 1

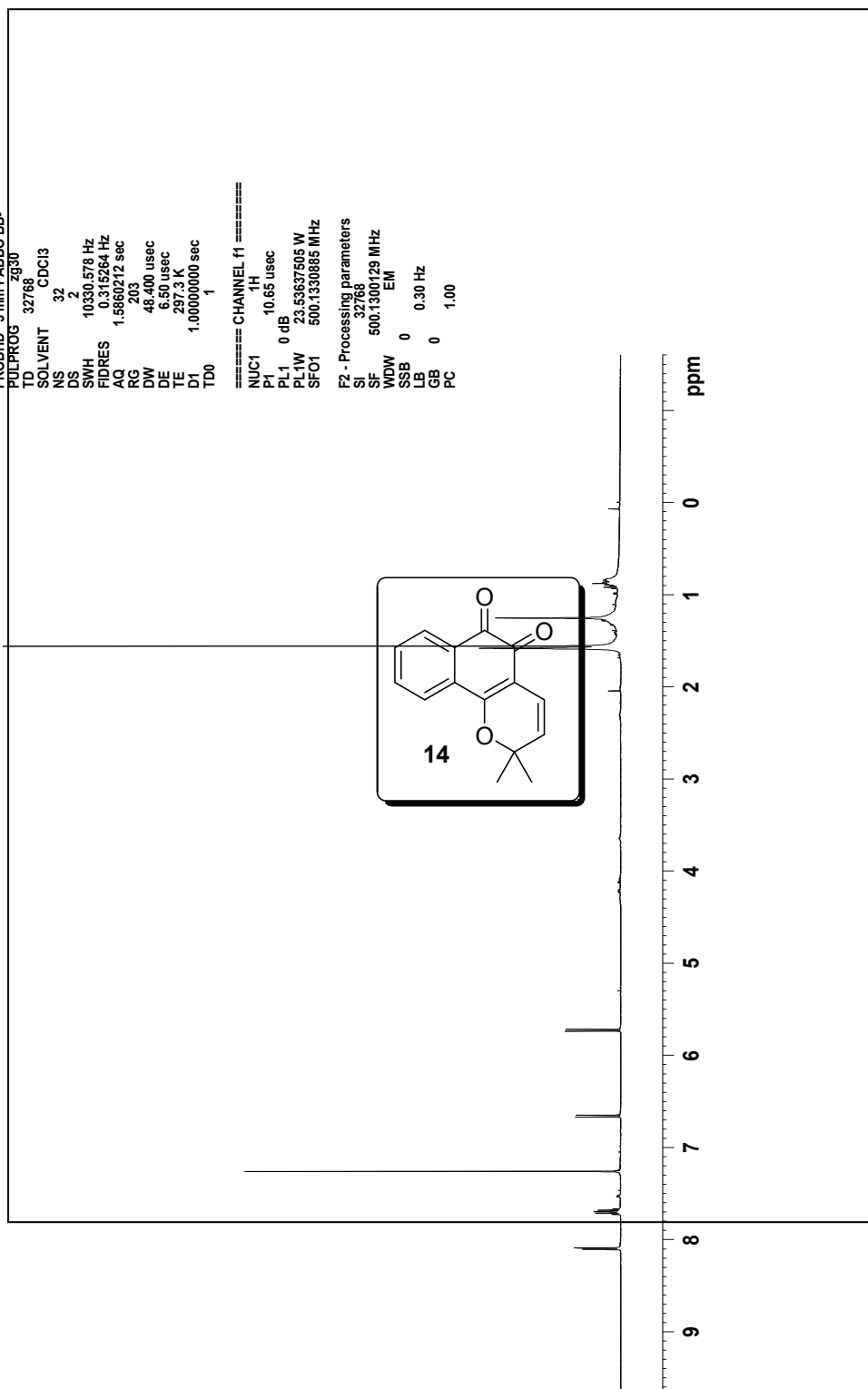
===== CHANNEL f1 =====

NUC1 1H
P1 10.65 usec
PL1 0 dB
PL1W 23.53637505 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.089
8.085
7.729
7.726
7.715
7.712
7.700
7.697
7.694
7.683
7.680
7.668
7.665
7.260
6.669
6.649
5.737
5.717

1.557



¹H NMR spectrum of compound 14

¹H NMR expanded spectrum of compound **14**

