Exploring mutasynthesis to increase structural diversity in the synthesis of highly oxygenated polyketides lactones

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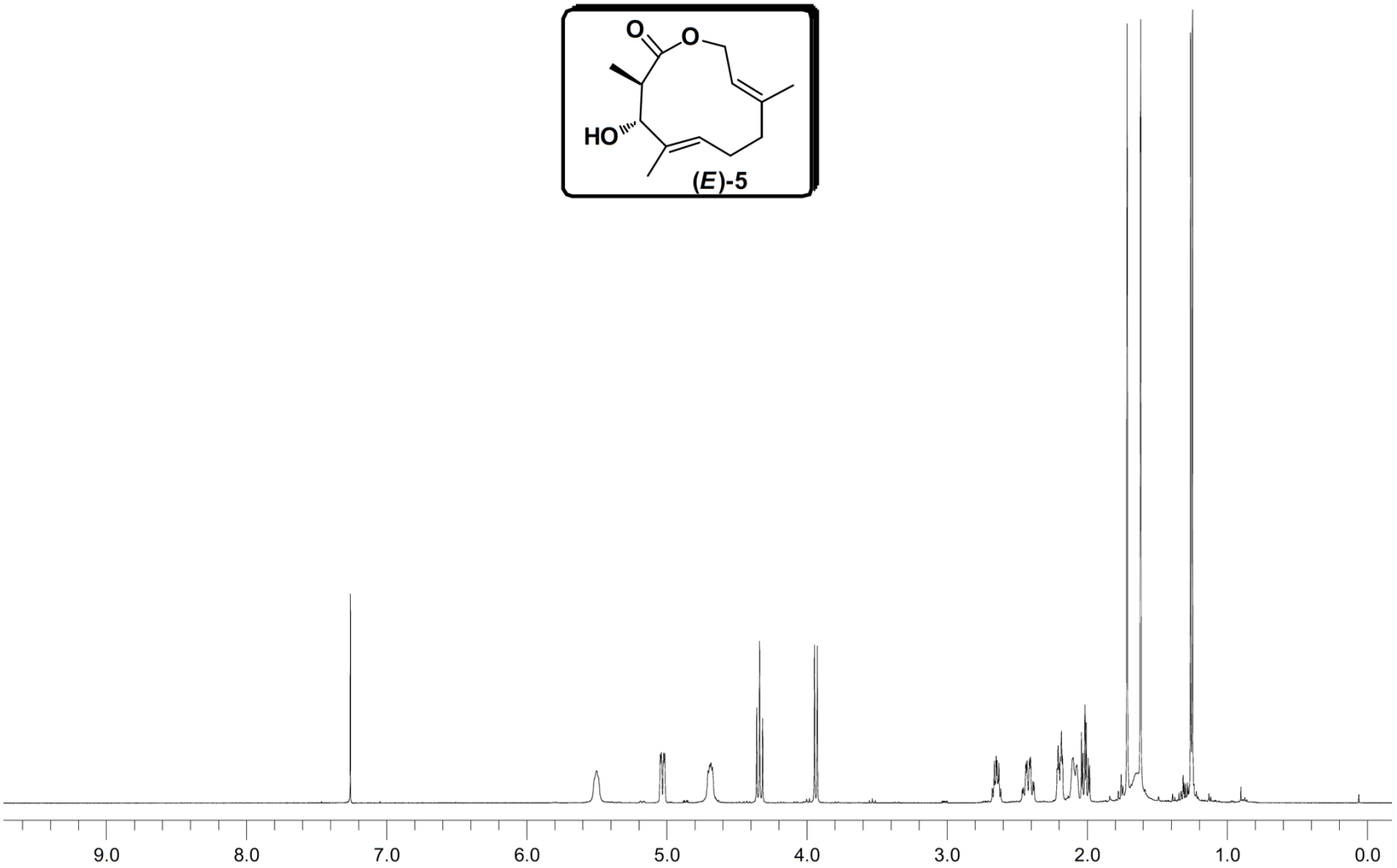
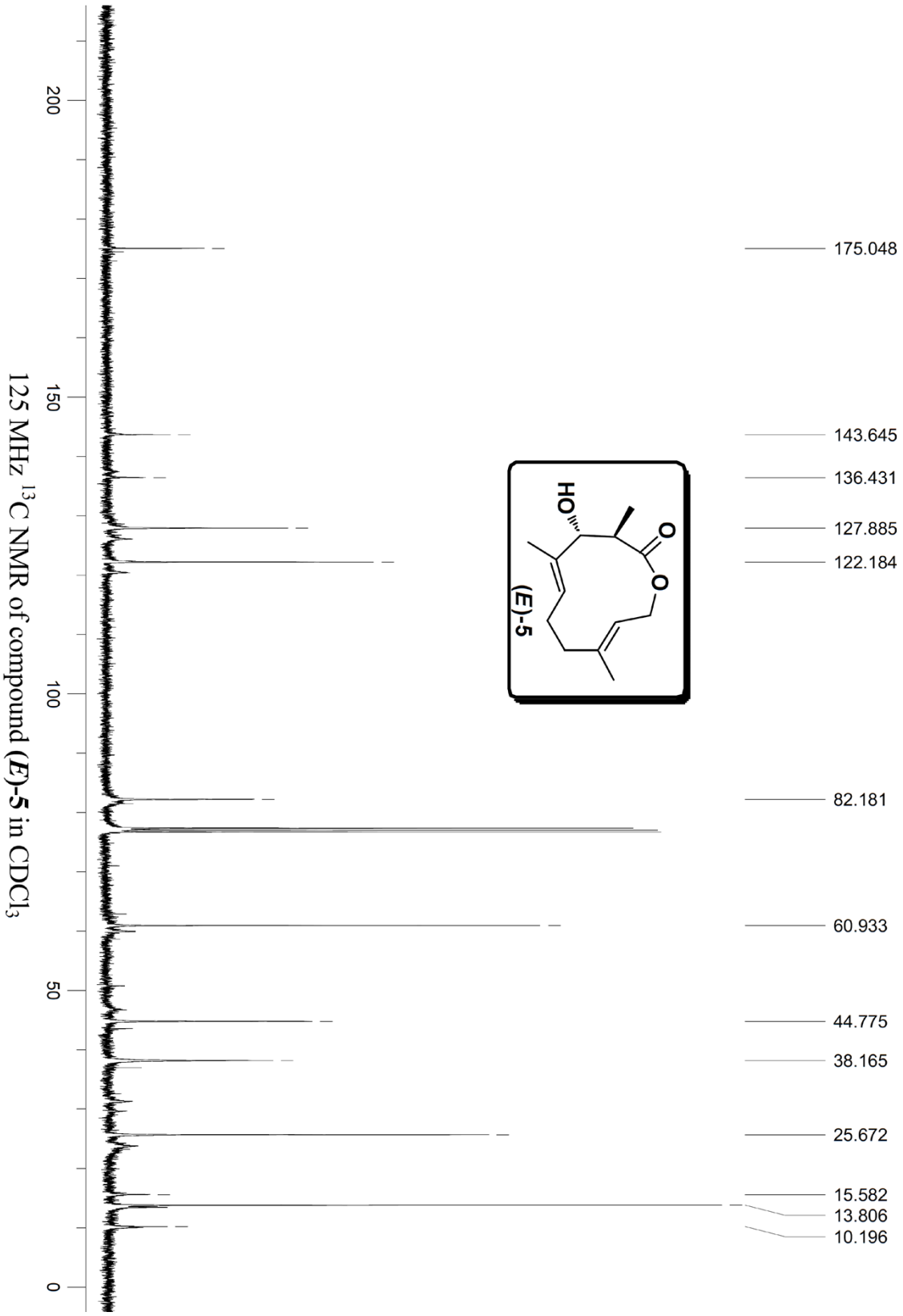
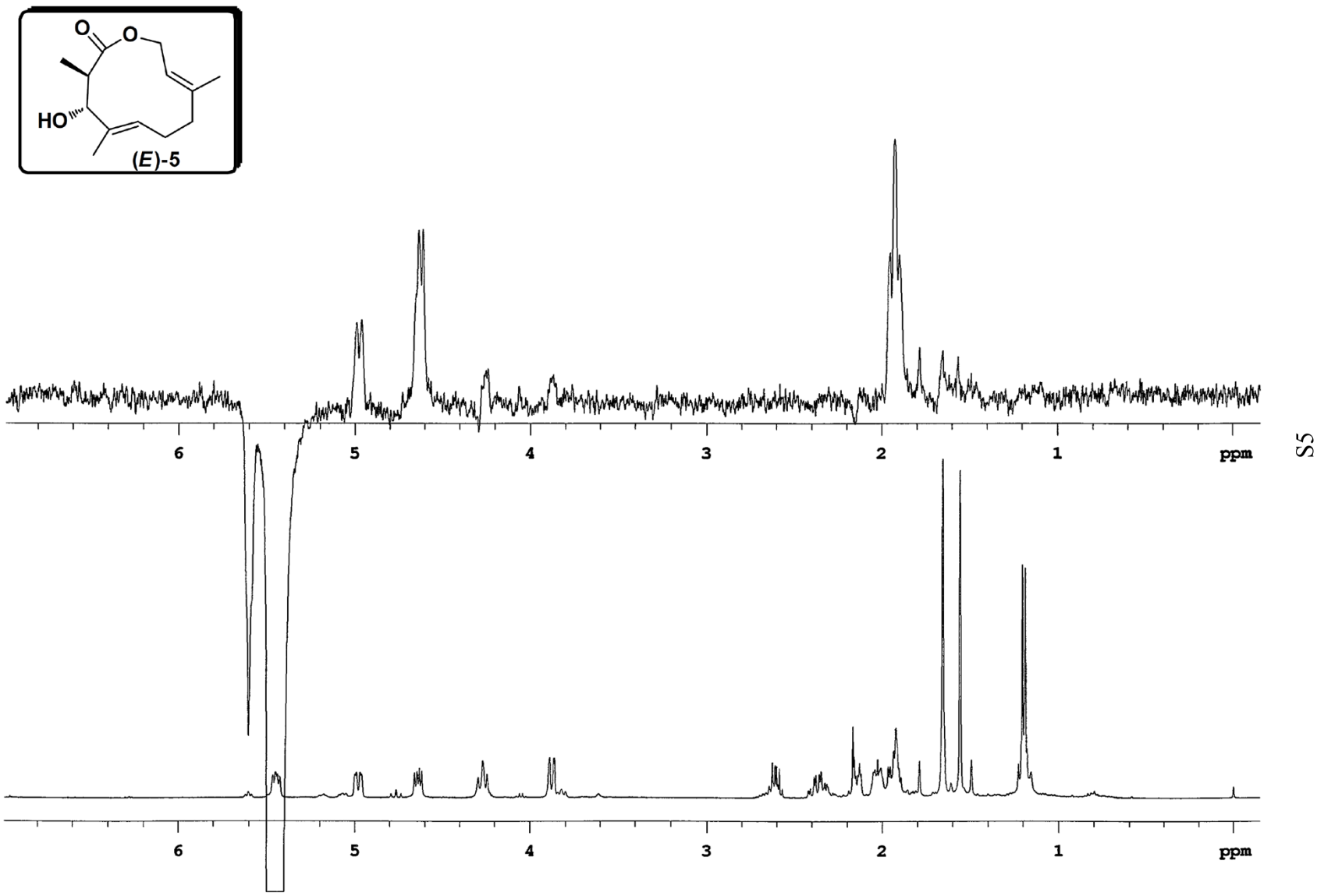
Supporting Information

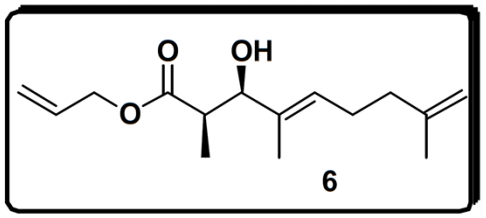
Table of contents:

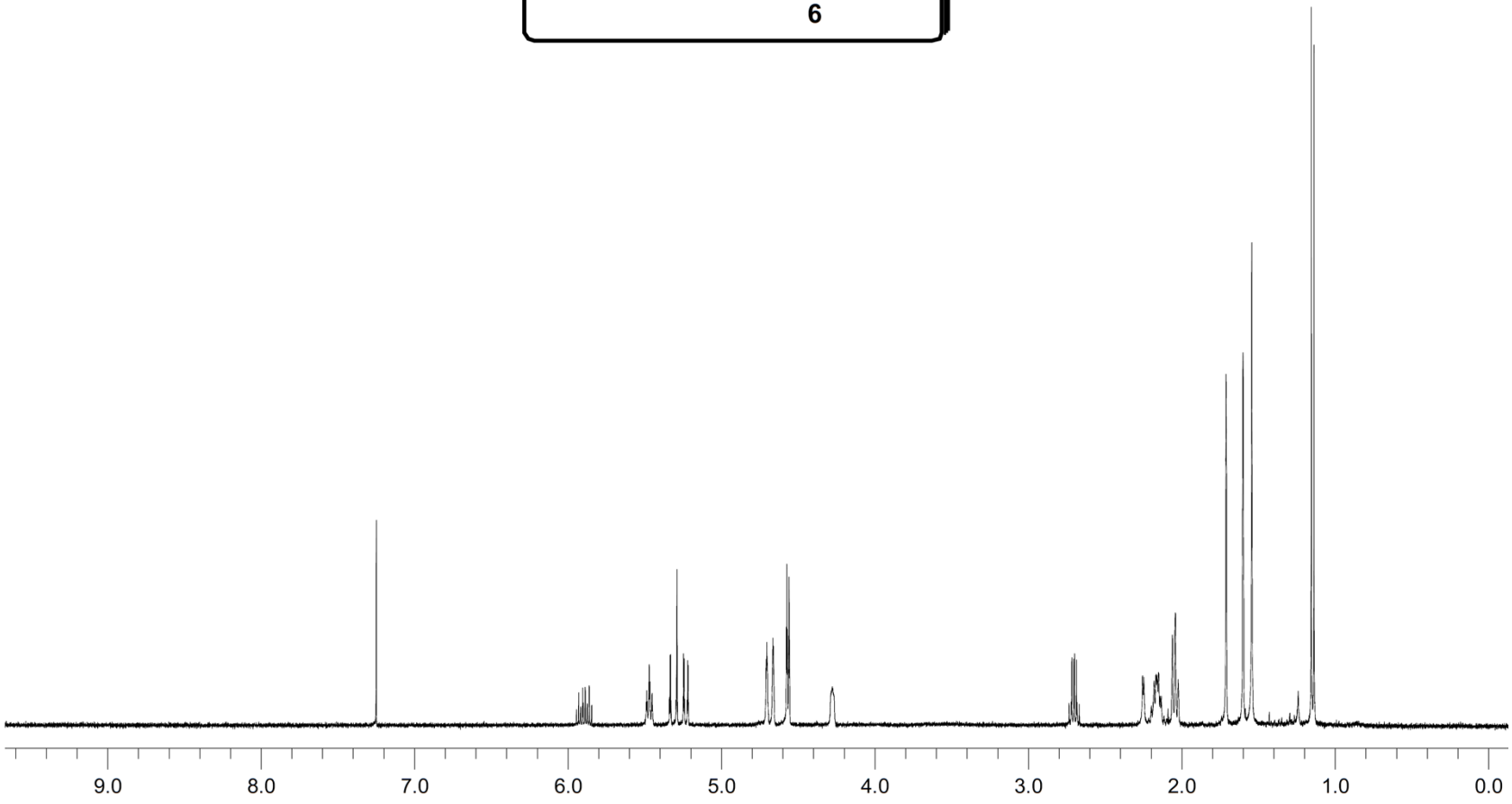


500 MHz ^{1}H NMR of compound **(*E*)-5** in $CDCl_3$

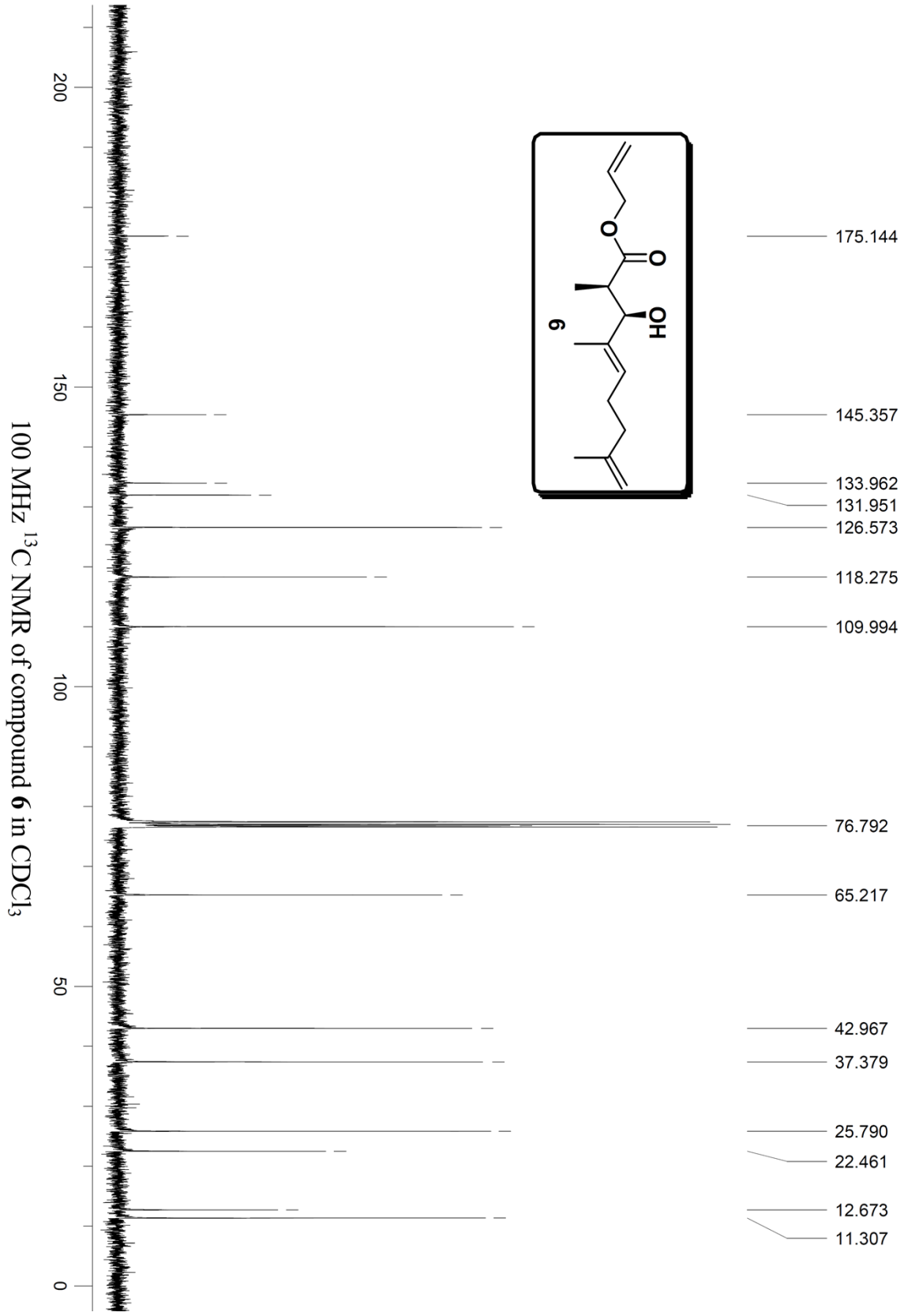

125 MHz ^{13}C NMR of compound (*E*)-**5** in $CDCl_3$
200
150
100
50
0
175.048
143.645
136.431
127.885
122.184
82.181
60.933
44.775
38.165
25.672
15.582
13.806
10.196
HO
O
O
(*E*)-5

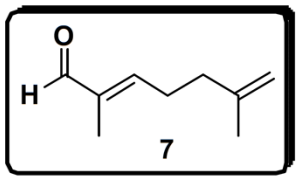

O
O
HO
(E)-5
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

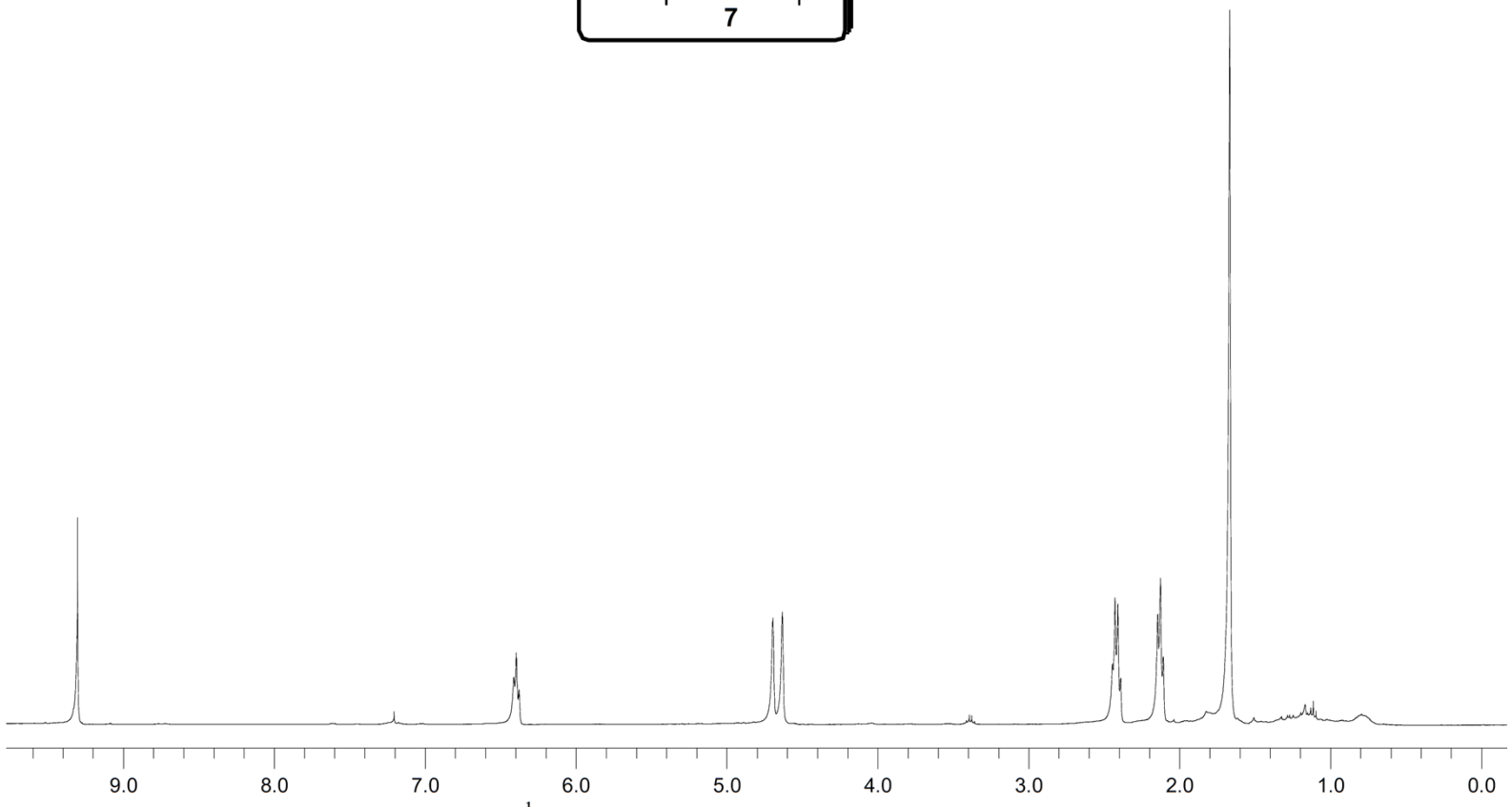




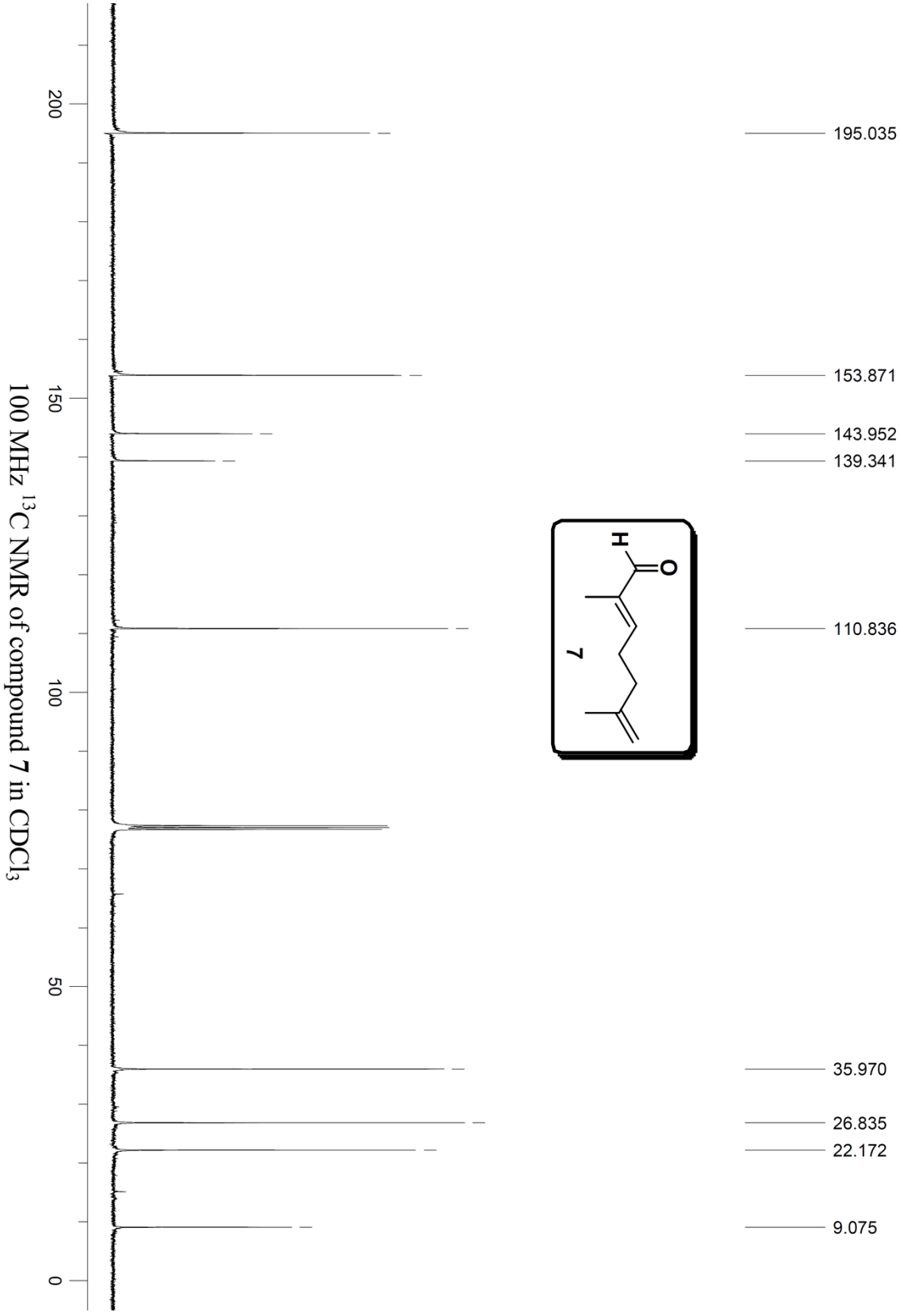
400 MHz ^{1}H NMR of compound **6** in $CDCl_3$

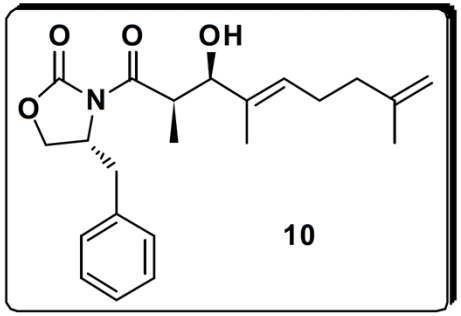

100 MHz ^{13}C NMR of compound **6** in $CDCl_3$
200
150
100
50
0
O
O
OH
6
175.144
145.357
133.962
131.951
126.573
118.275
109.994
76.792
65.217
42.967
37.379
25.790
22.461
12.673
11.307

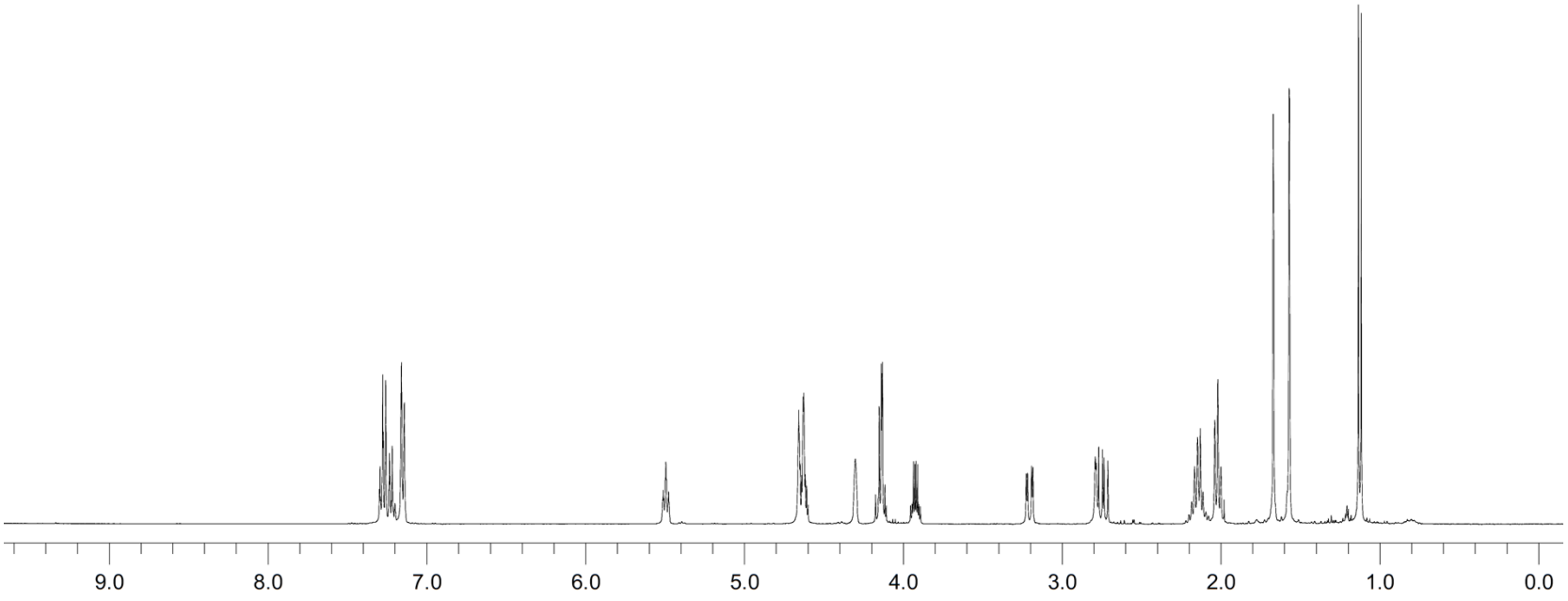




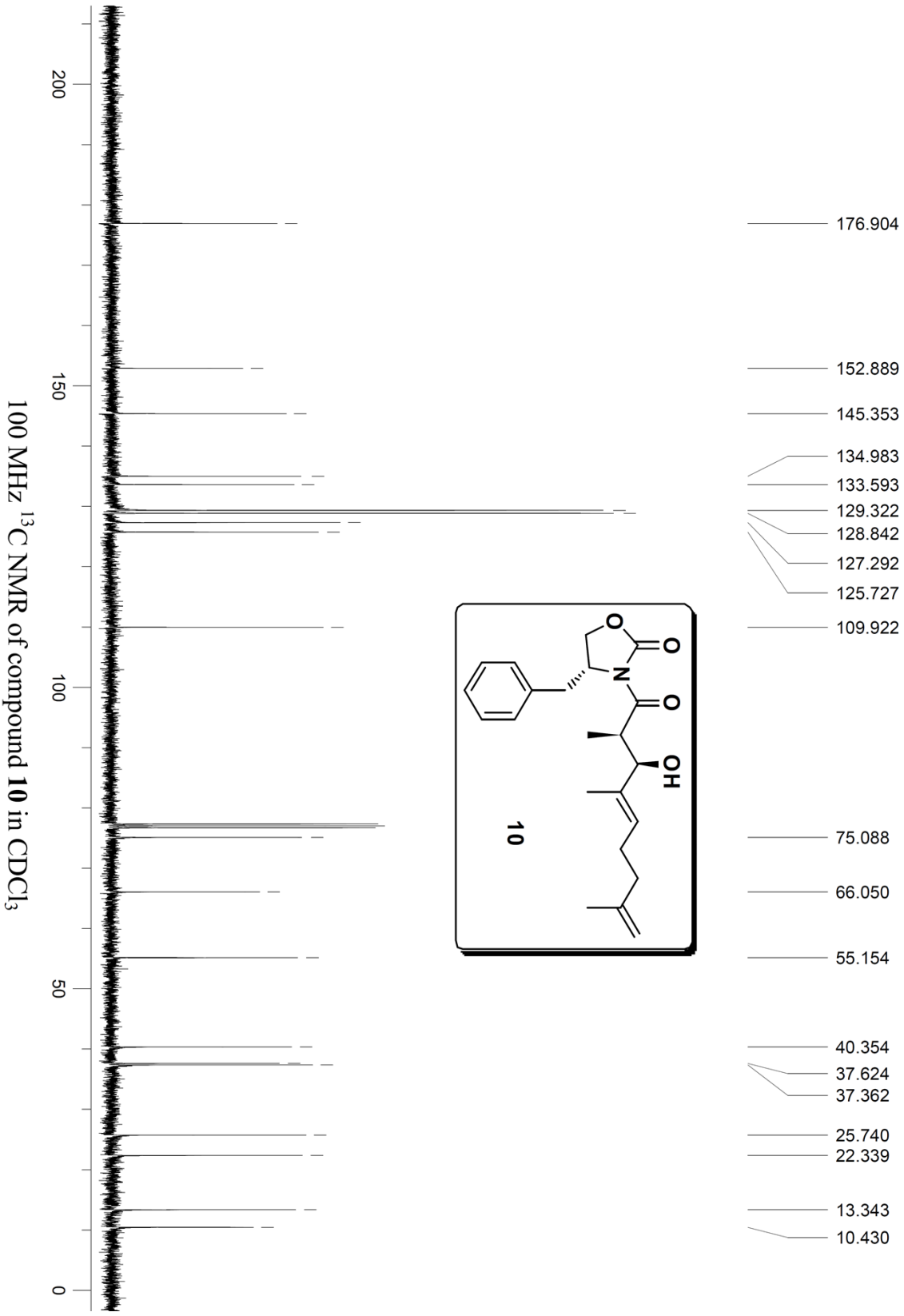
400 MHz ^{1}H NMR of compound **7** in $CDCl_3$

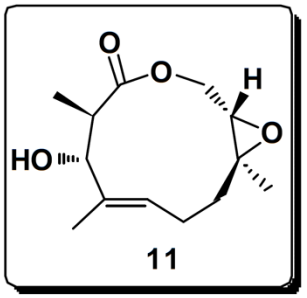

100 MHz ^{13}C NMR of compound **7** in $CDCl_3$
200
150
100
50
0
195.035
153.871
143.952
139.341
110.836
35.970
26.835
22.172
9.075
H
O
7





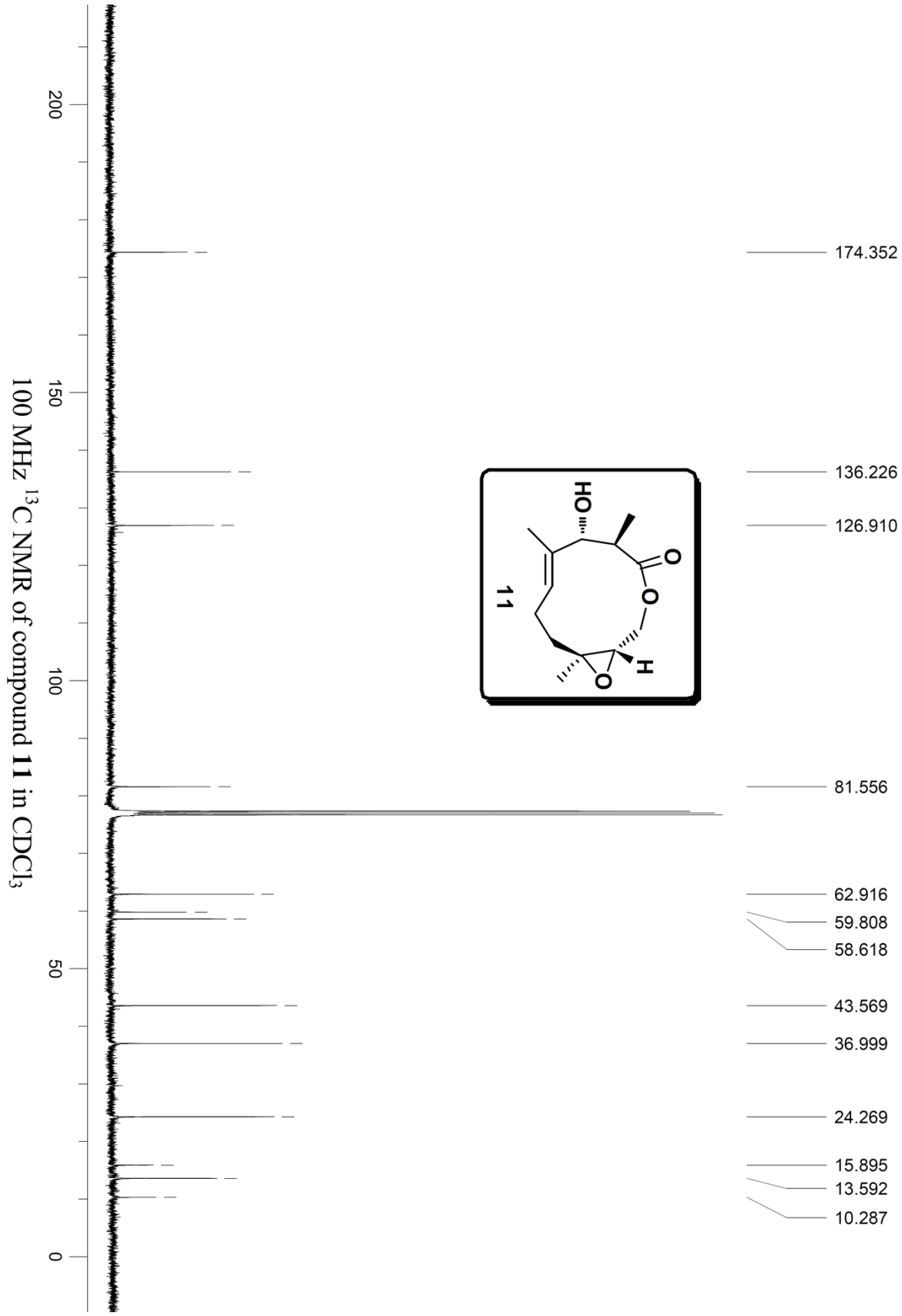
400 MHz ^{1}H NMR of compound **10** in $CDCl_3$


100 MHz ^{13}C NMR of compound **10** in $CDCl_3$
200
150
100
50
0
176.904
152.889
145.353
134.983
133.593
129.322
128.842
127.292
125.727
109.922
75.088
66.050
55.154
40.354
37.624
37.362
25.740
22.339
13.343
10.430
O
O
N
O
O
OH
10



11

400 MHz ^{1}H NMR of compound **11** in $CDCl_3$


100 MHz ^{13}C NMR of compound **11** in $CDCl_3$
200
150
100
50
0
174.352
136.226
126.910
81.556
62.916
59.808
58.618
43.569
36.999
24.269
15.895
13.592
10.287
HO
O
O
H
O
11

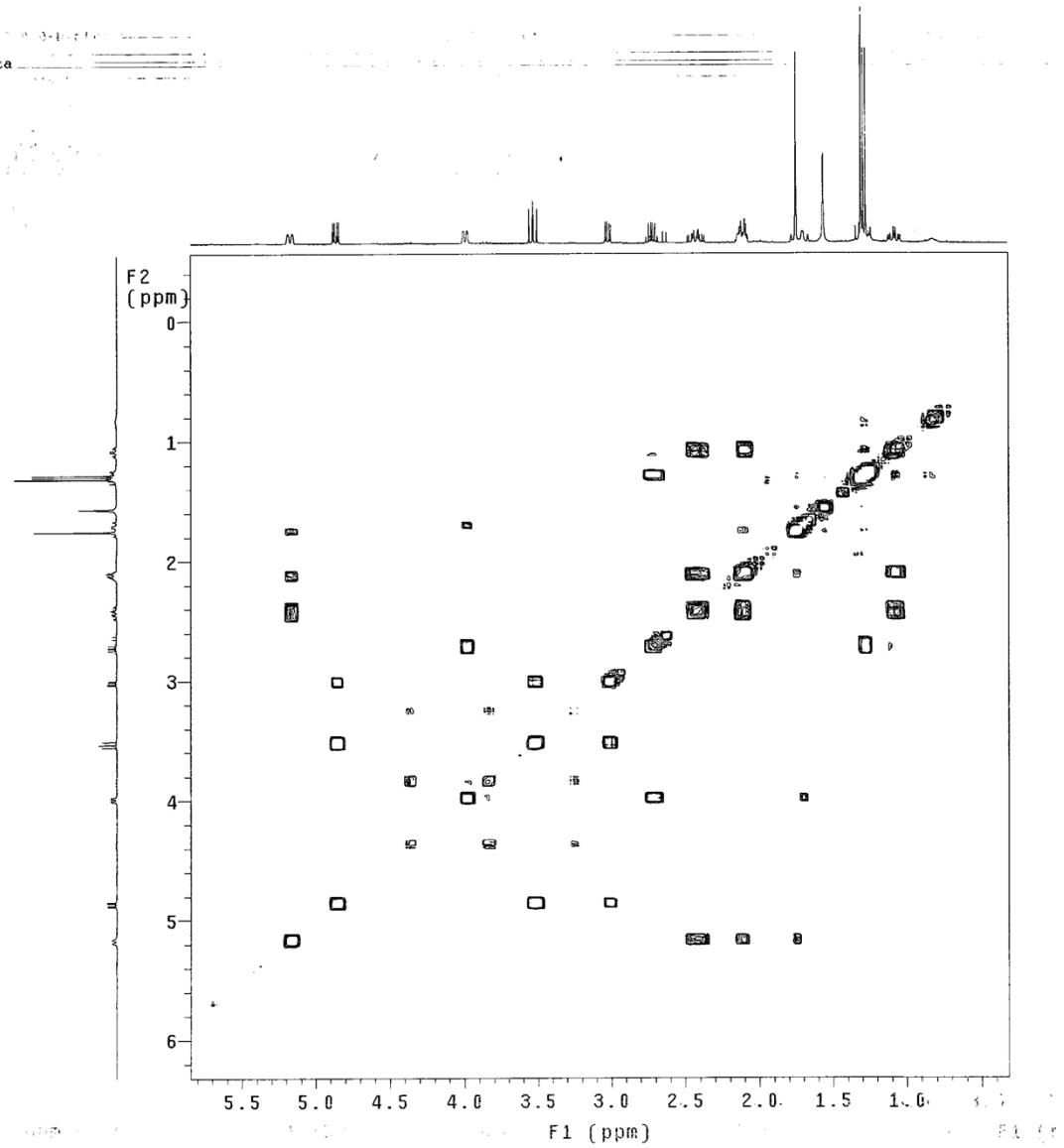
030910-biotransf-31-38-HPLC27min-cosy

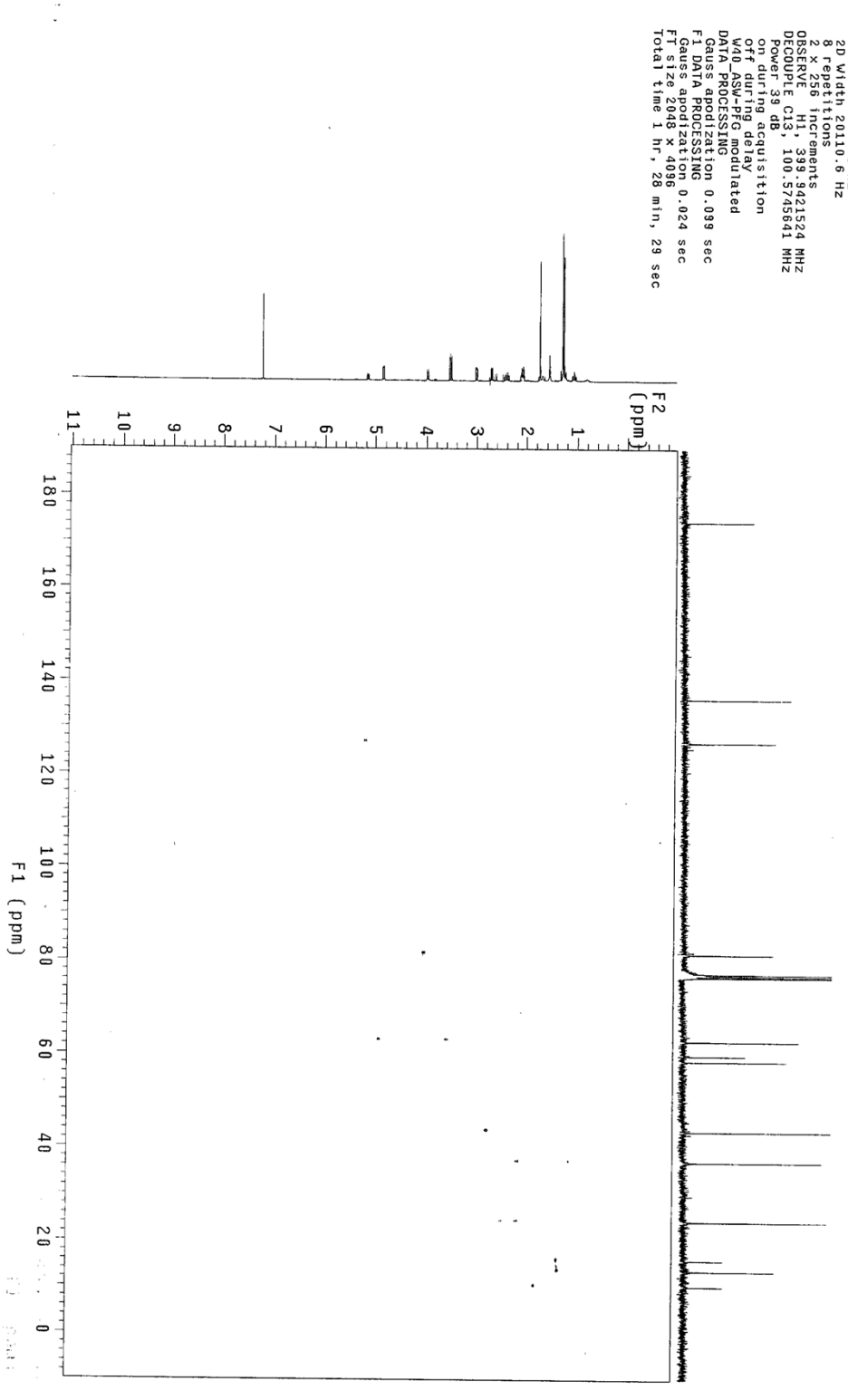
Archive directory: /export/home/hongos/vnmrsys/data
Sample directory:

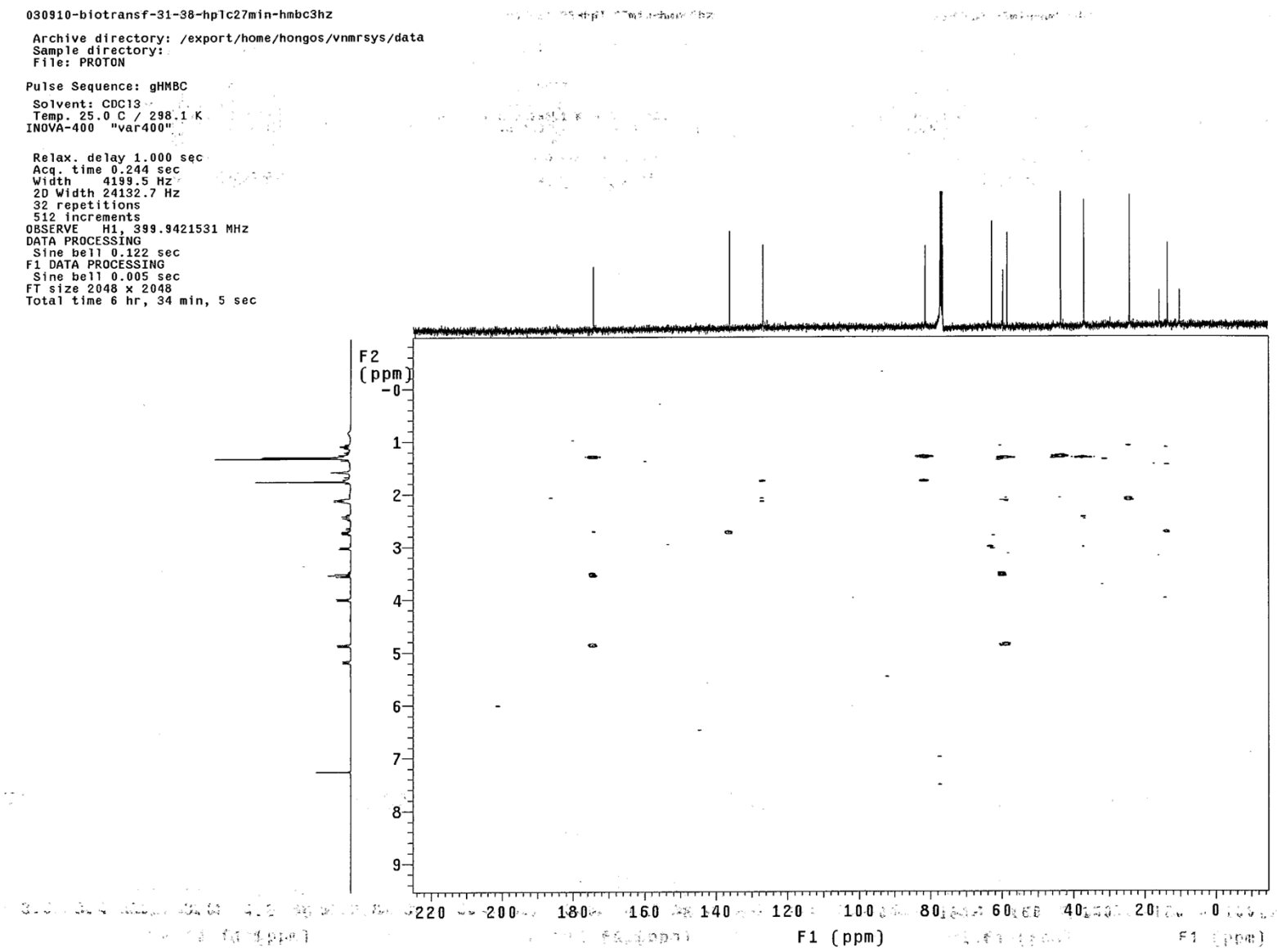
Pulse Sequence: gCOSY

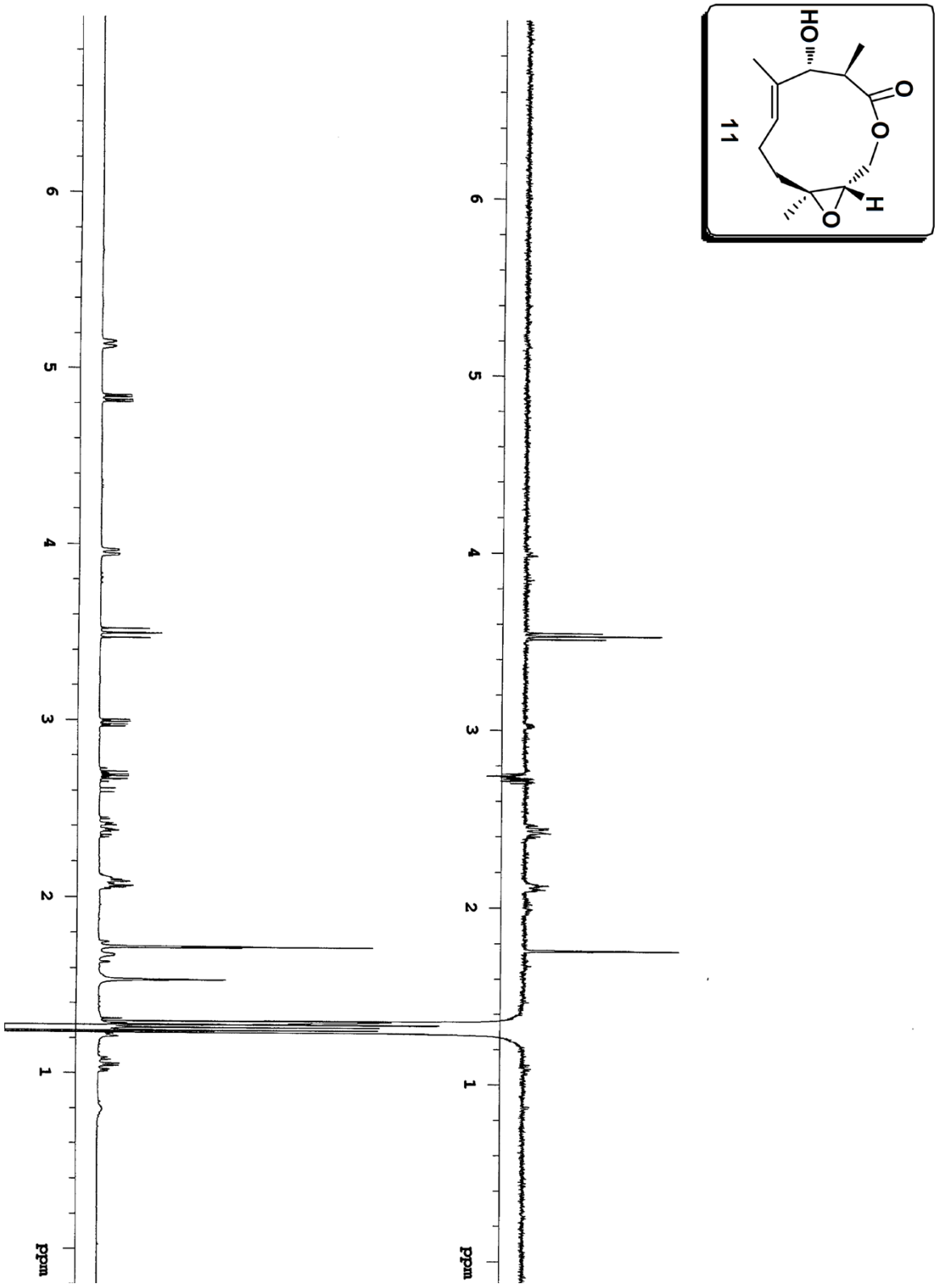
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 030910-biotransf-31-38-HPLC27min-cosy
INOVA-600 "rmnproc1"

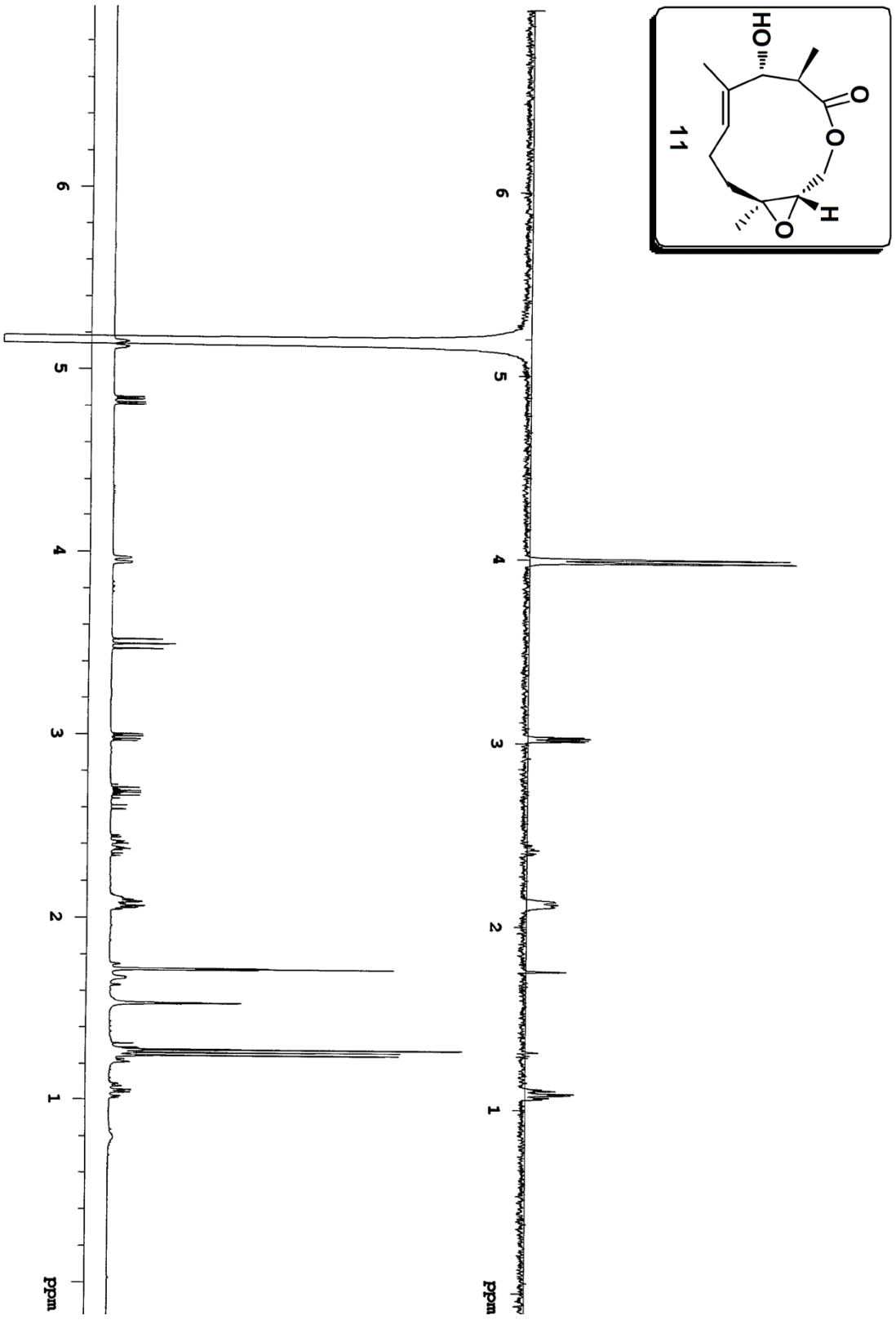
Relax. delay 1.000 sec
Acq. time 0.213 sec
Width 4799.3 Hz
2D Width 4799.3 Hz
4 repetitions
128 increments
OBSERVE H1, 399.9421527 MHz
DATA PROCESSING
Sq. sine bell 0.107 sec
F1 DATA PROCESSING
Sq. sine bell 0.027 sec
FT size 2048 x 2048
Total time 10 min, 54 sec

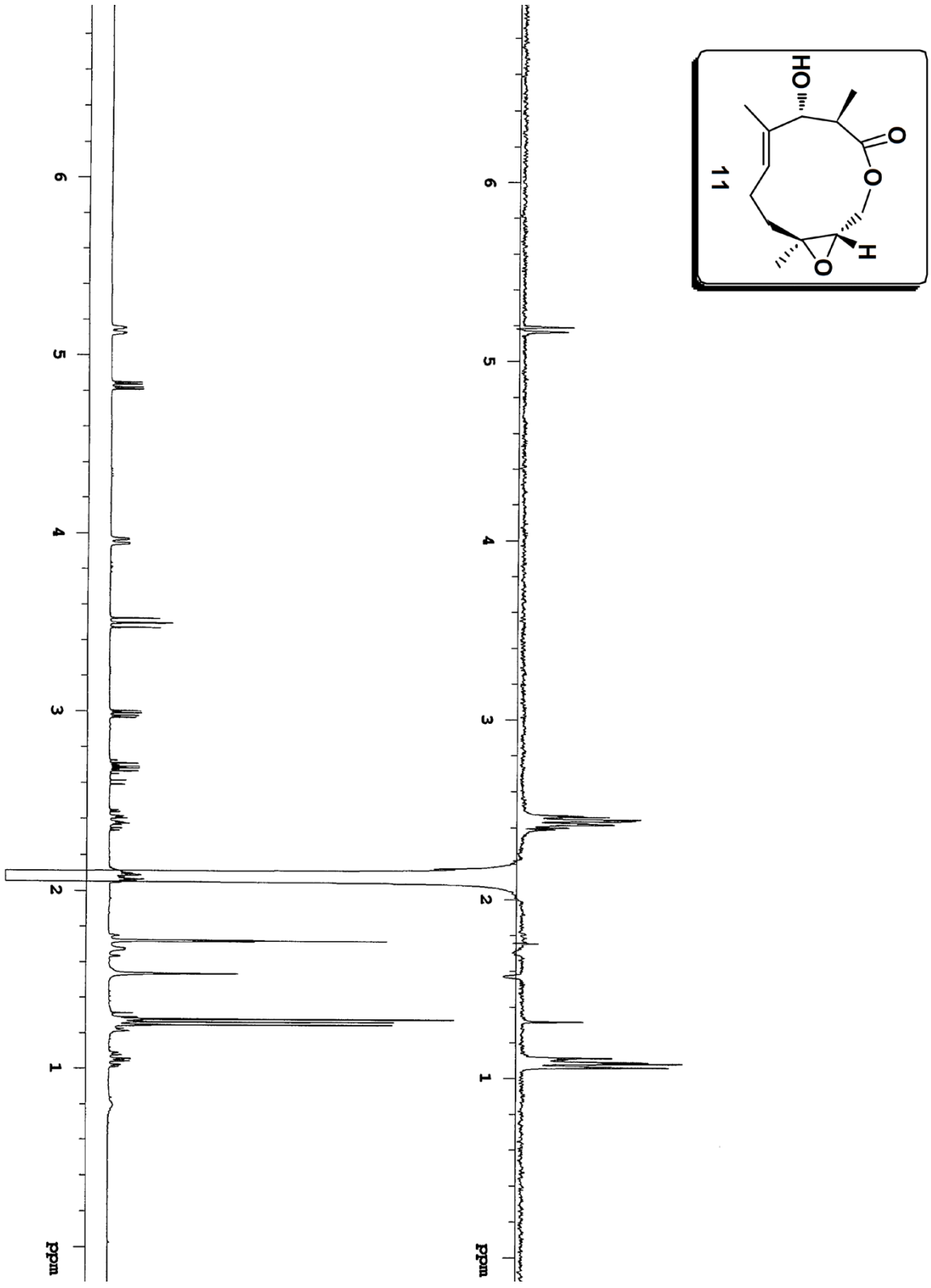


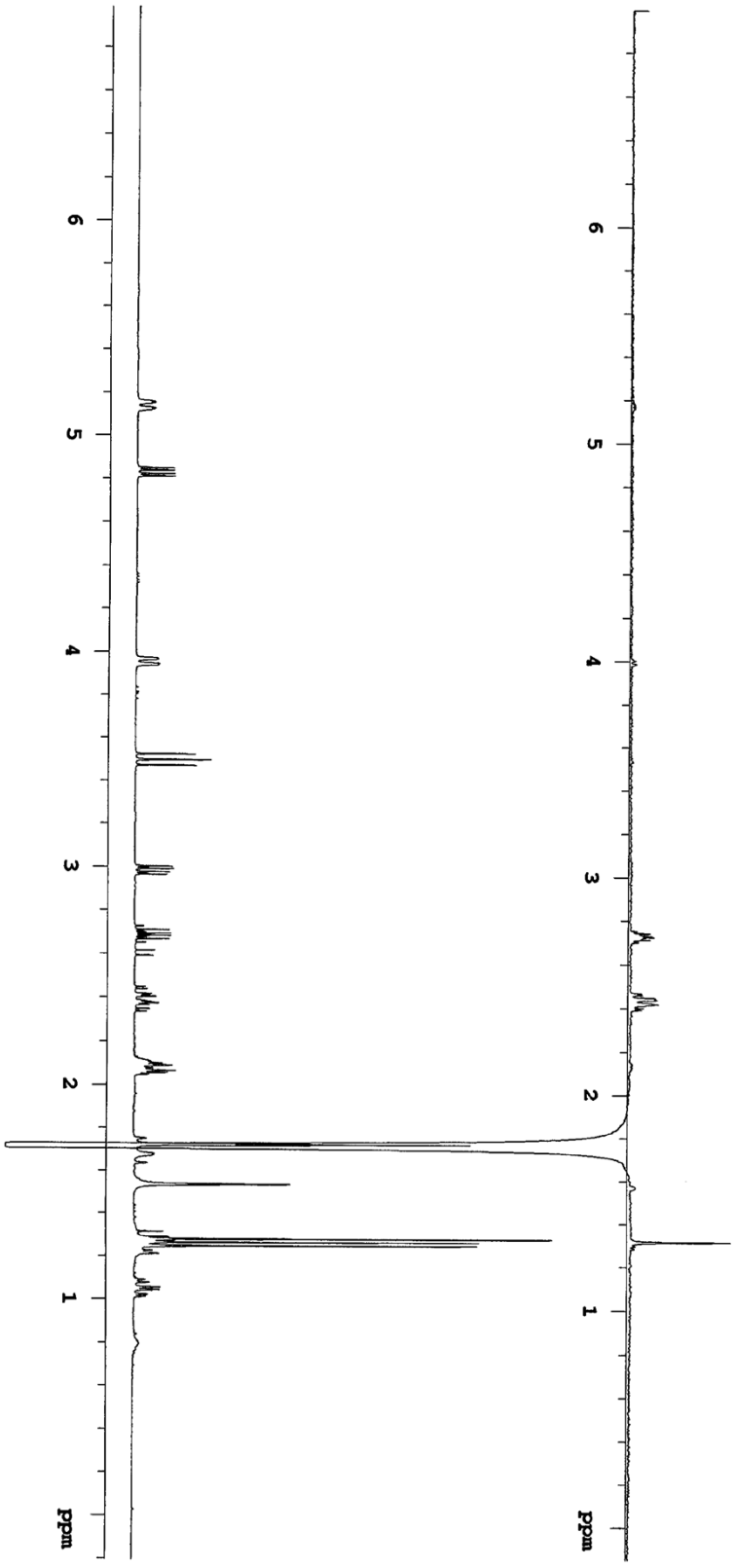

030910-biotransf-botes31-38-hplc27min-hsqc
Archive directory: /export/home/bongos/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: gHSQC
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-400 "var400"
Relax. delay 1.000 sec
Acq. time 0.213 sec
Width 4799.3 Hz
2D Width 20110.6 Hz
8 repetitions
2 x 256 increments
OBSERVE H1, 399.9421524 MHz
DECOUPLE C13, 100.5745641 MHz
Power 39 dB
on during acquisition
off during delay
W10_ASW-PFG modulated
DATA PROCESSING
Gauss apodization 0.099 sec
F1 DATA PROCESSING
Gauss apodization 0.024 sec
FT size 2048 x 4096
Total time 1 hr, 28 min, 29 sec
F2 (ppm)
F1 (ppm)

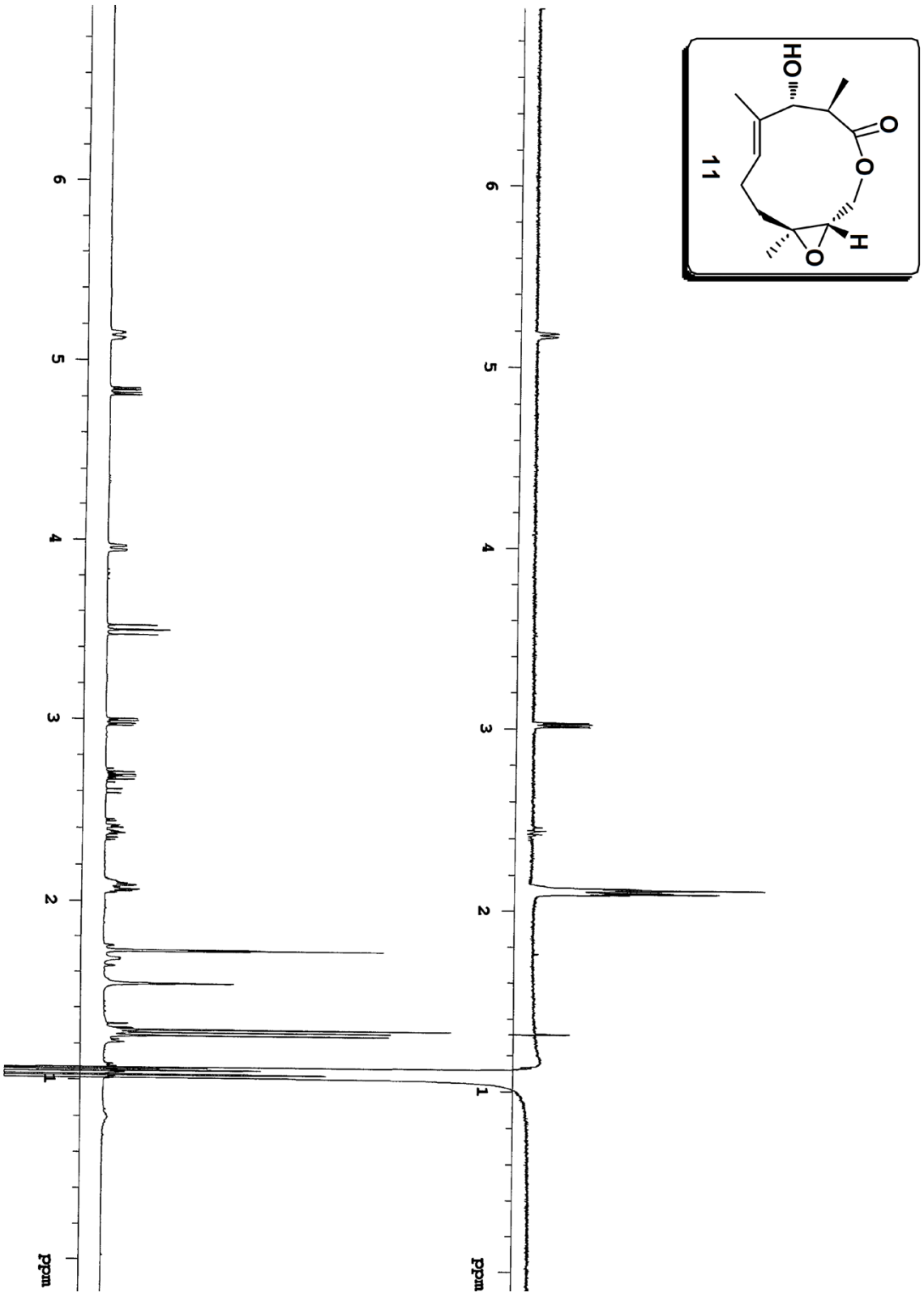

030910-biotransf-31-38-hplc27min-hmbc3hz
Archive directory: /export/home/hongos/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: gHMBC
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-400 "var400"
Relax. delay 1.000 sec
Acq. time 0.244 sec
Width 4199.5 Hz
2D Width 24132.7 Hz
32 repetitions
512 increments
OBSERVE H1, 399.9421531 MHz
DATA PROCESSING
Sine bell 0.122 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 2048
Total time 6 hr, 34 min, 5 sec
F2 (ppm)
F1 (ppm)

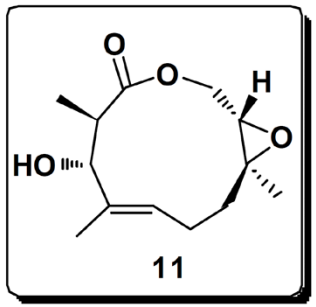

HO
O
O
H
O
11
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm


HO
O
O
H
O
11
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

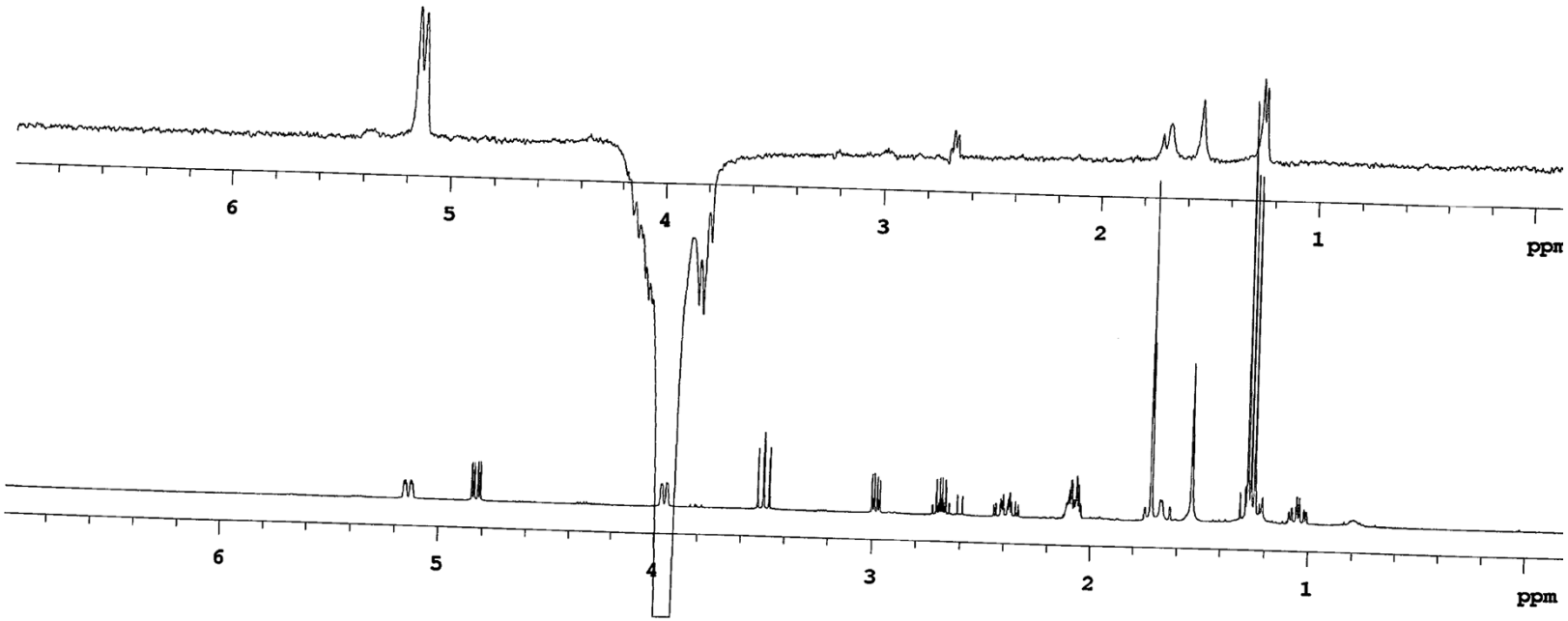

HO
O
O
H
O
11
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

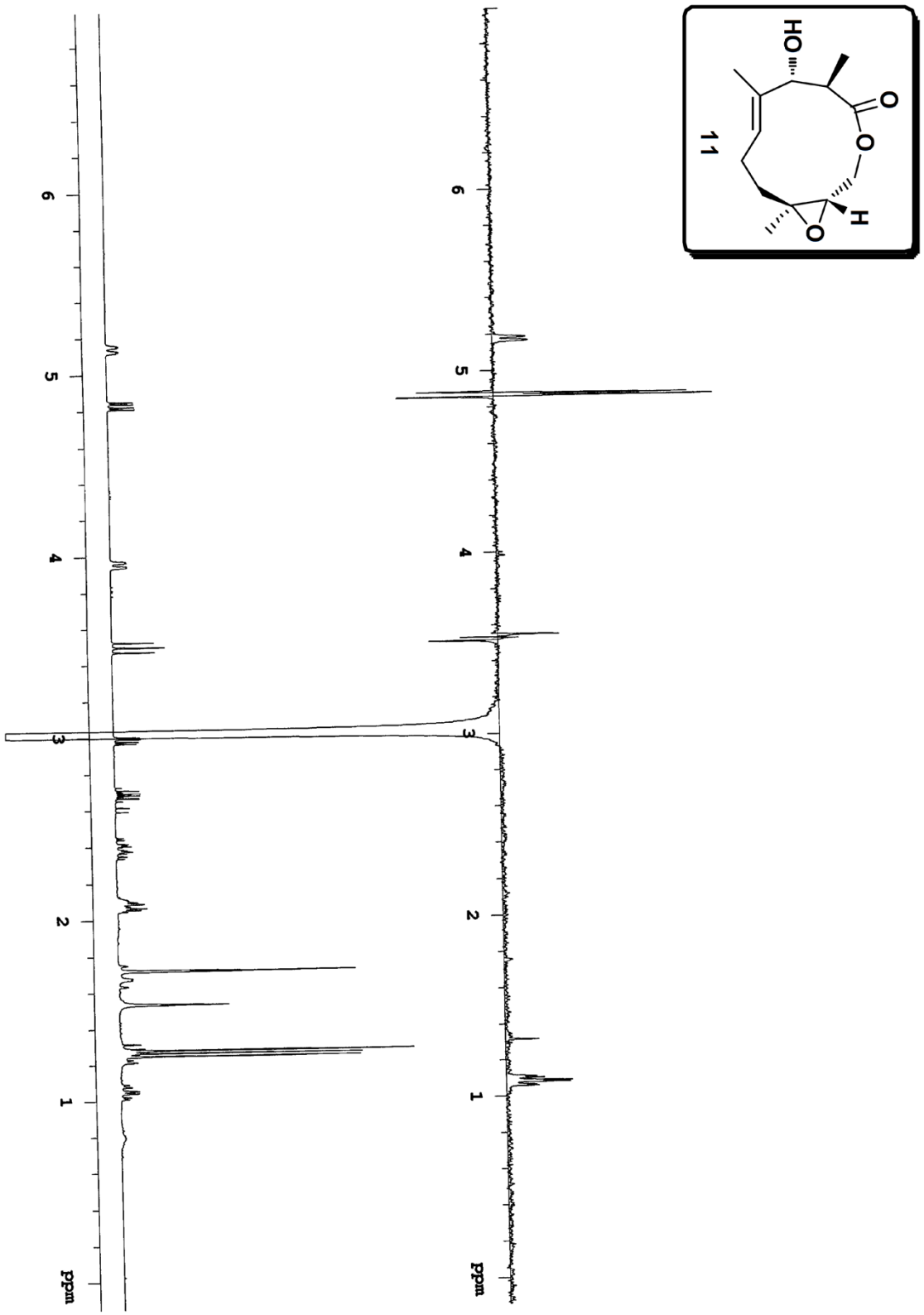

HO
O
O
H
O
11
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

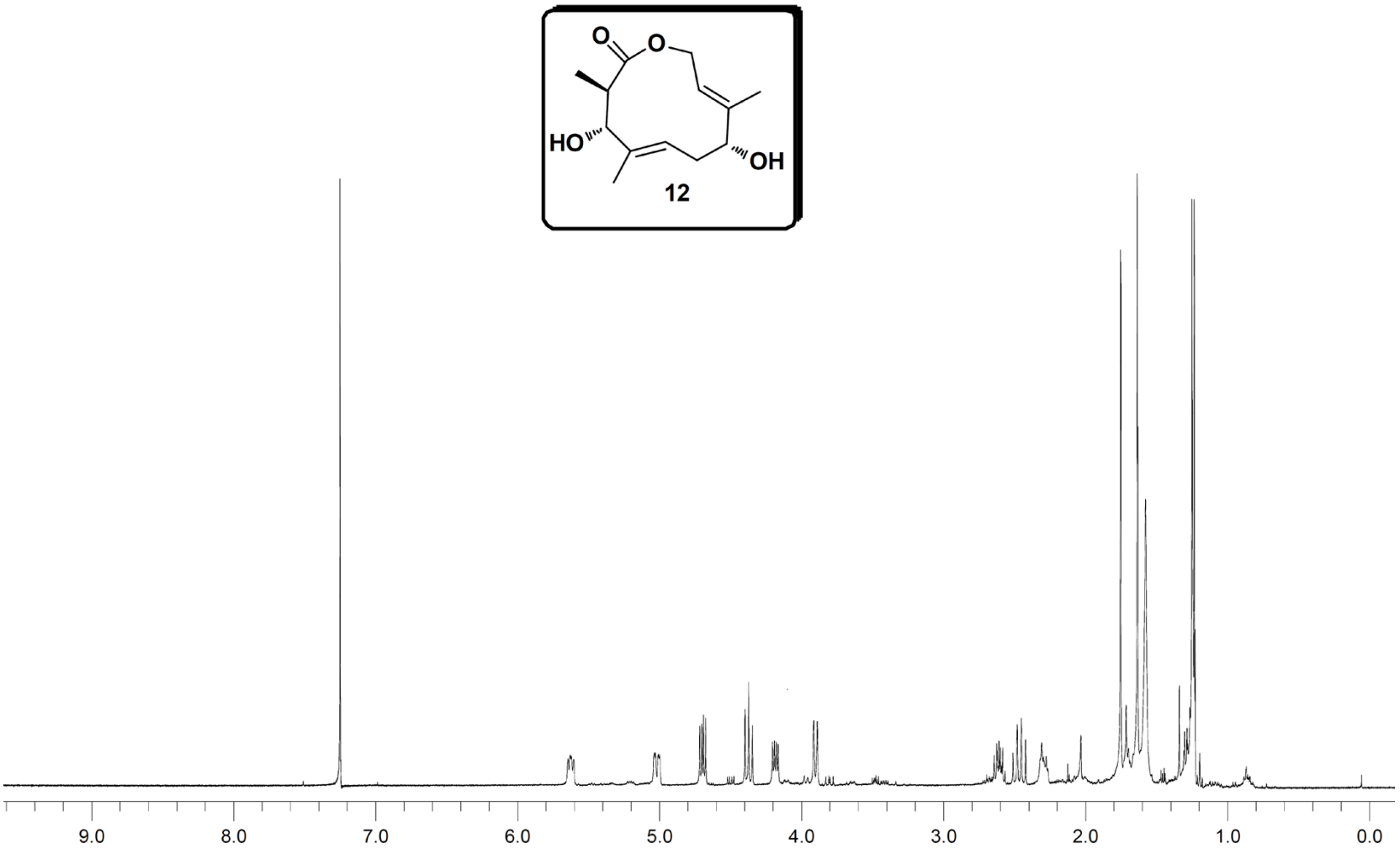

HO
O
O
H
O
11
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm



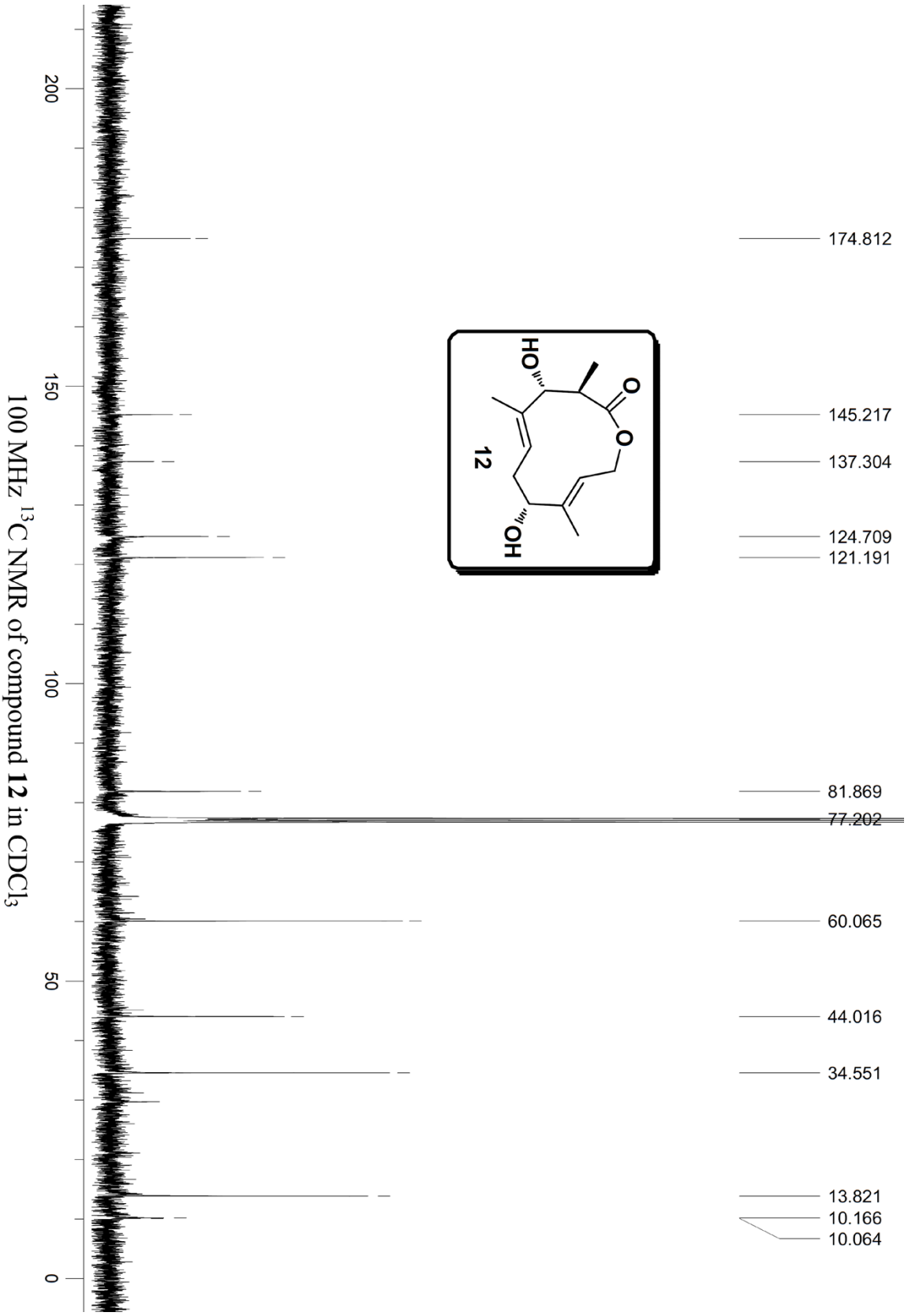
11

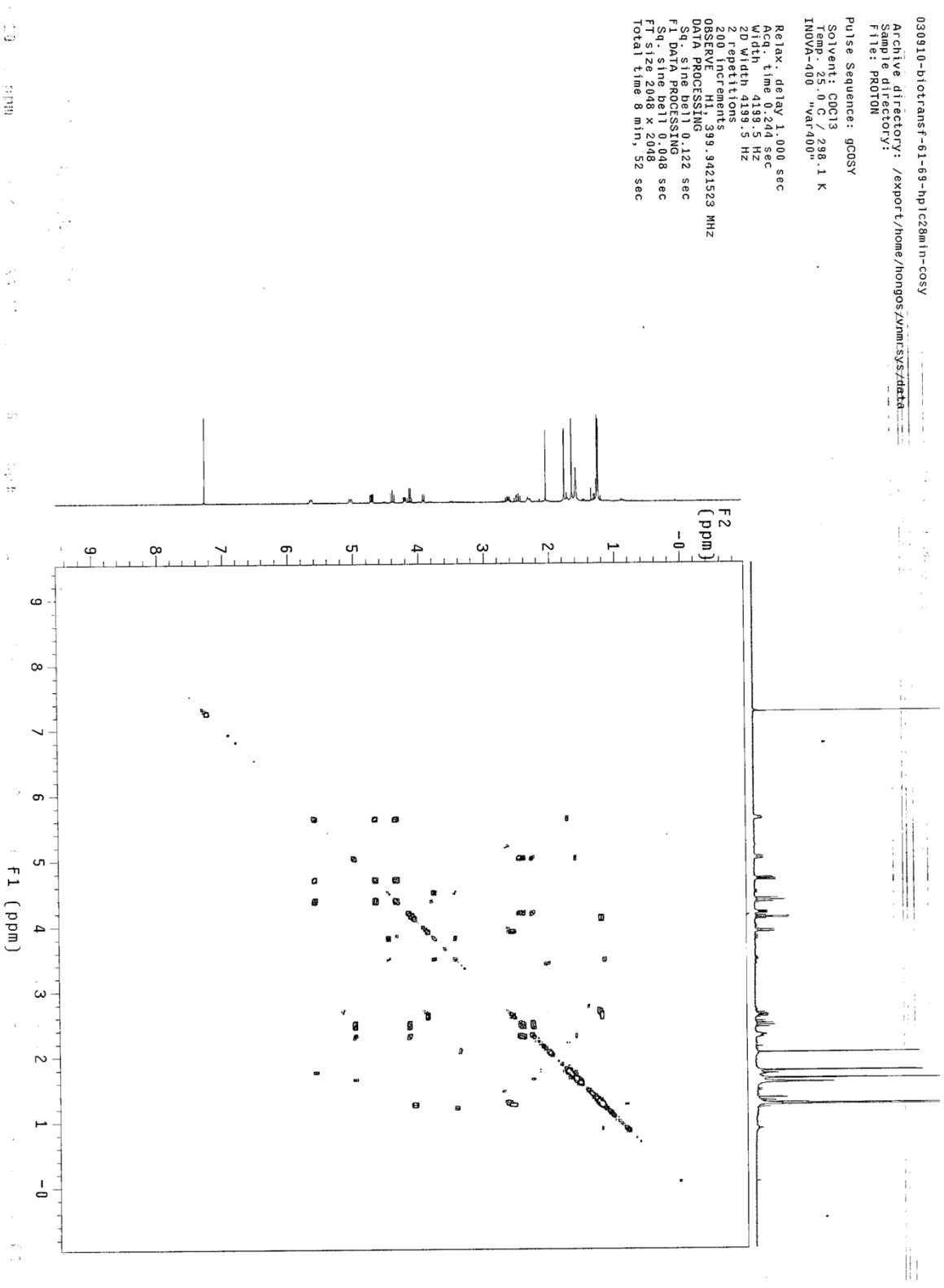



HO
O
O
H
O
11
6
5
4
3
2
1
ppm



400 MHz ^{1}H NMR of compound **12** in $CDCl_3$


100 MHz ^{13}C NMR of compound **12** in $CDCl_3$
200
150
100
50
0
HO
OH
O
O
12
174.812
145.217
137.304
124.709
121.191
81.869
77.202
60.065
44.016
34.551
13.821
10.166
10.064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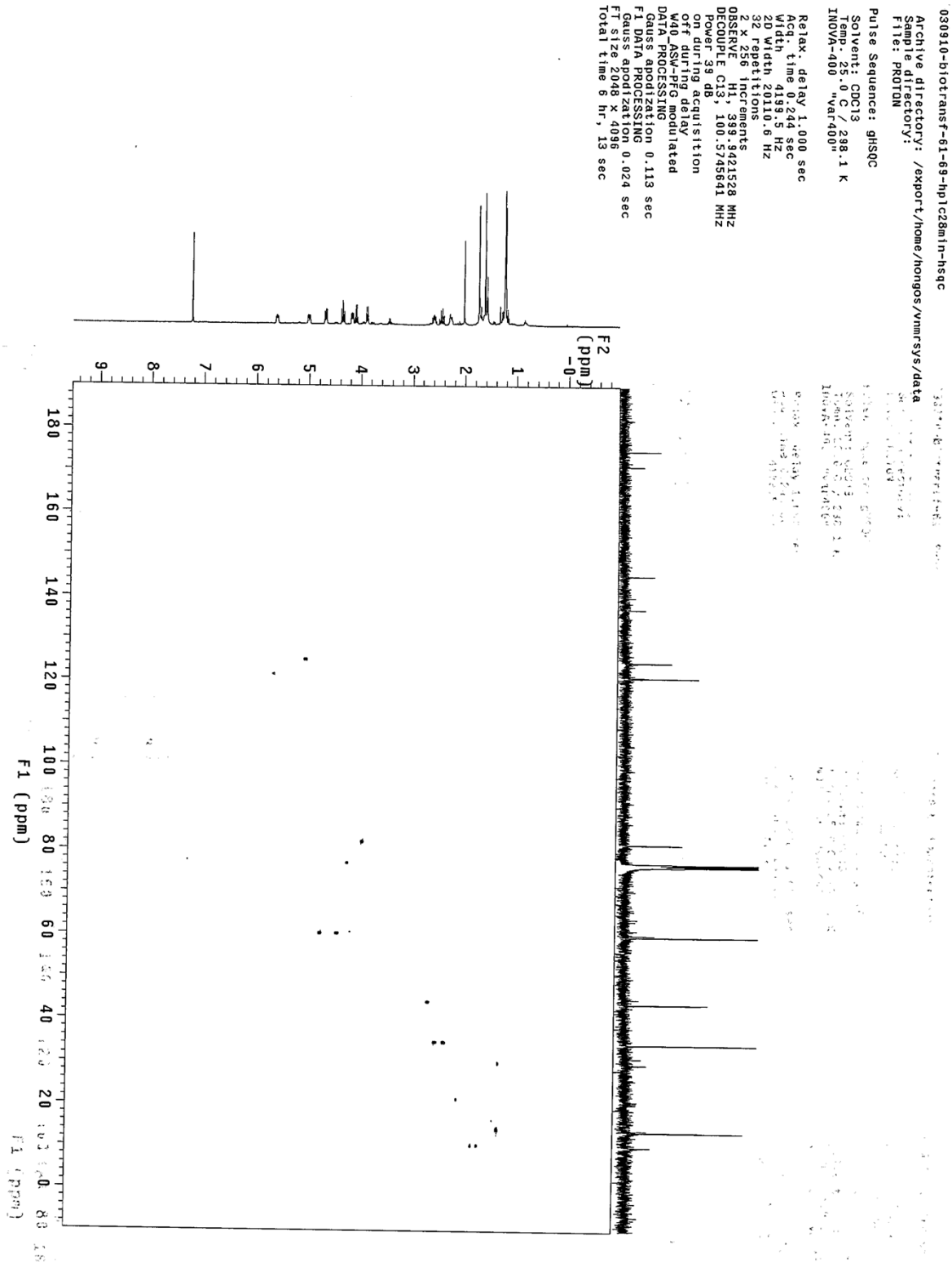
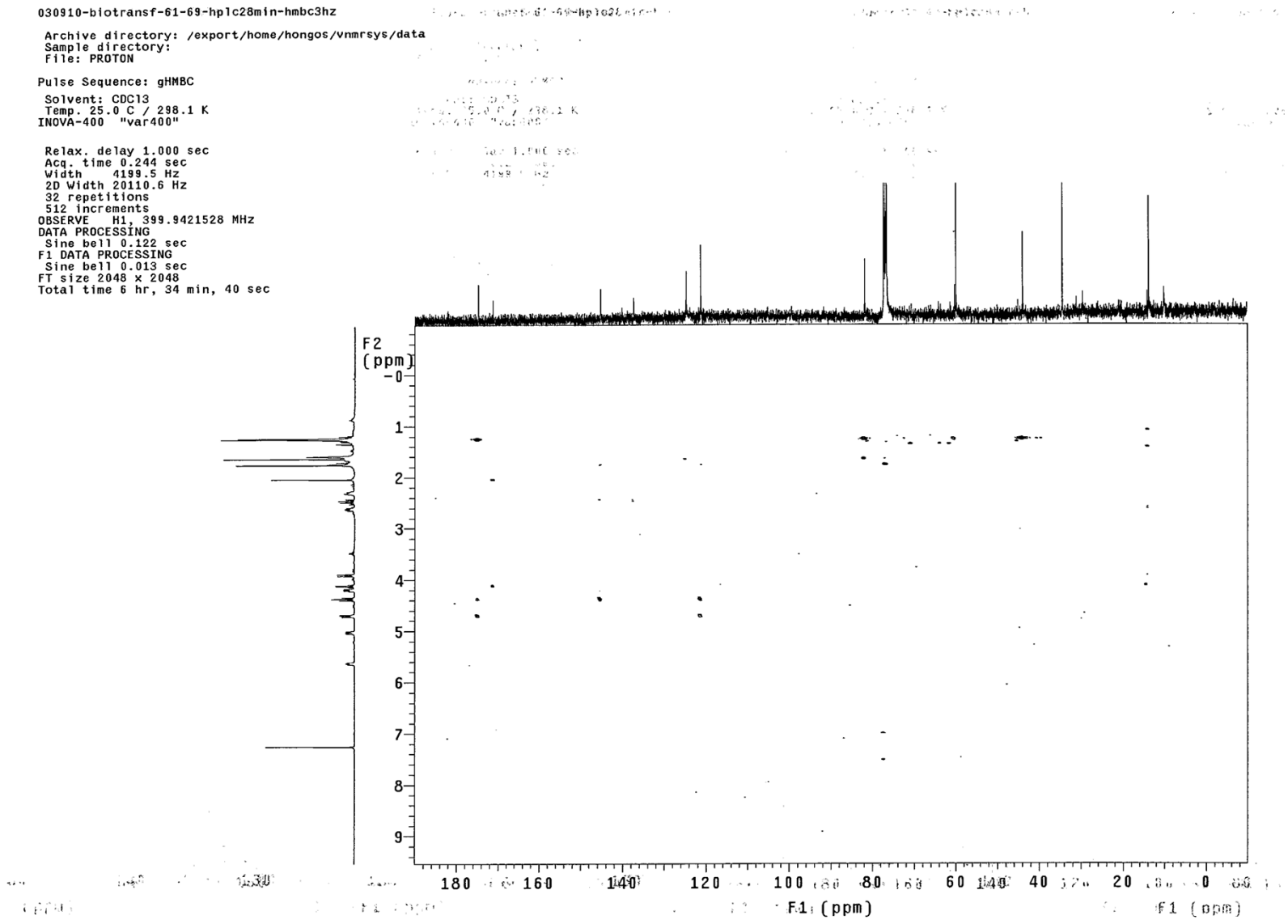
Sample directory:
File: PROTON
Pulse Sequence: gCOSY
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-400 "var400"
Relax. delay 1.000 sec
Acq. time 0.244 sec
Width 4199.5 Hz
2D width 4199.5 Hz
2 repetitions
200 increments
OBSERVE H1, 399.9421523 MHz
DATA PROCESSING
Sq. sine bell 0.122 sec
F1 DATA PROCESSING
Sq. sine bell 0.048 sec
FT size 2048 x 2048
Total time 8 min, 52 sec
F2 (ppm)
F1 (ppm)


030910-biotransf-61-69-hplc28min-hsqc
Archive directory: /export/home/hongos/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: gHSQC
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-400 "var400"
Relax. delay 1.000 sec
Acq. time 0.244 sec
Width 4199.5 Hz
2D Width 20110.6 Hz
32 repetitions
256 x 256 increments
OBSERVE H1, 399.9421528 MHz
DECOUPLE C13, 100.5745641 MHz
Power 39 dB
on during acquisition
off during delay
W40_ASW-PFG modulated
DATA PROCESSING
Gauss apodization 0.113 sec
F1 DATA PROCESSING
Gauss apodization 0.024 sec
FT size 2048 x 4096
Total time 6 hr, 13 sec
F2 (ppm)
F1 (ppm)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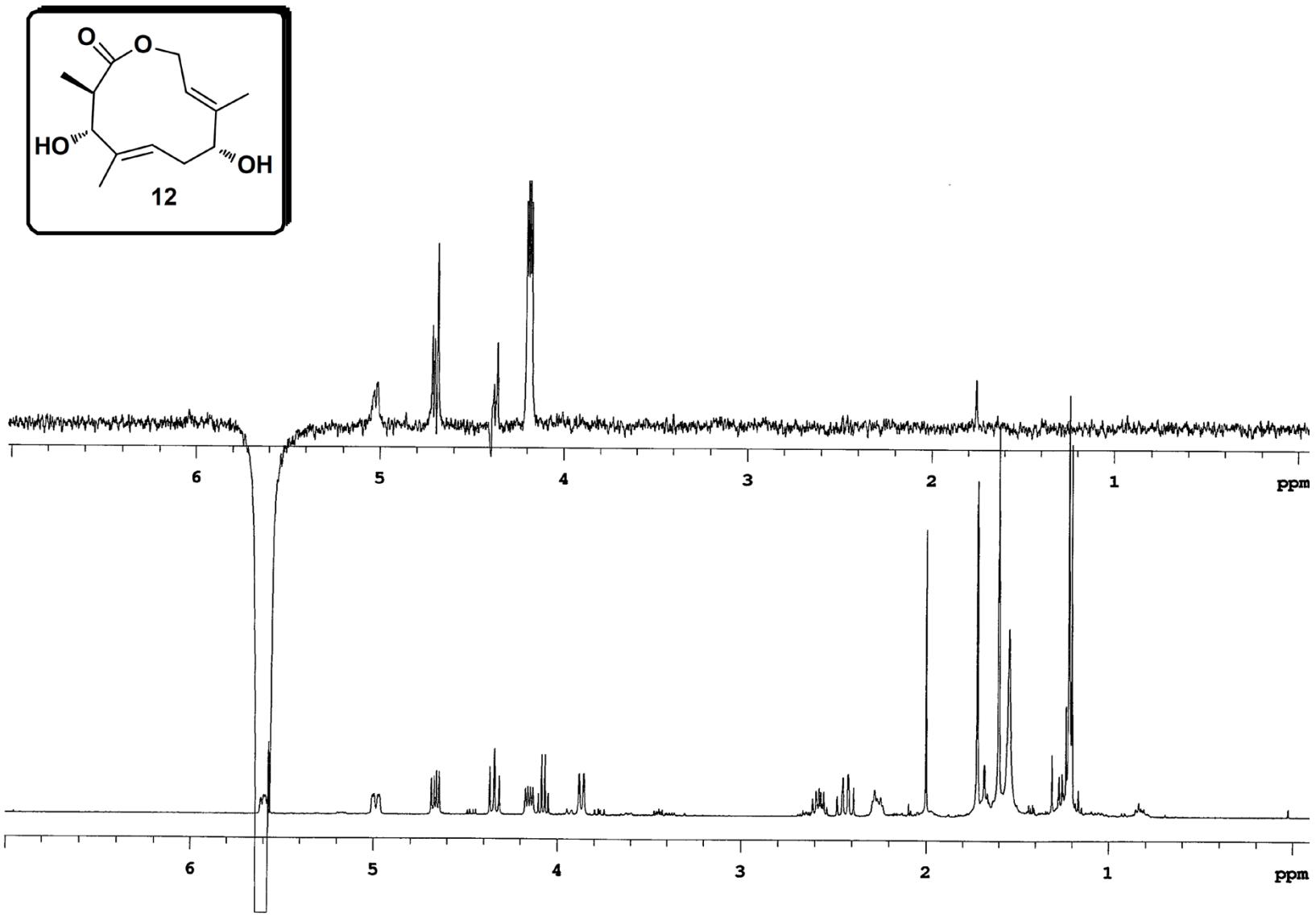
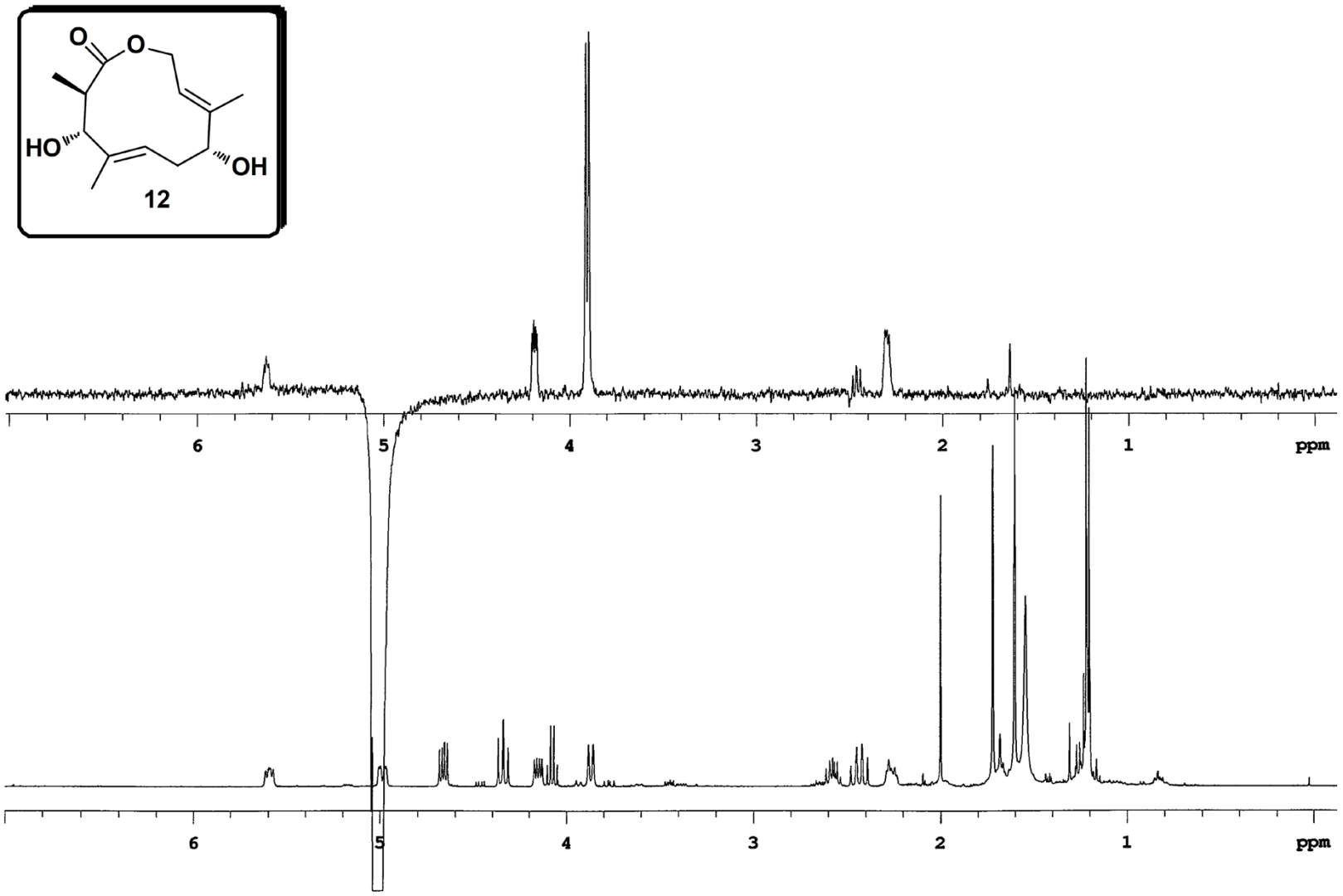
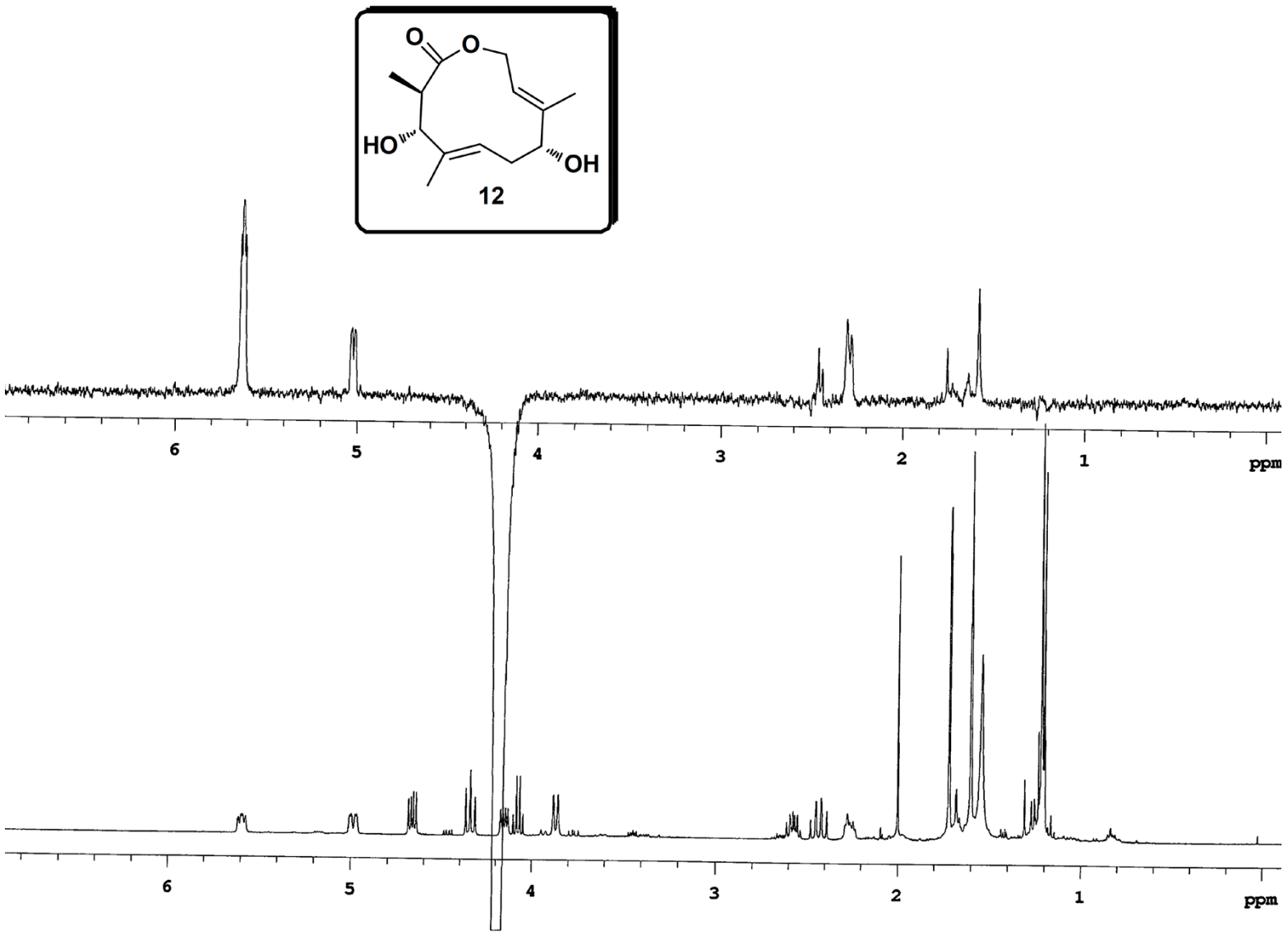
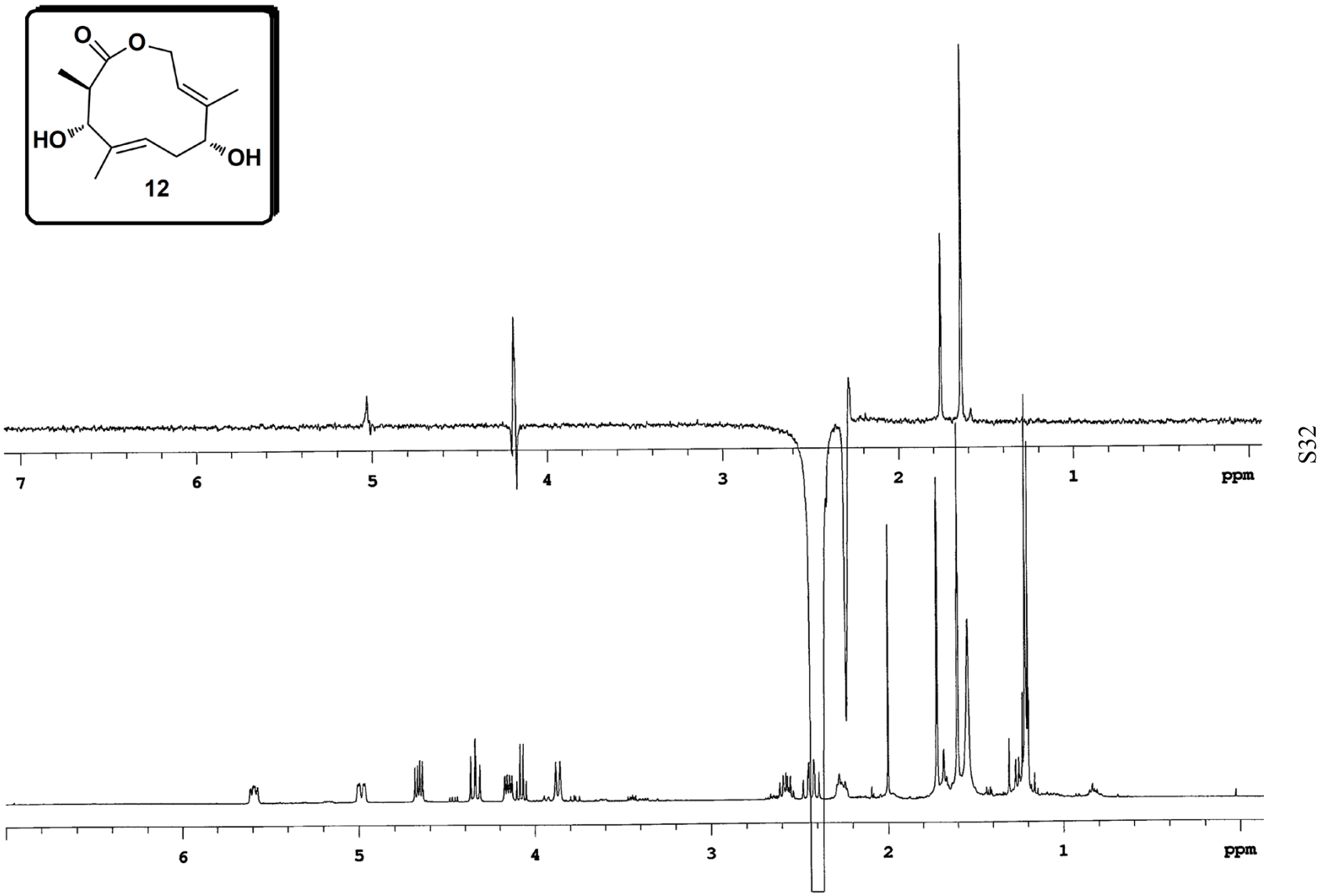
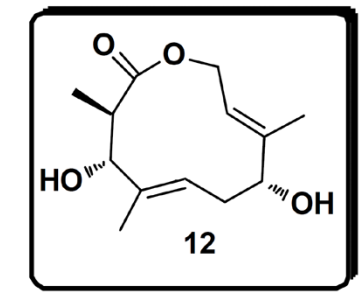
Archive directory: /export/home/hongos/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: gHMBC
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-400 "var400"
Relax. delay 1.000 sec
Acq. time 0.244 sec
Width 4199.5 Hz
2D Width 20110.6 Hz
32 repetitions
512 increments
OBSERVE H1, 399.9421528 MHz
DATA PROCESSING
Sine bell 0.122 sec
F1 DATA PROCESSING
Sine bell 0.013 sec
FT size 2048 x 2048
Total time 6 hr, 34 min, 40 sec
F2 (ppm)
F1 (ppm)


O
O
HO
OH
12
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

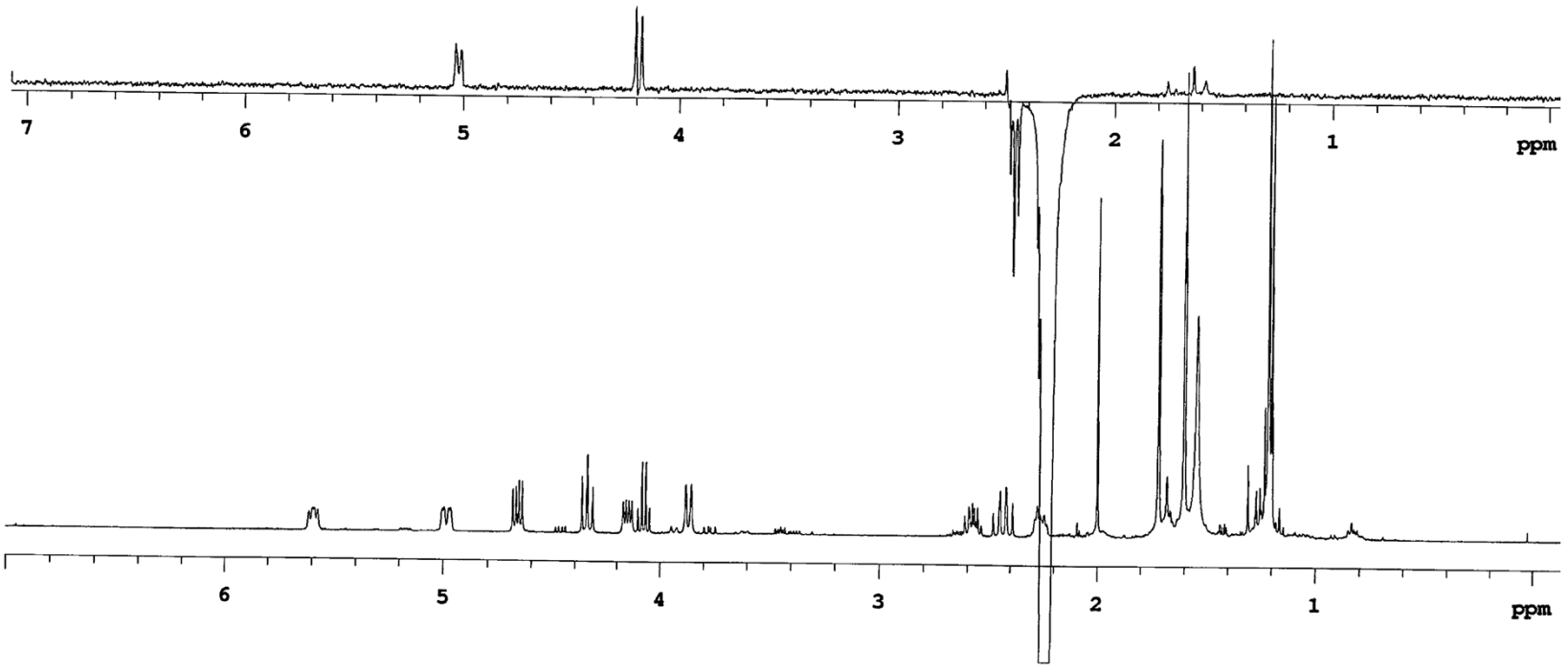

O
O
HO
OH
12
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

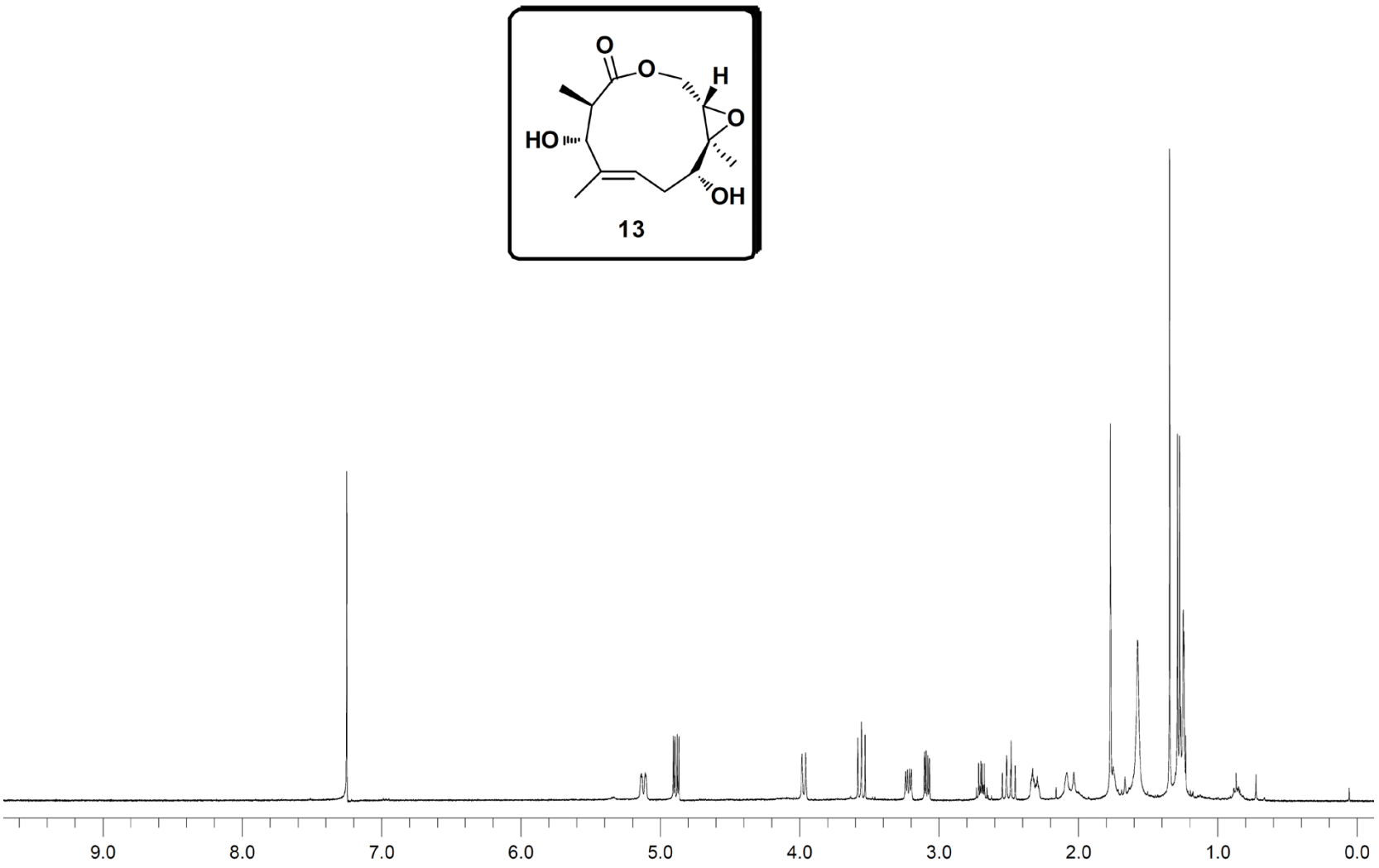

O
O
HO
OH
12
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm


O
O
HO
OH
12
7
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

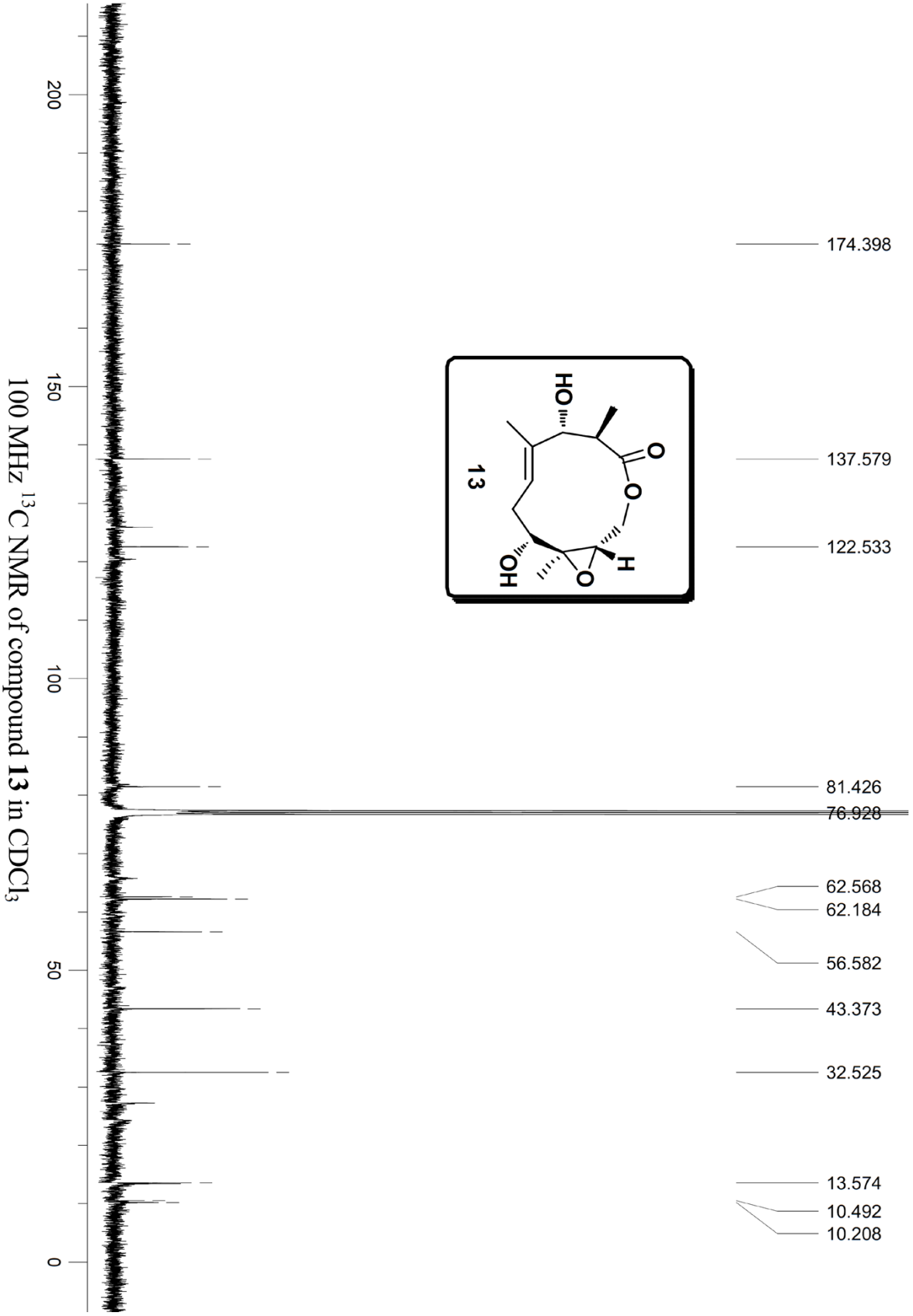


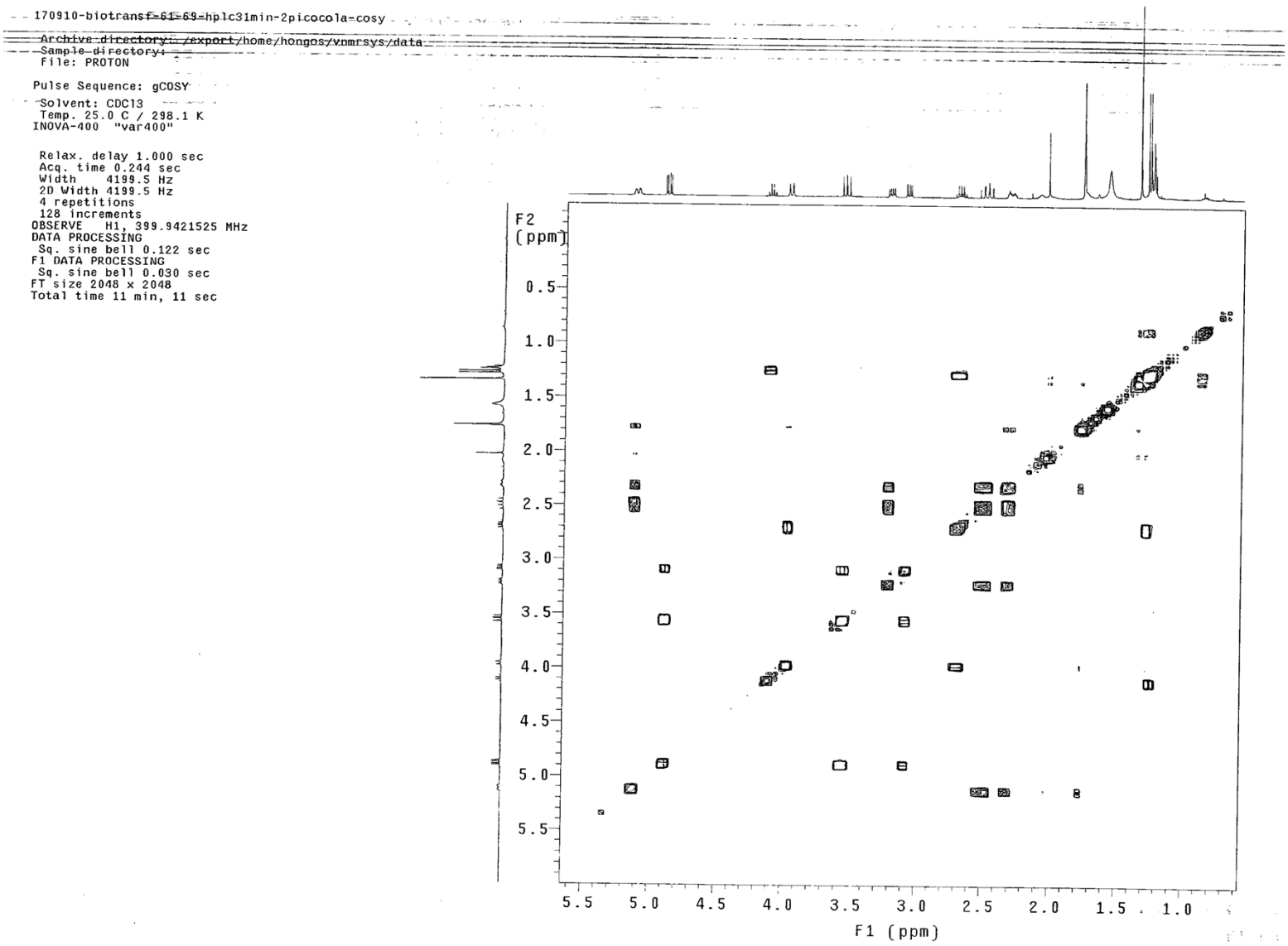
12





400 MHz ^{1}H NMR of compound **13** in $CDCl_3$

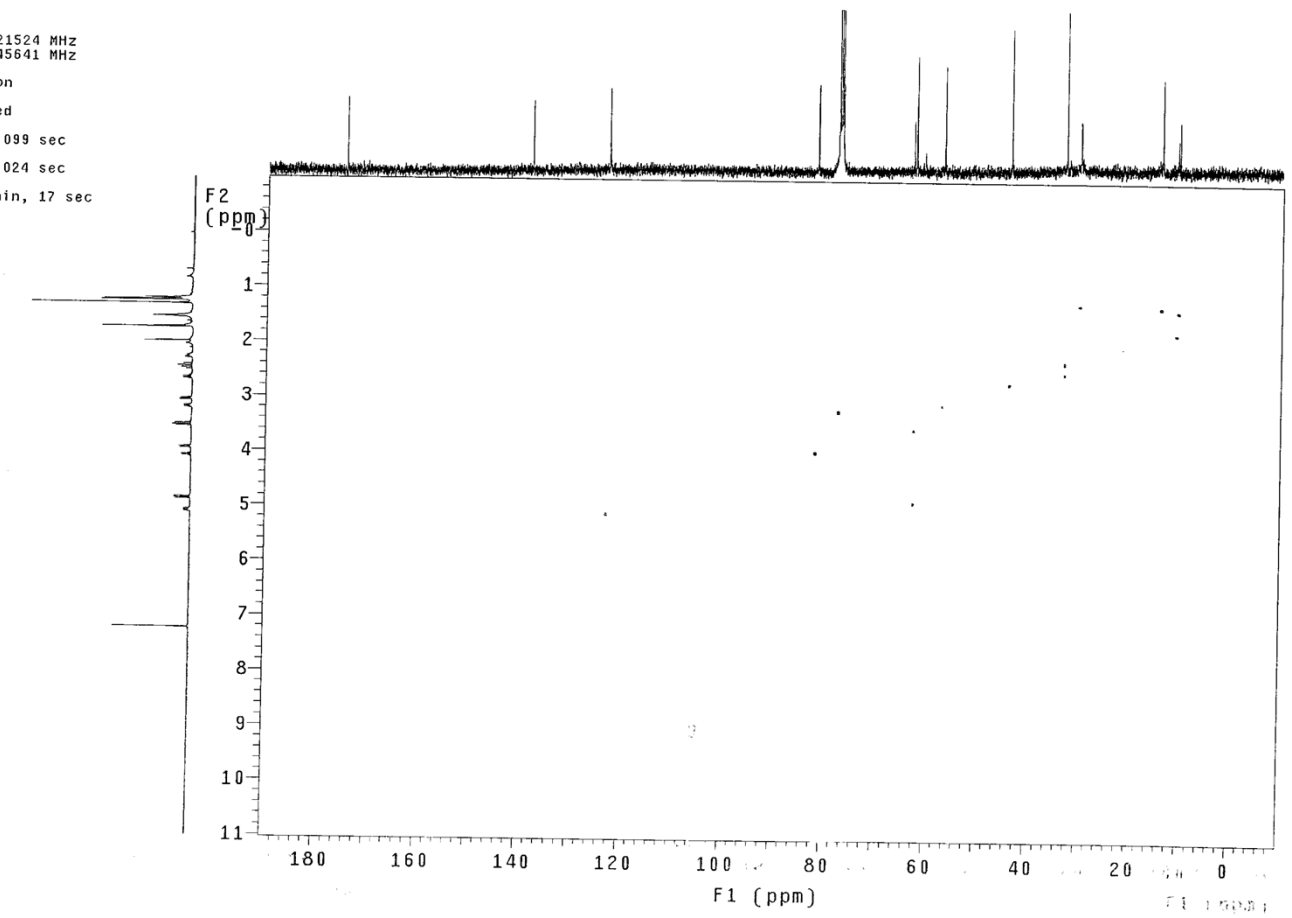

100 MHz ^{13}C NMR of compound **13** in $CDCl_3$
200
150
100
50
0
174.398
137.579
122.533
81.426
76.928
62.568
62.184
56.582
43.373
32.525
13.574
10.492
10.208
13
HO
OH
O
O
O
H

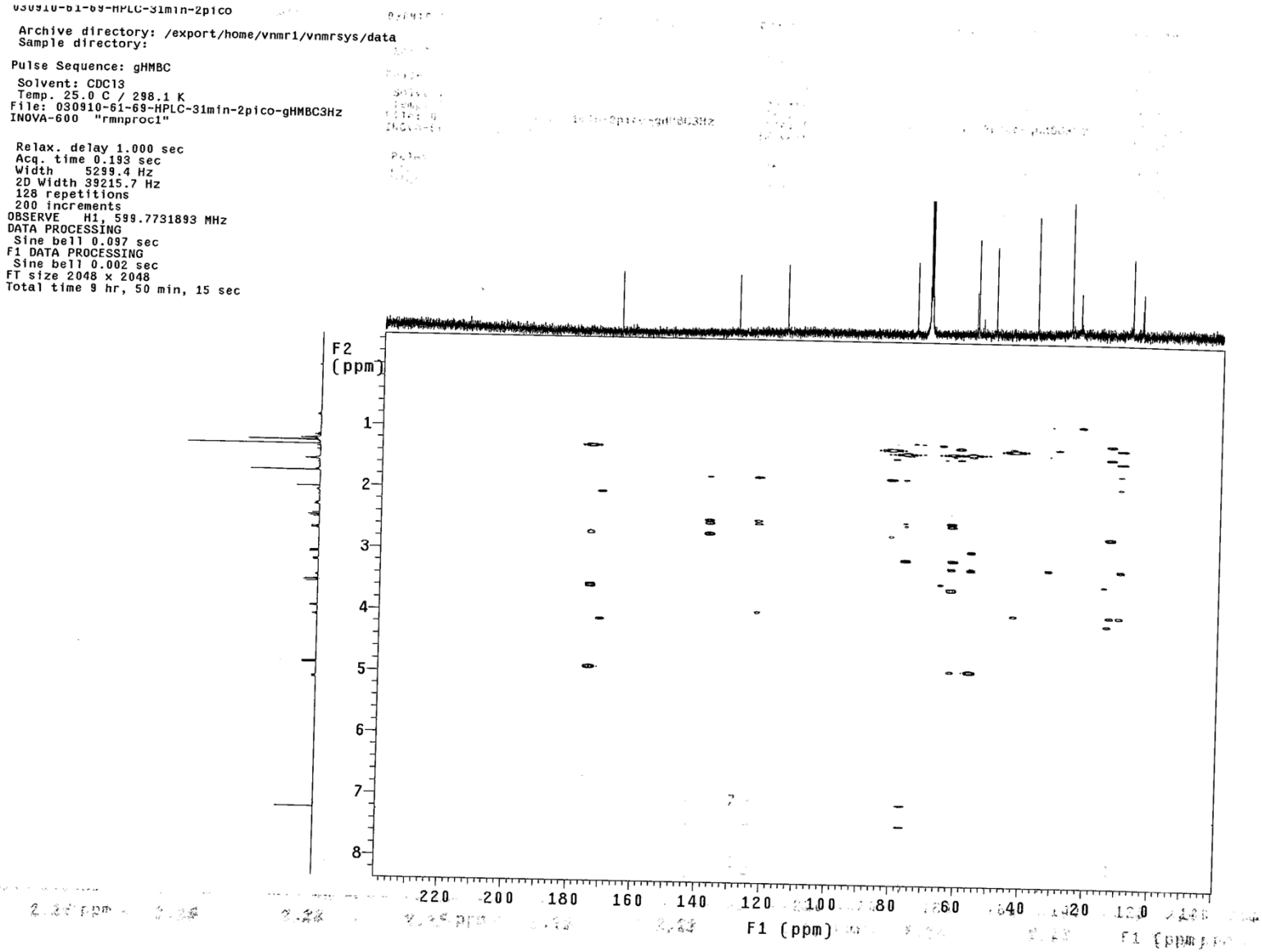

170910-biotransf-61-69-hplc31min-2picocola-cosy
Archive directory: /export/home/hongos/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: gCOSY
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-400 "var400"
Relax. delay 1.000 sec
Acq. time 0.244 sec
Width 4199.5 Hz
2D Width 4199.5 Hz
4 repetitions
128 increments
OBSERVE H1, 399.9421525 MHz
DATA PROCESSING
Sq. sine bell 0.122 sec
F1 DATA PROCESSING
Sq. sine bell 0.030 sec
FT size 2048 x 2048
Total time 11 min, 11 sec
F2 (ppm)
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
F1 (ppm)

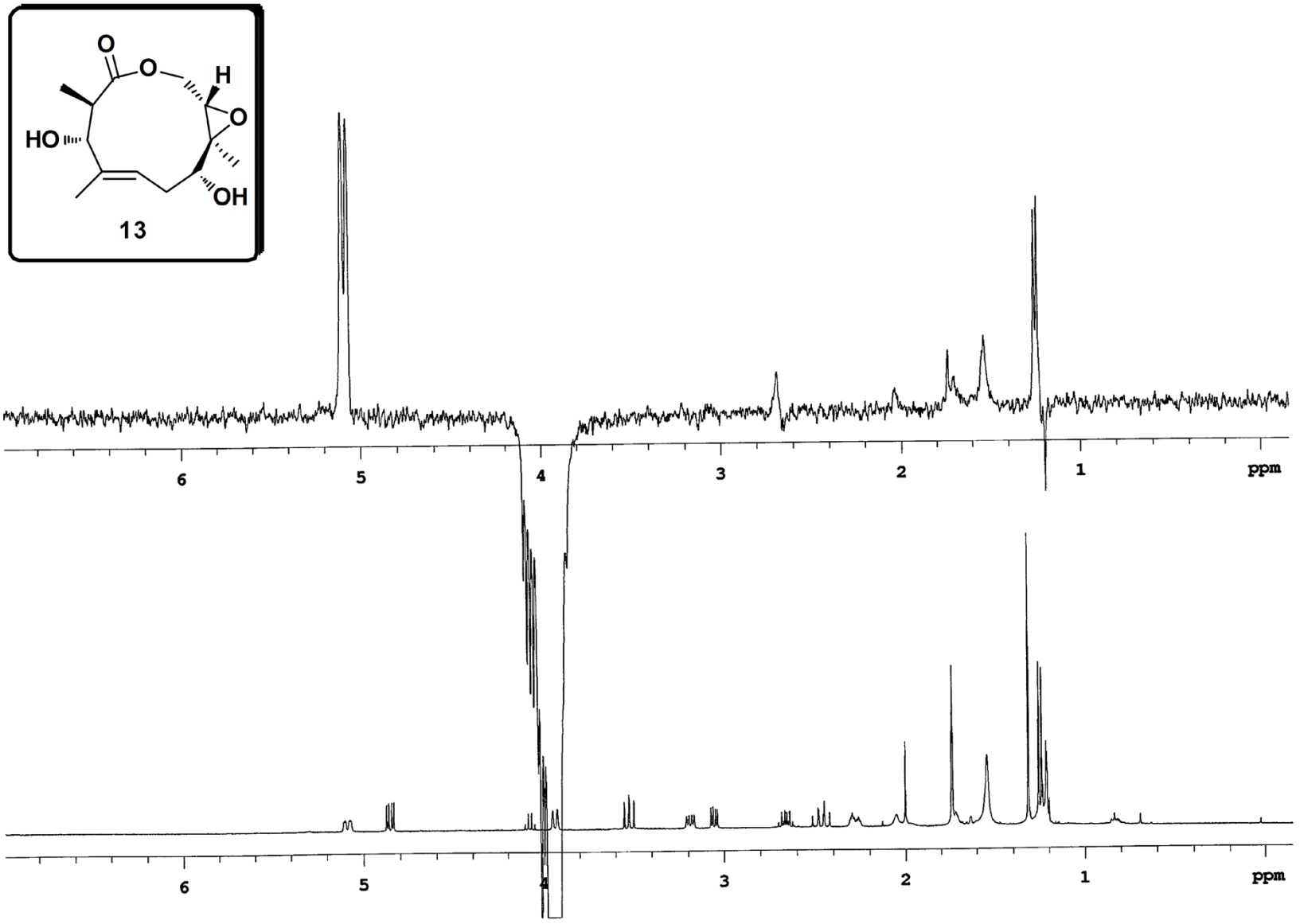
190910=biotransf-61-69-hplc31min-2picocola=hsqc
Archive directory: /export/home/hongos/vnmrsys/data
Sample directory:

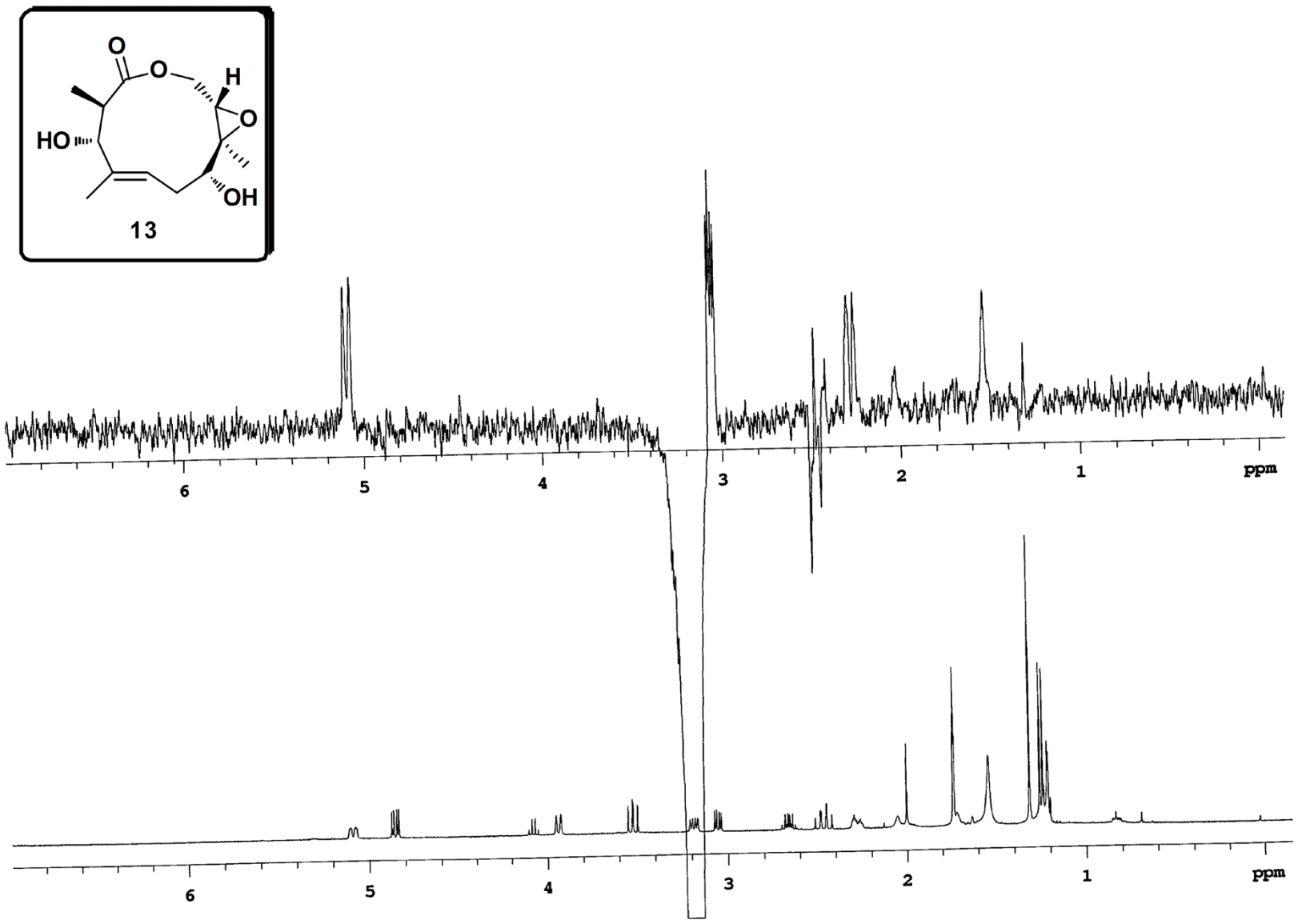
Pulse Sequence: gHSQC
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 190910-biotransf-61-69-hplc31min-2picocola-hsqc
INOVA-600 "rmnproc1"

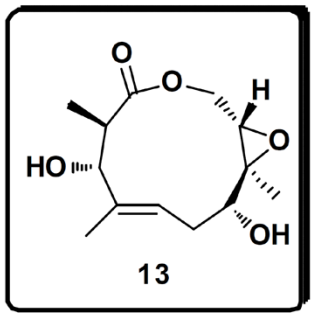
Relax. delay 1.000 sec
Acq. time 0.213 sec
Width 4799.3 Hz
2D Width 20110.6 Hz
16 repetitions
2 x 256 increments
OBSERVE H1, 399.9421524 MHz
DECOUPLE C13, 100.5745641 MHz
Power 39 dB
on during acquisition
off during delay
W40_ASW-PFG modulated
DATA PROCESSING
Gauss apodization 0.099 sec
F1 DATA PROCESSING
Gauss apodization 0.024 sec
FT size 2048 x 4096
Total time 2 hr, 56 min, 17 sec



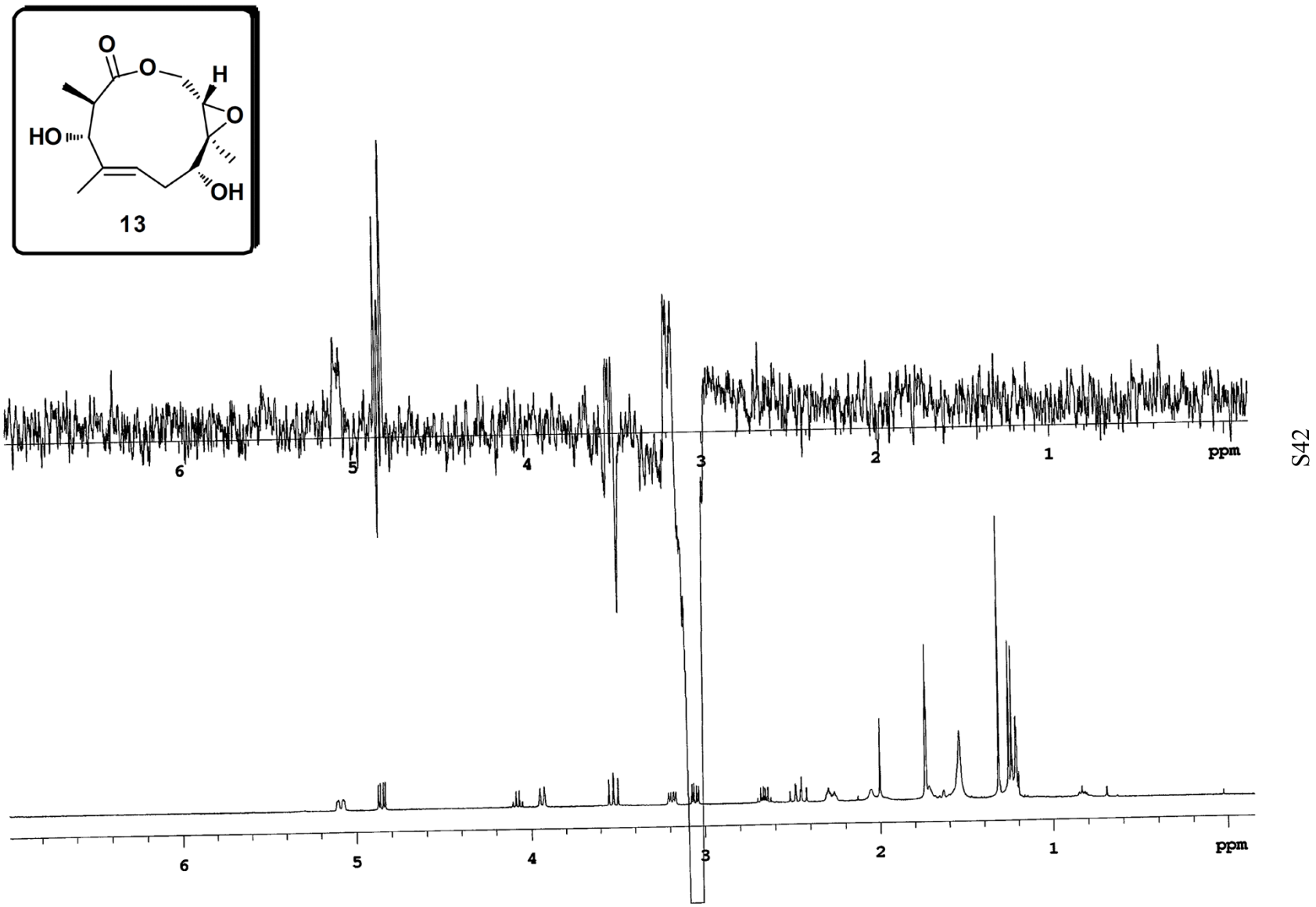

030910-61-69-HPLC-31min-2pico
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: gHMBC
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 030910-61-69-HPLC-31min-2pico-gHMBC3Hz
INOVA-600 "rmnproc1"
Relax. delay 1.000 sec
Acq. time 0.193 sec
Width 5299.4 Hz
2D Width 39215.7 Hz
128 repetitions
200 increments
OBSERVE H1, 599.7731893 MHz
DATA PROCESSING
Sine bell 0.097 sec
F1 DATA PROCESSING
Sine bell 0.002 sec
FT size 2048 x 2048
Total time 9 hr, 50 min, 15 sec
F2 (ppm)
1
2
3
4
5
6
7
8
220
200
180
160
140
120
100
80
60
40
20
0
F1 (ppm)

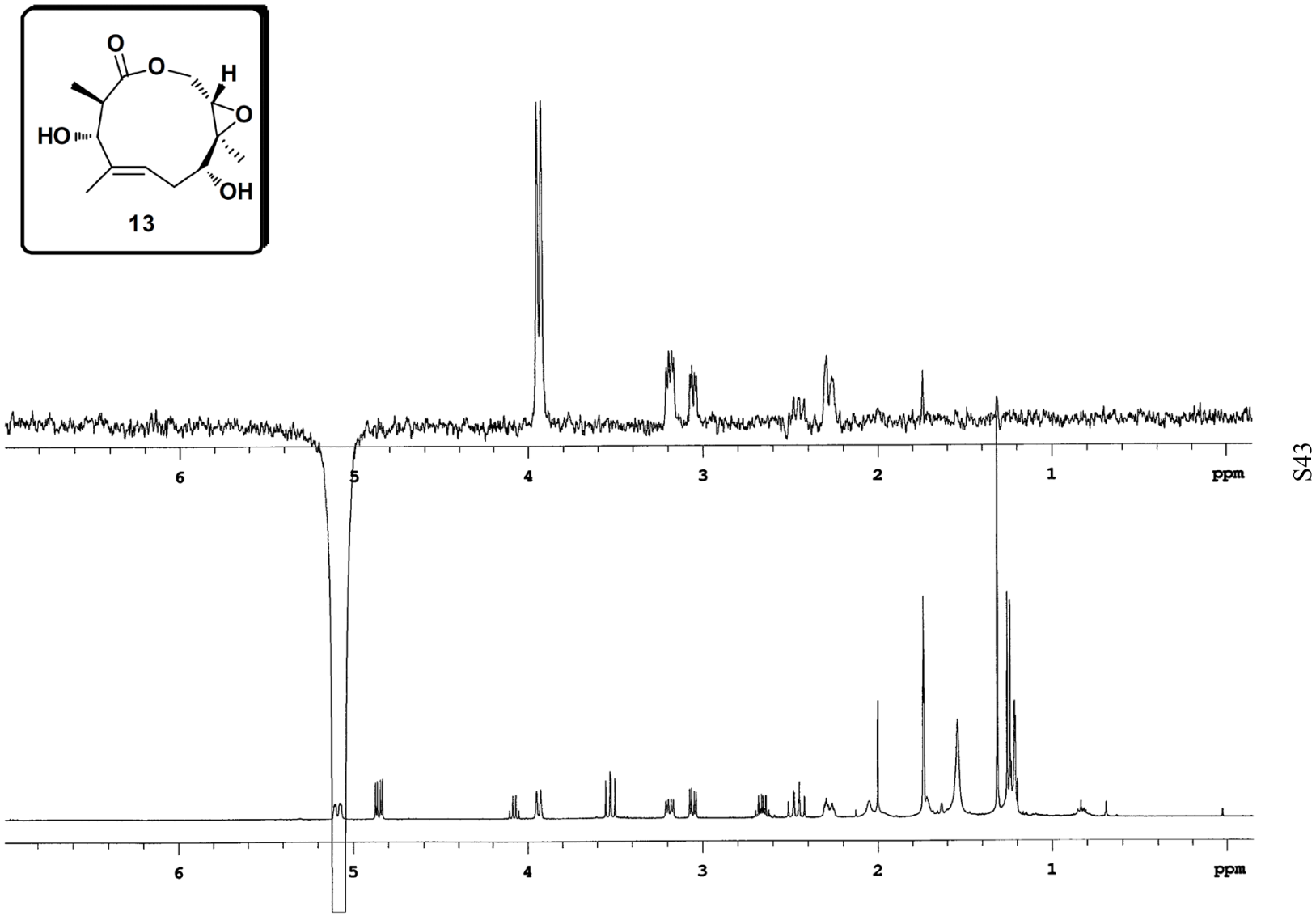

O
O
H
O
HO
OH
13
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

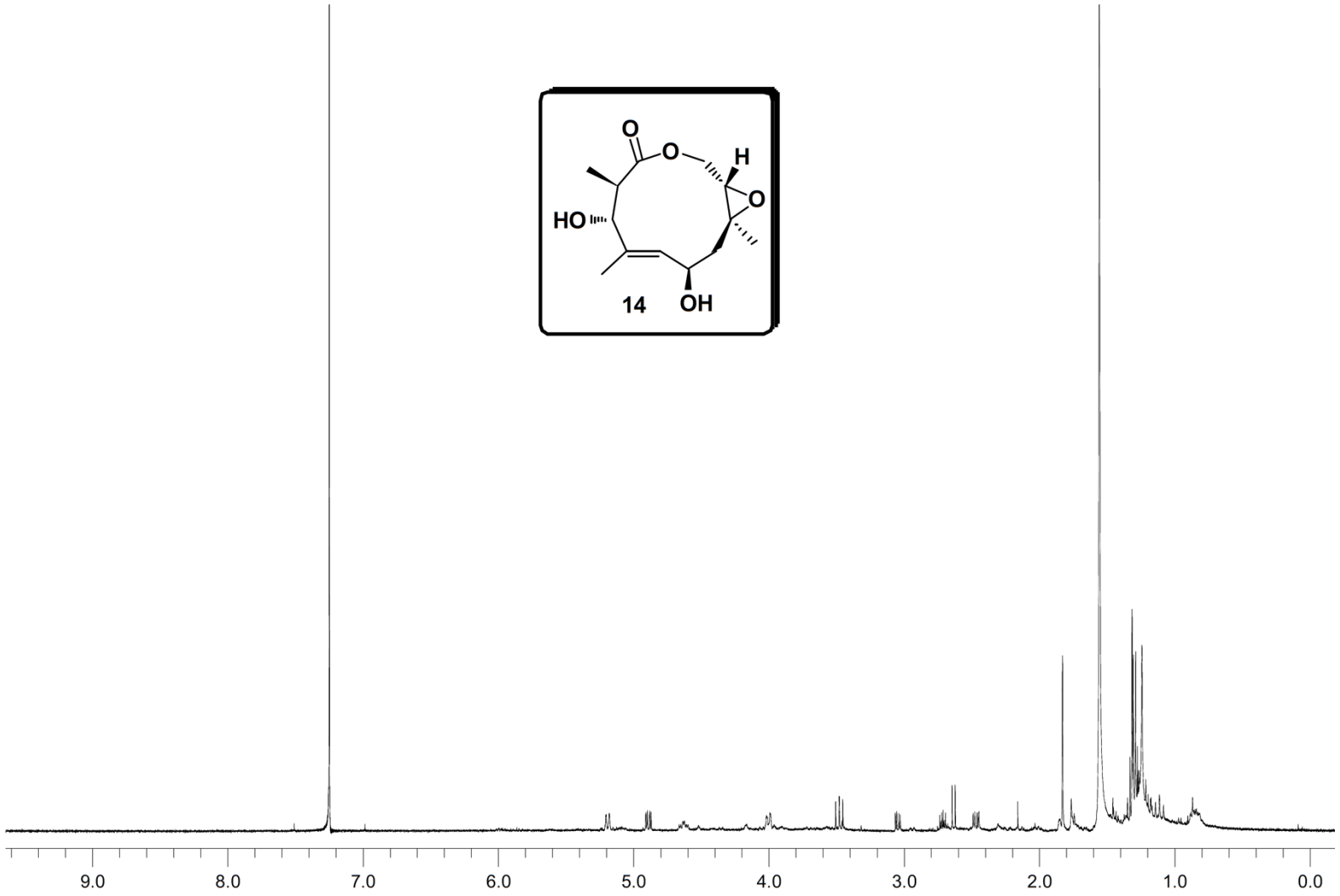

O
O
H
O
HO
OH
13
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm



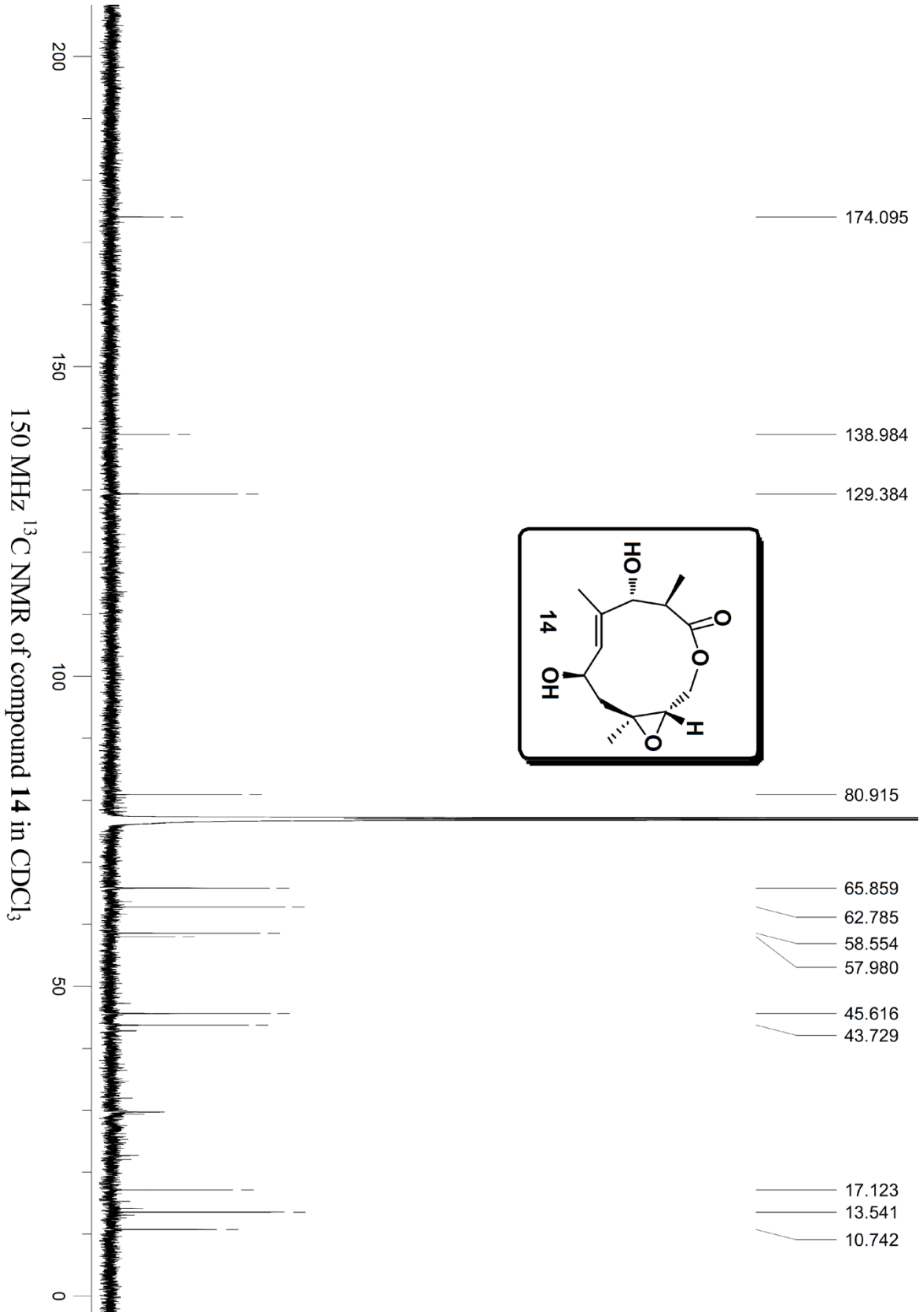
13

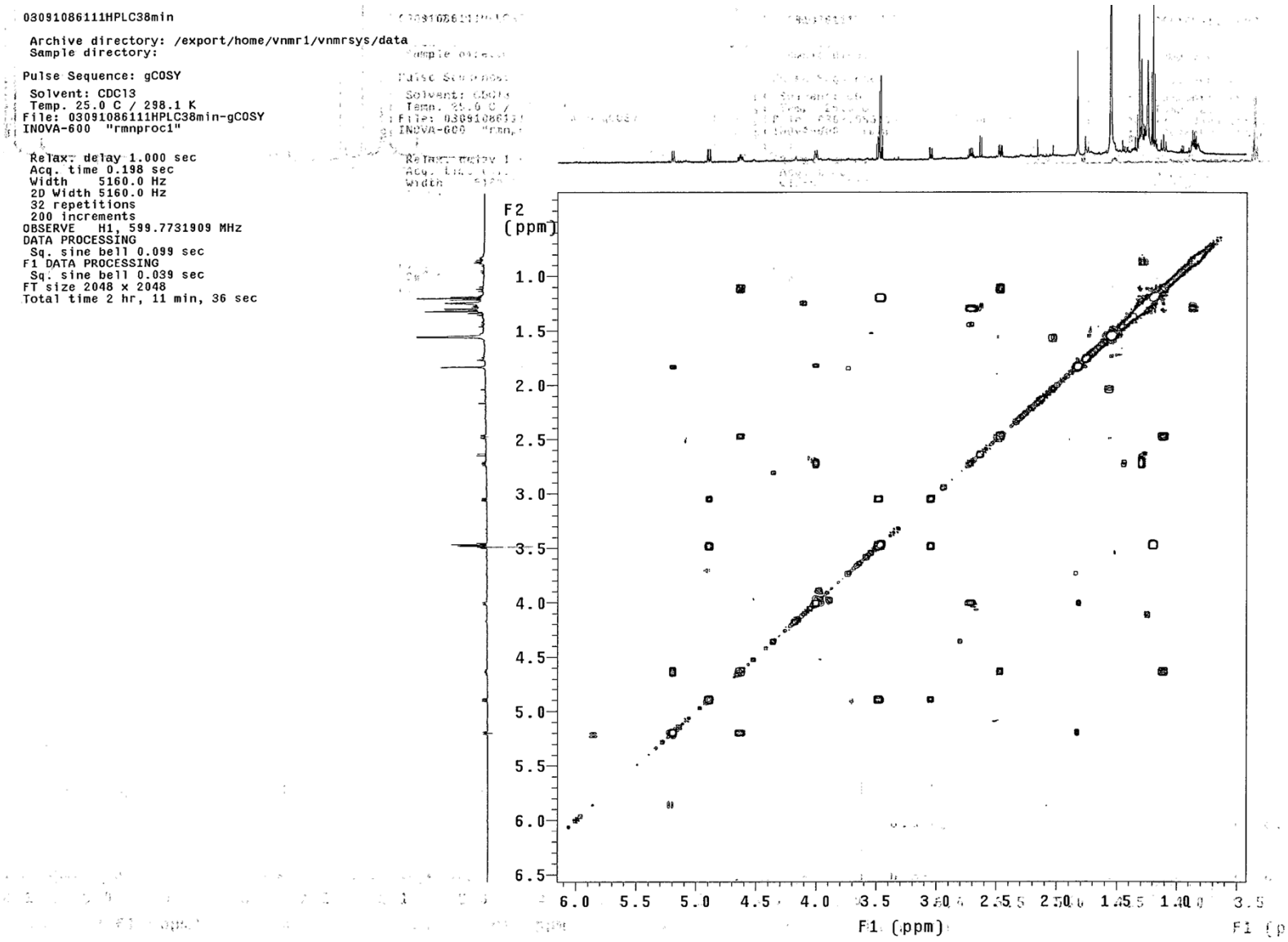

O
O
H
O
HO
OH
13
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

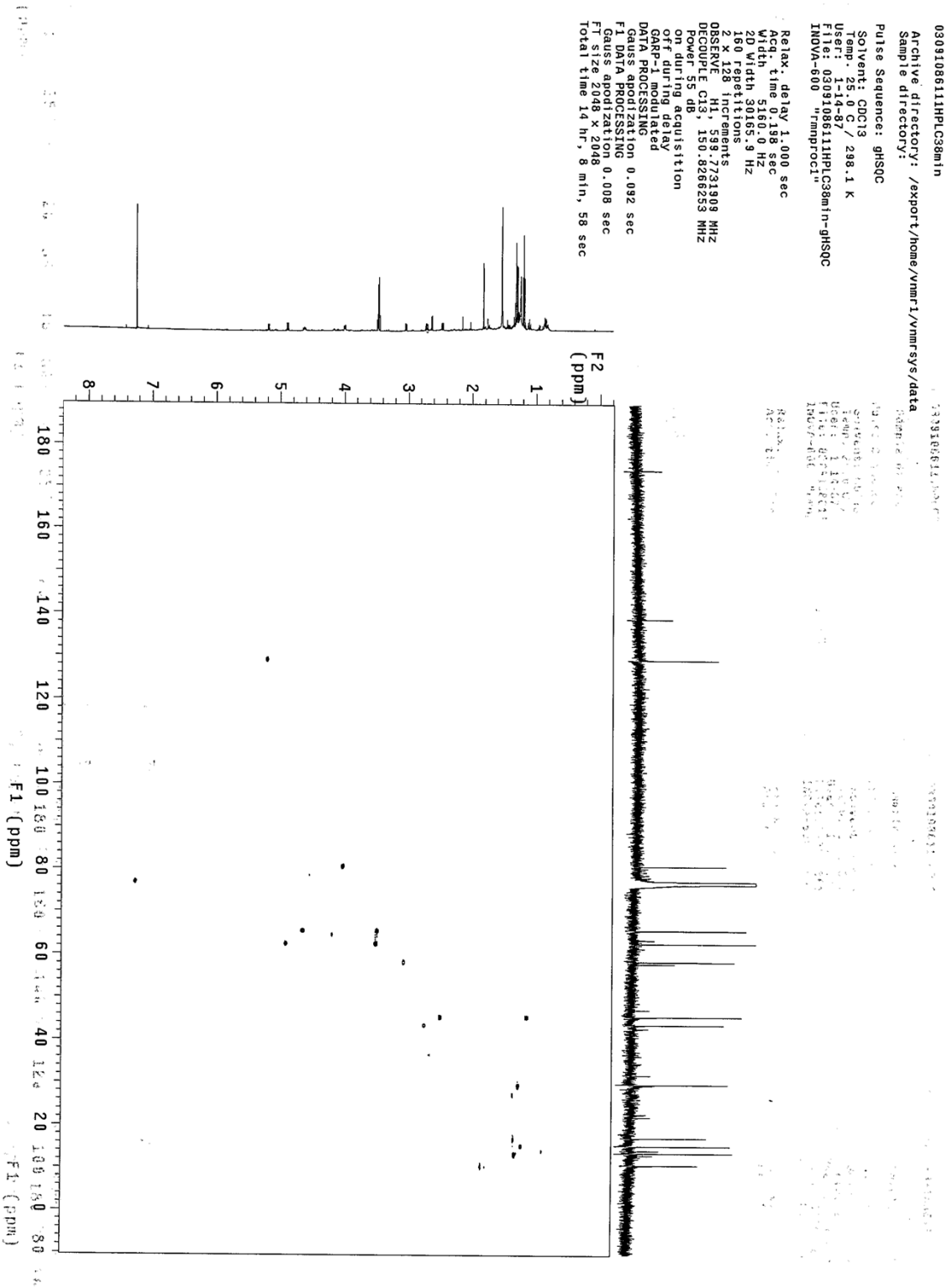

O
O
H
O
HO
OH
13
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm

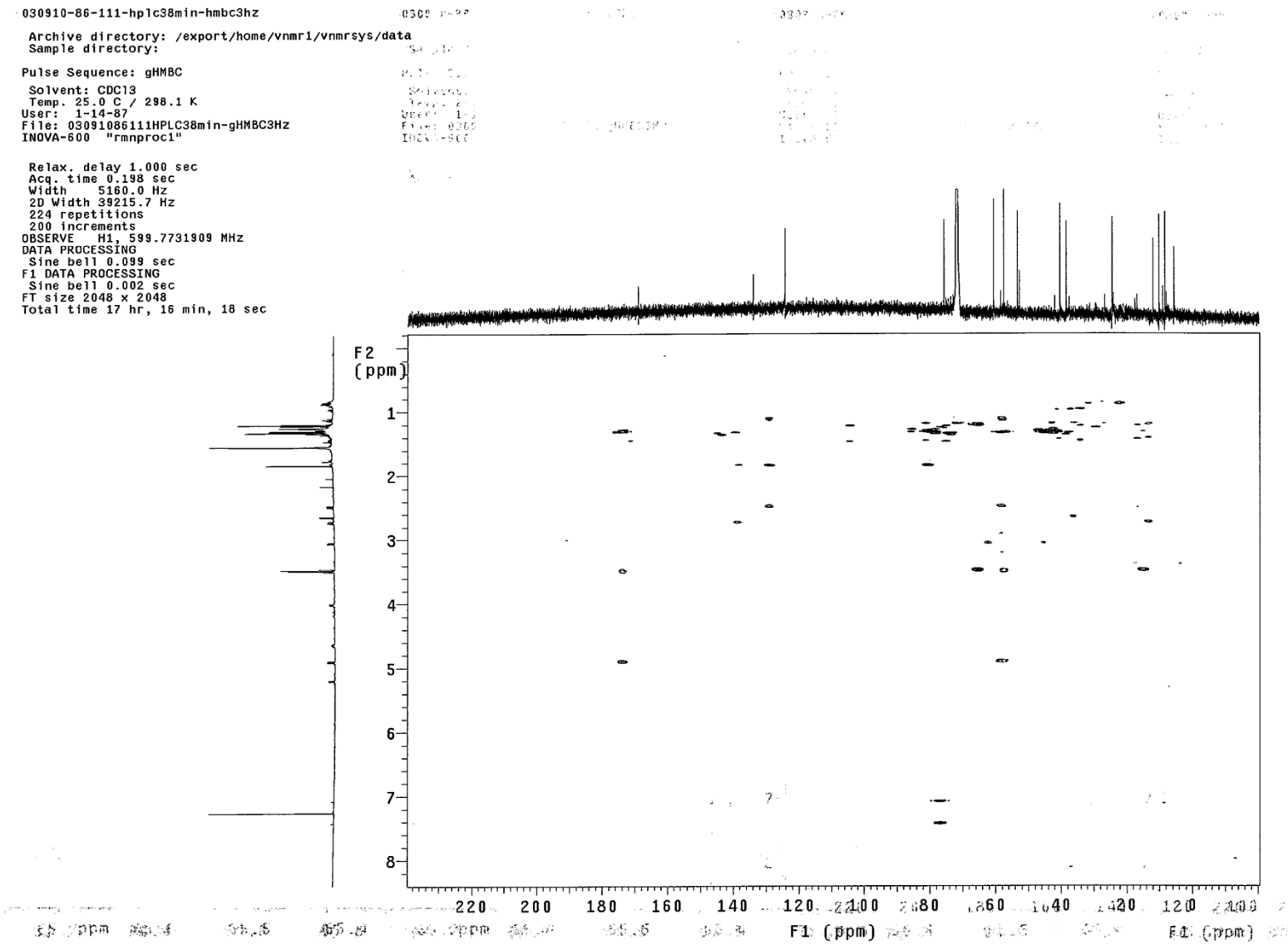


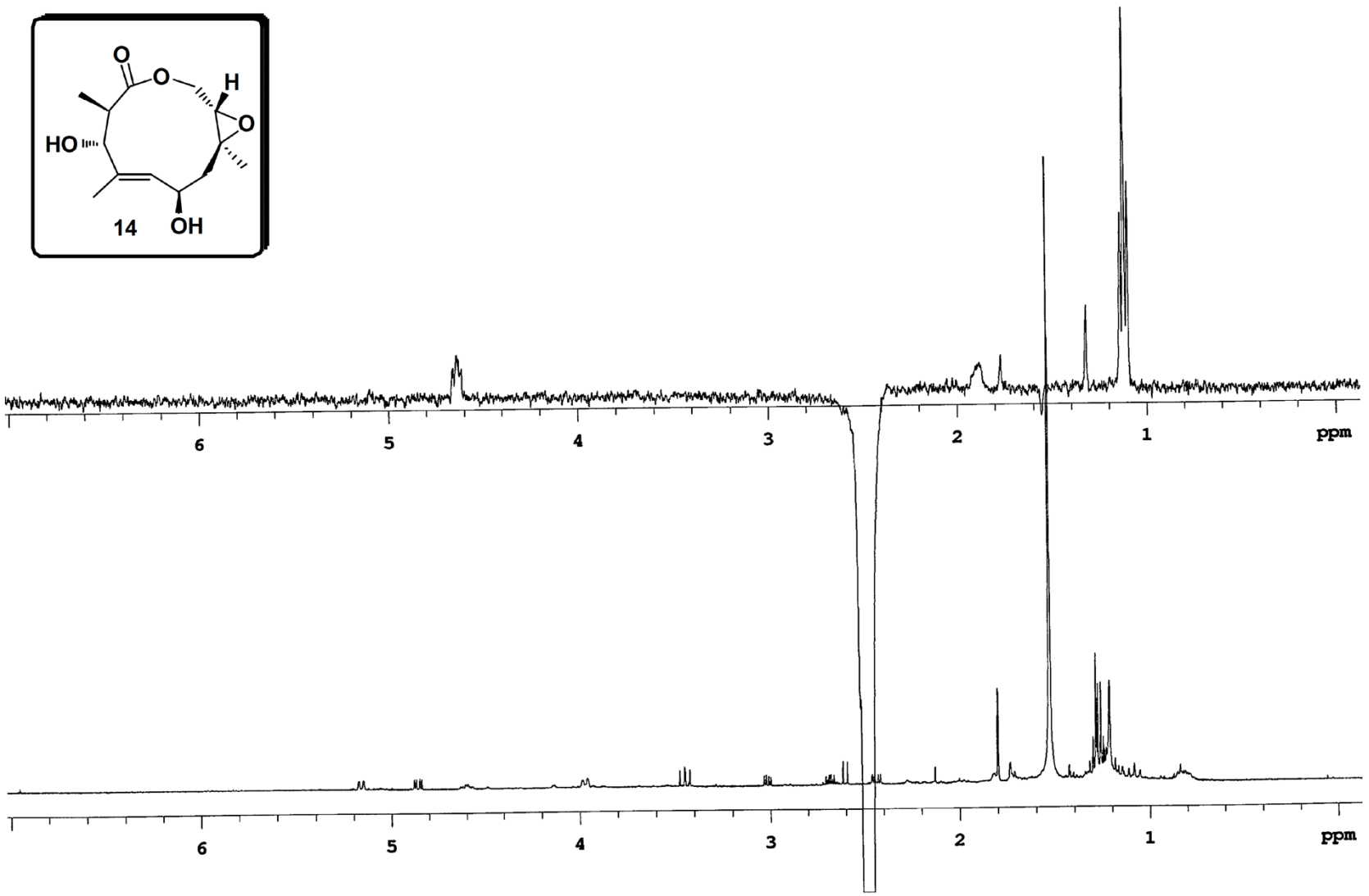
400 MHz ^{1}H NMR of compound **14** in $CDCl_3$

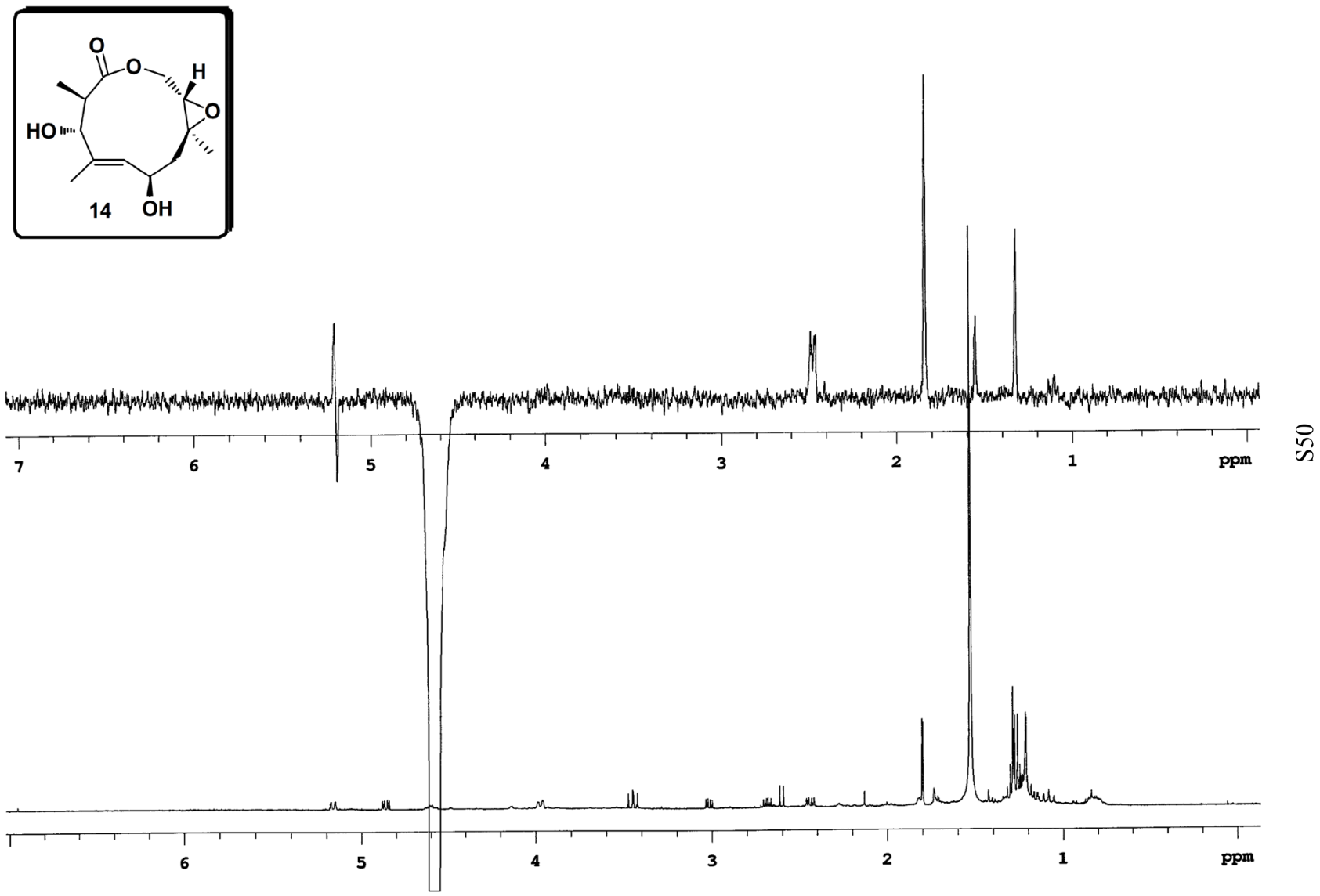

150 MHz ^{13}C NMR of compound **14** in $CDCl_3$
200
150
100
50
0
174.095
138.984
129.384
80.915
65.859
62.785
58.554
57.980
45.616
43.729
17.123
13.541
10.742
HO
14
OH
O
O
H
O

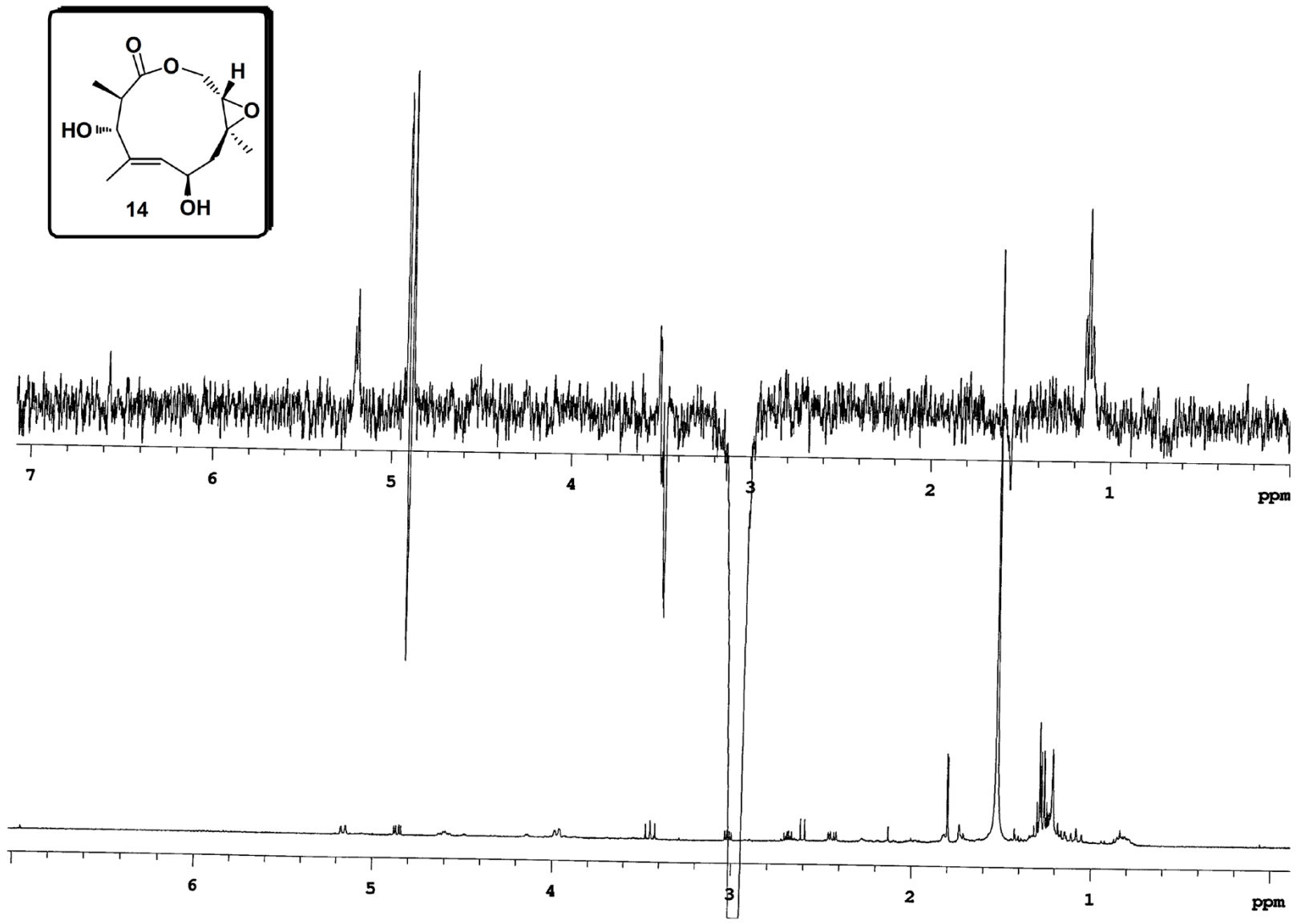

030910861111HPLC38min
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: gCOSY
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 030910861111HPLC38min-gCOSY
INOVA-600 "rmnproc1"
Relax. delay 1.000 sec
Acq. time 0.198 sec
Width 5160.0 Hz
2D Width 5160.0 Hz
32 repetitions
200 increments
OBSERVE H1, 599.7731909 MHz
DATA PROCESSING
Sq. sine bell 0.099 sec
F1 DATA PROCESSING
Sq. sine bell 0.039 sec
FT size 2048 x 2048
Total time 2 hr, 11 min, 36 sec
F2 (ppm)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
F1 (ppm)


0309108611HPLC38min
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: gHSQC
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: 0309108611HPLC38min-gHSQC
INOVA-600 "rmnproc1"
Relax. delay 1.000 sec
Acq. time 0.198 sec
Width 5160.0 Hz
2D Width 30165.9 Hz
160 repetitions
2 x 128 increments
OBSERVE H1, 599.7731909 MHz
DECOUPLE C13, 150.8266253 MHz
Power 55 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Gauss apodization 0.092 sec
F1 DATA PROCESSING
Gauss apodization 0.008 sec
FT size 2048 x 2048
Total time 14 hr, 8 min, 58 sec
F2 (ppm)
F1 (ppm)


030910-86-111-hplc38min-hmbc3hz
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
Pulse Sequence: gHMBC
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: 03091086111HPLC38min-gHMBC3Hz
INOVA-600 "rmnproc1"
Relax. delay 1.000 sec
Acq. time 0.198 sec
Width 5160.0 Hz
2D Width 39215.7 Hz
224 repetitions
200 increments
OBSERVE H1, 599.7731909 MHz
DATA PROCESSING
Sine bell 0.099 sec
F1 DATA PROCESSING
Sine bell 0.002 sec
FT size 2048 x 2048
Total time 17 hr, 16 min, 18 sec
F2 (ppm)
1
2
3
4
5
6
7
8
220
200
180
160
140
120
100
80
60
40
20
0
F1 (ppm)


O
O
H
O
HO
14
OH
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm


O
O
H
O
HO
14
OH
7
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm


O
O
H
O
HO
14
OH
7
6
5
4
3
2
1
ppm
6
5
4
3
2
1
ppm