

## Supporting Information

### Modeling, Synthesis and Biological Evaluation of Potential Retinoid-X-Receptor (RXR) Selective Agonists: Novel Bexarotene Analogs

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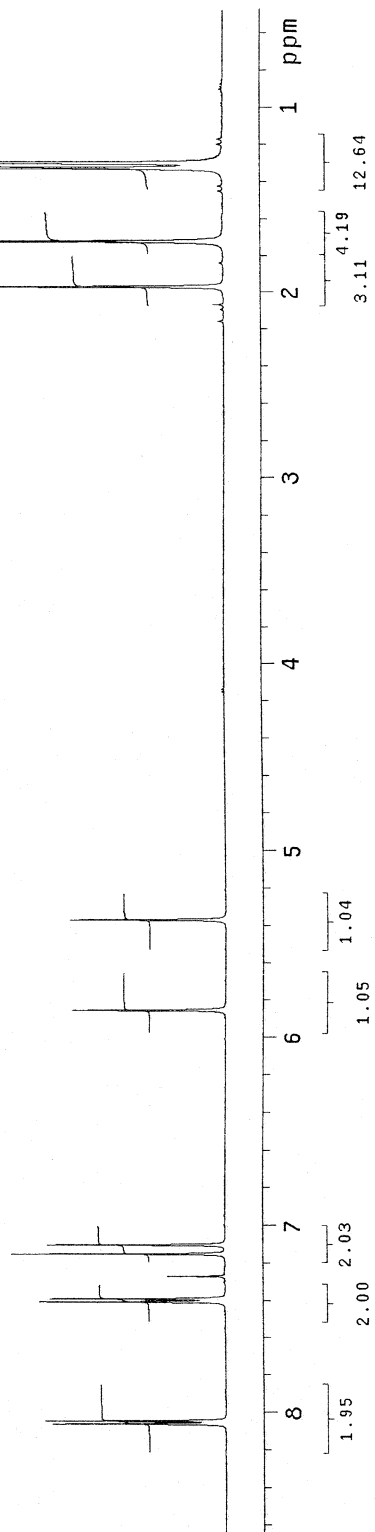
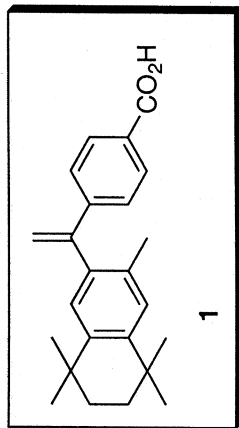
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cwI-039

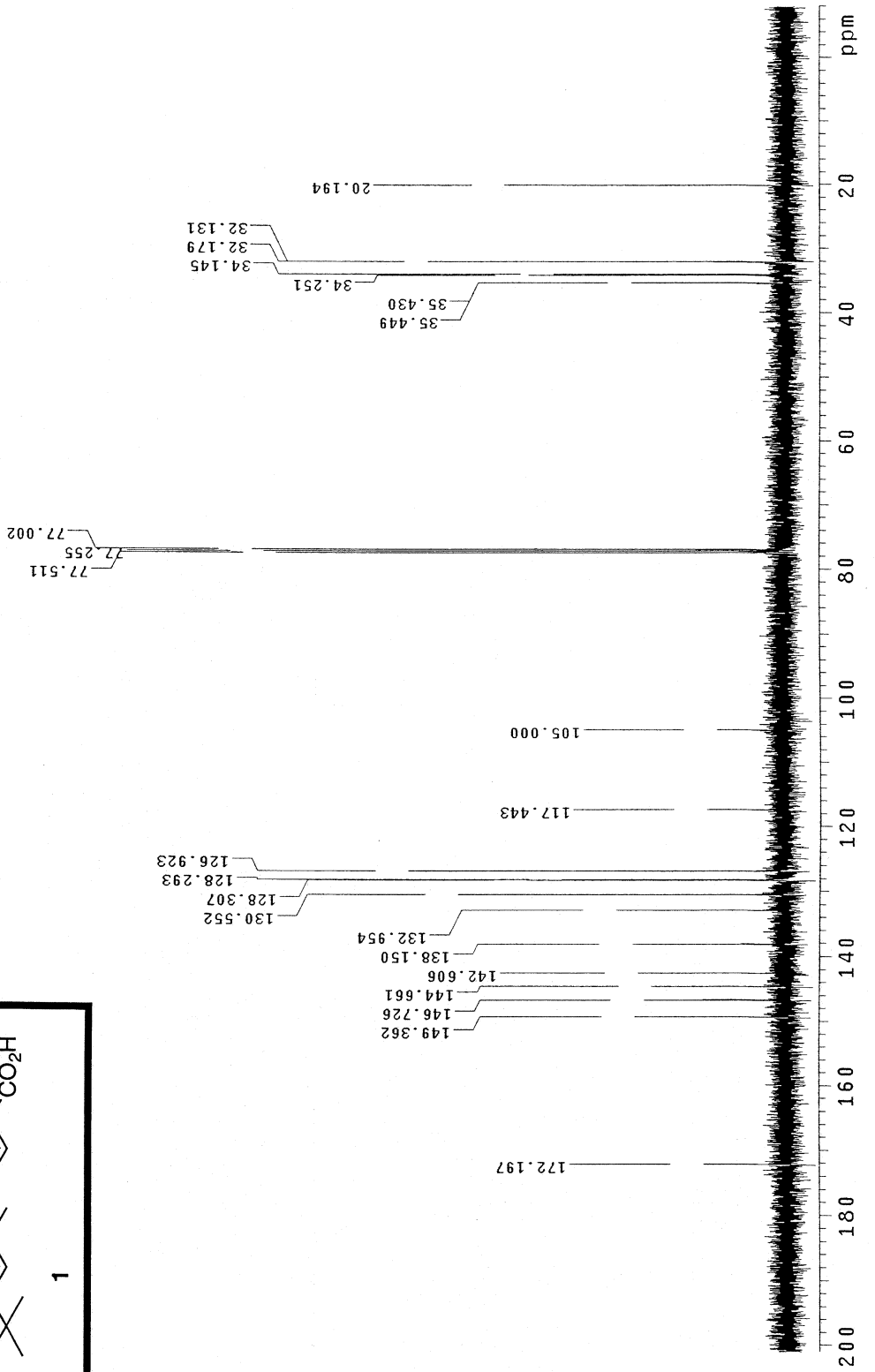
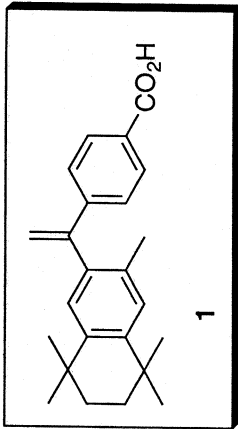
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Pulse Sequence: s2pul



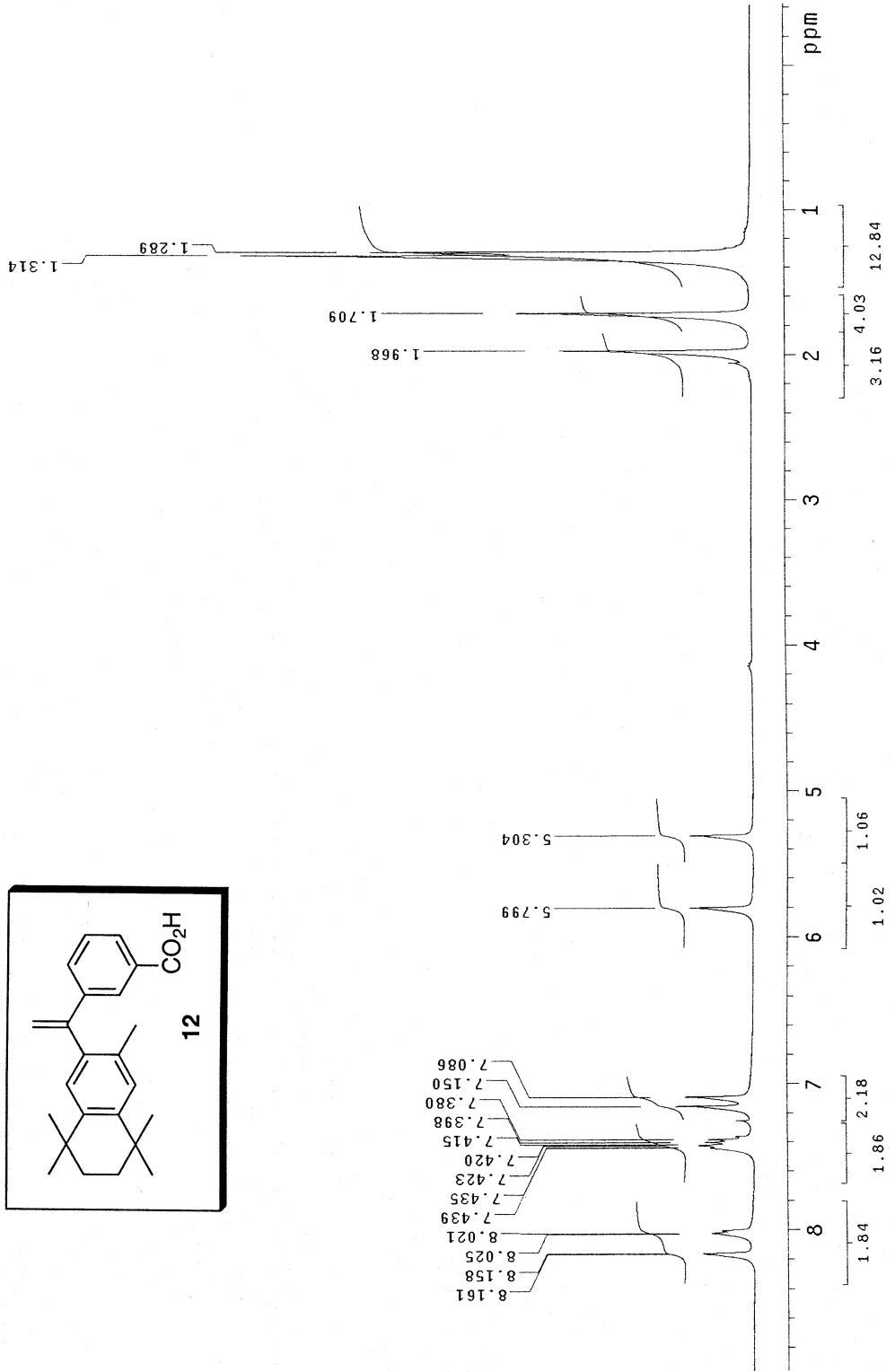
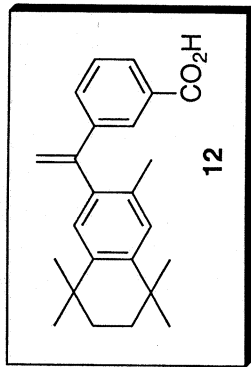
cwI-039

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cwI-131

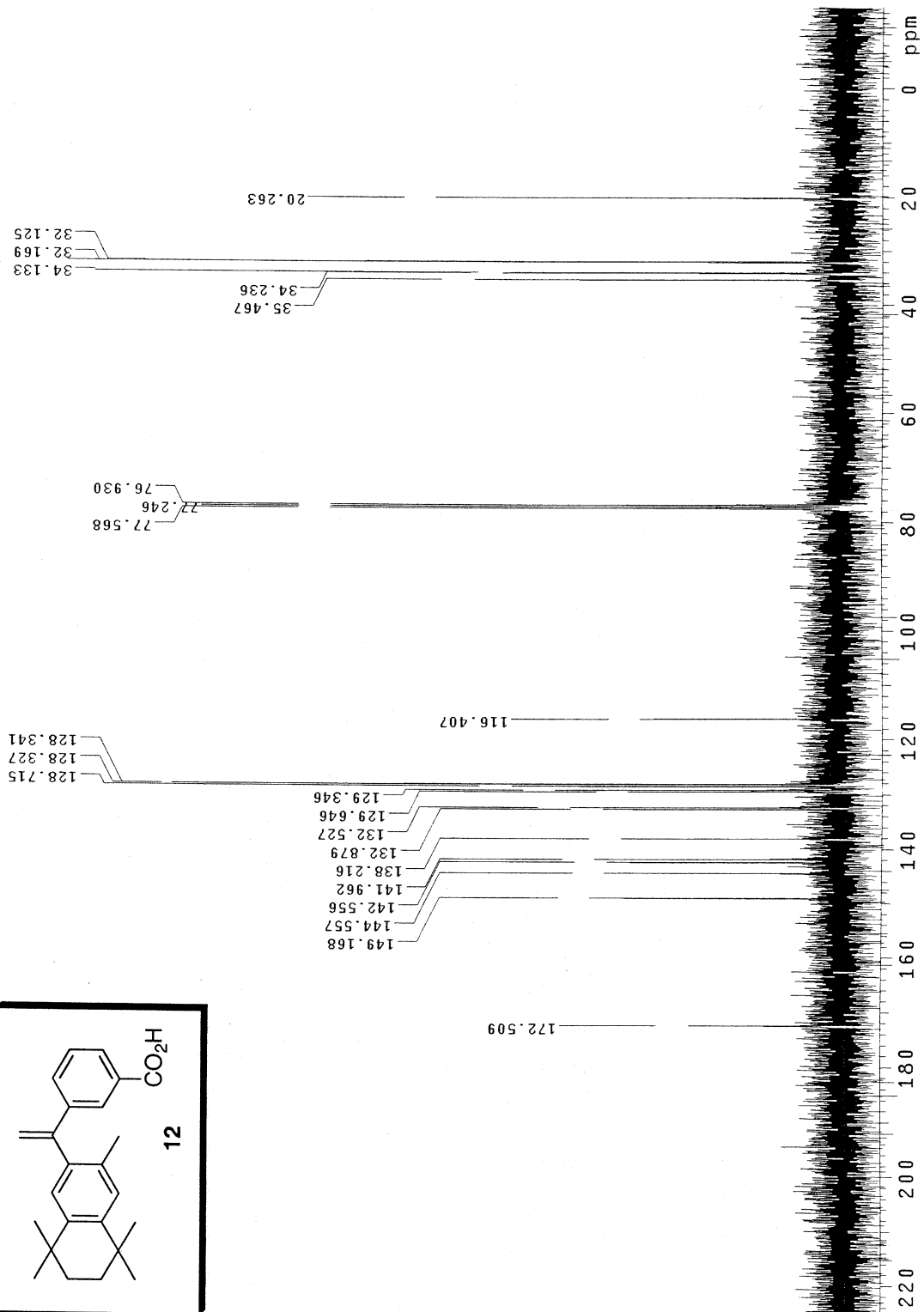
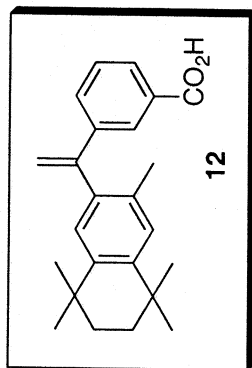
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cwi-131

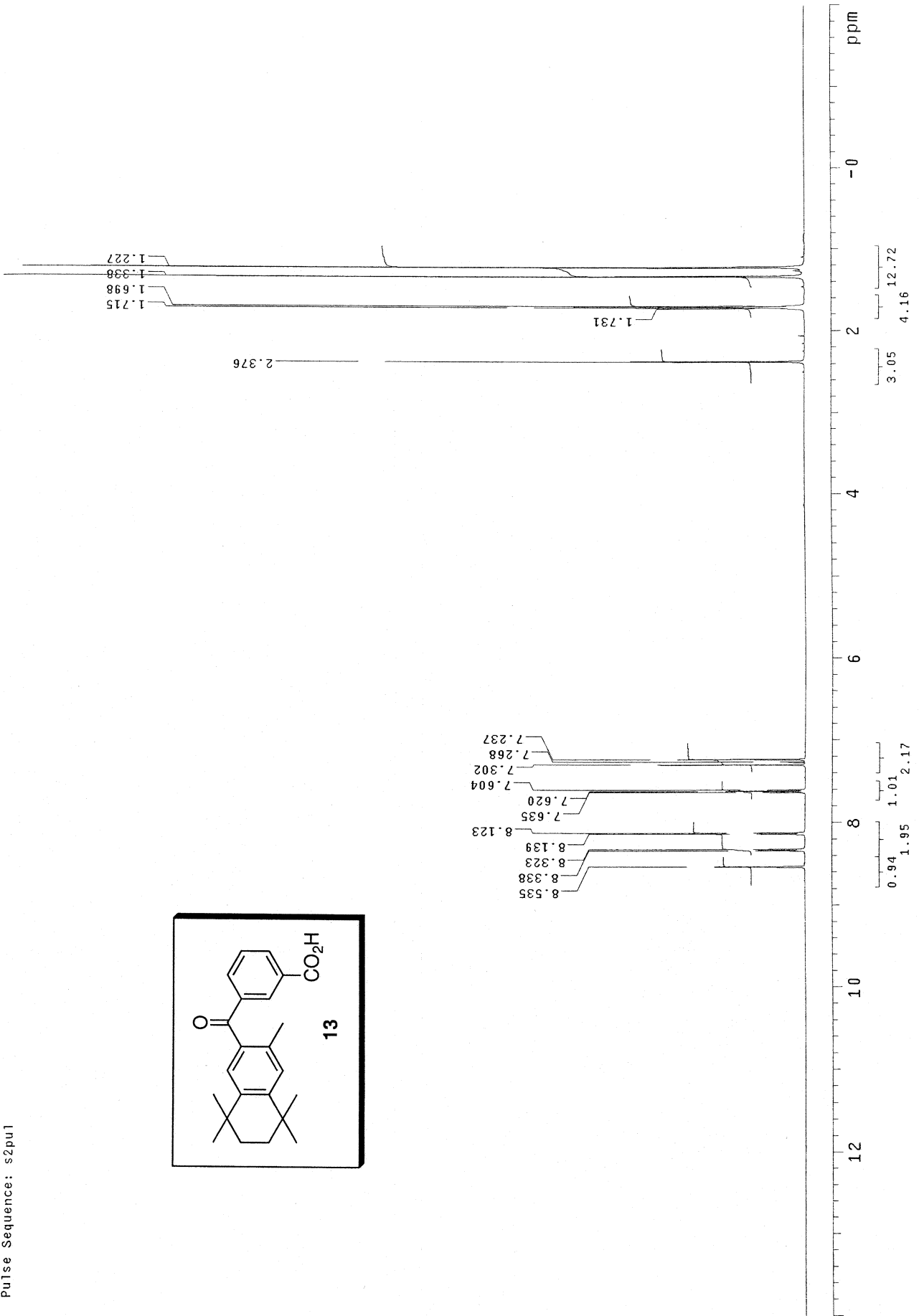
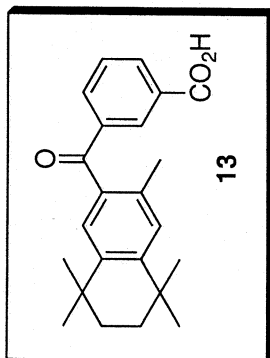
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cwi\_167

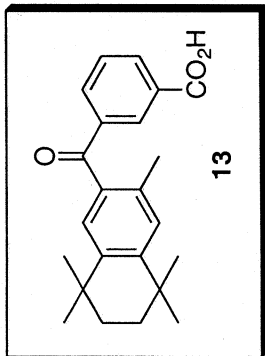
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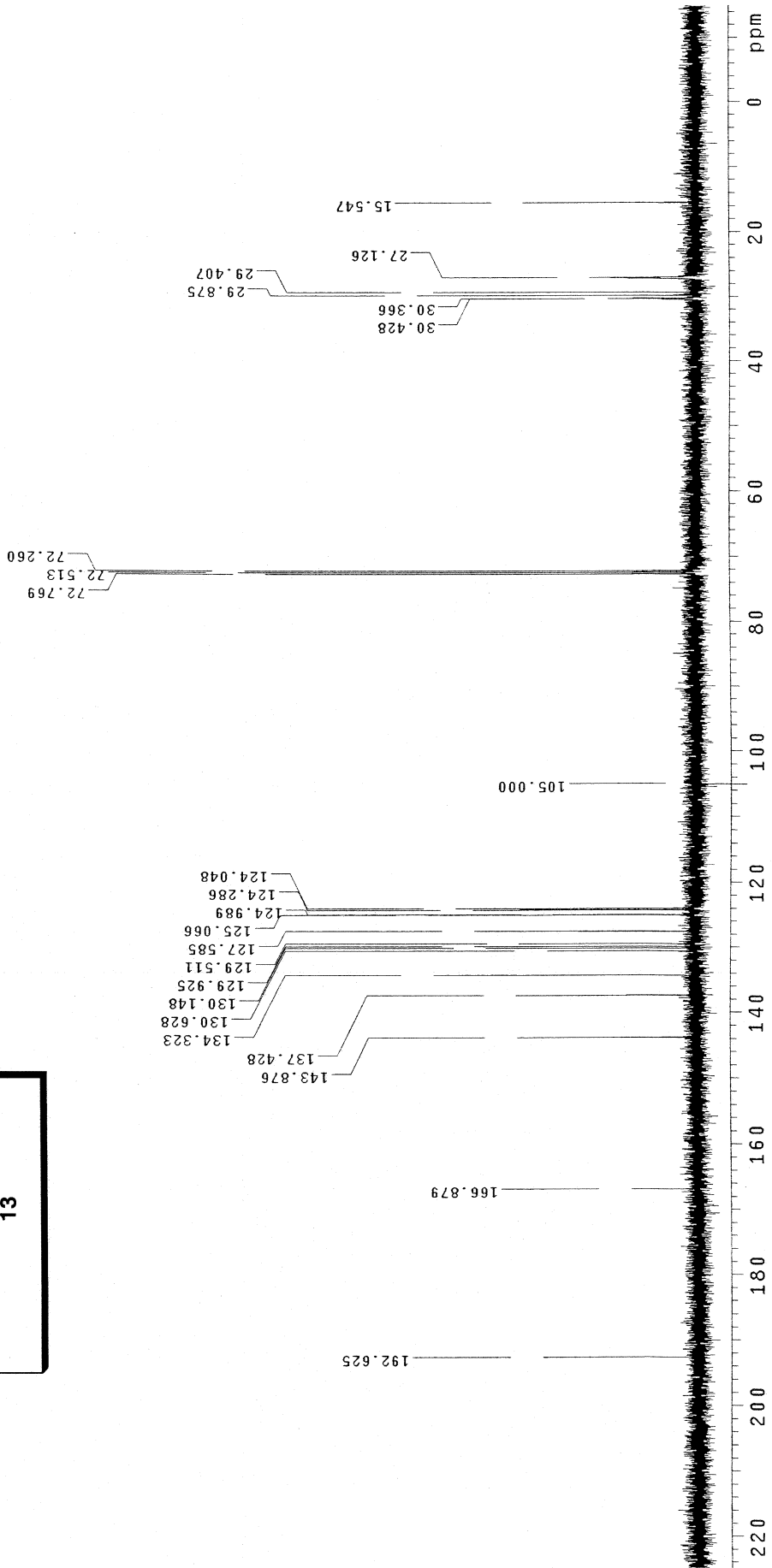
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Pulse Sequence: s2pu1

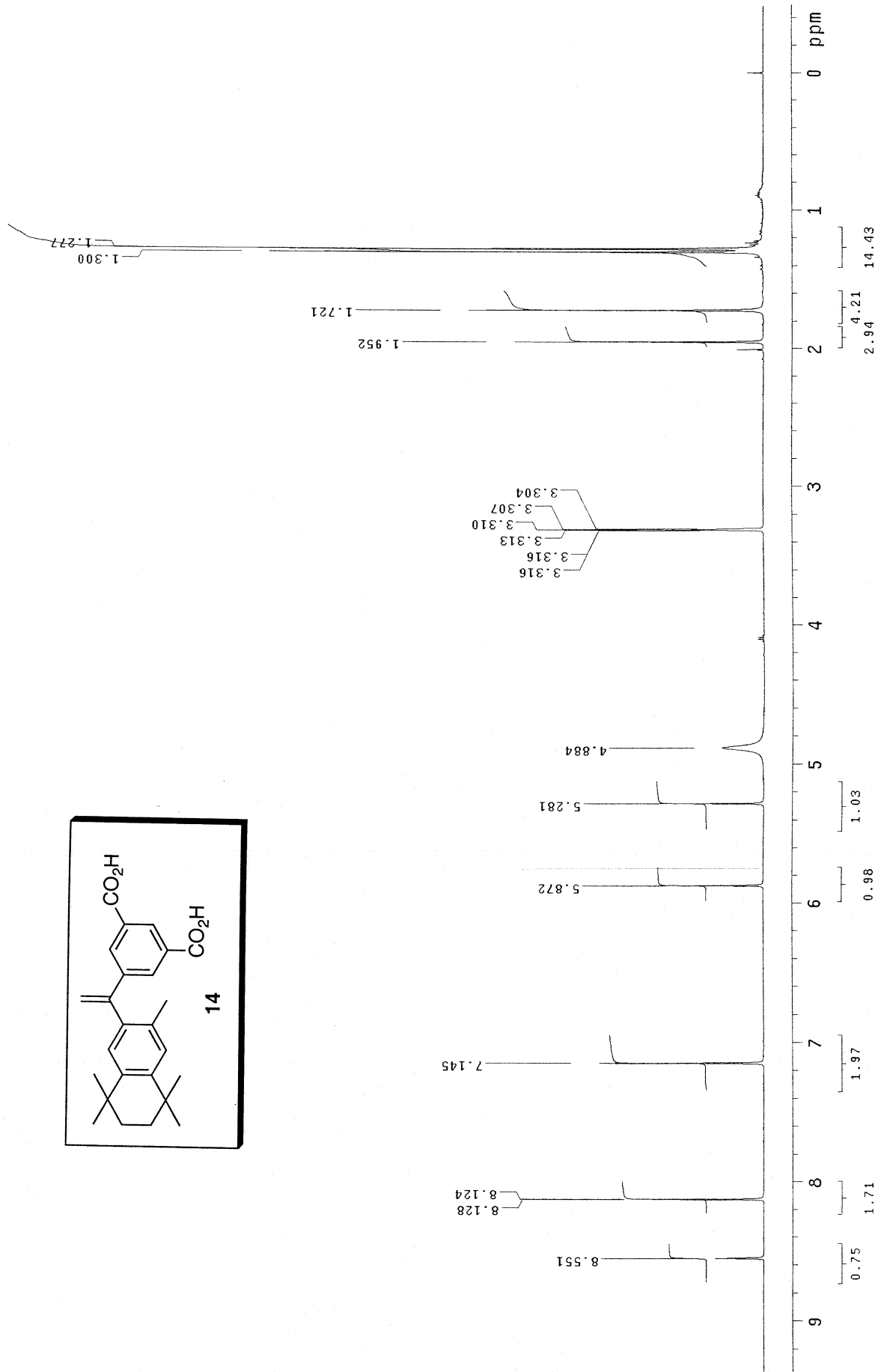
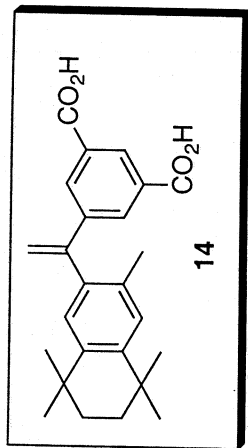


S7



CW-143

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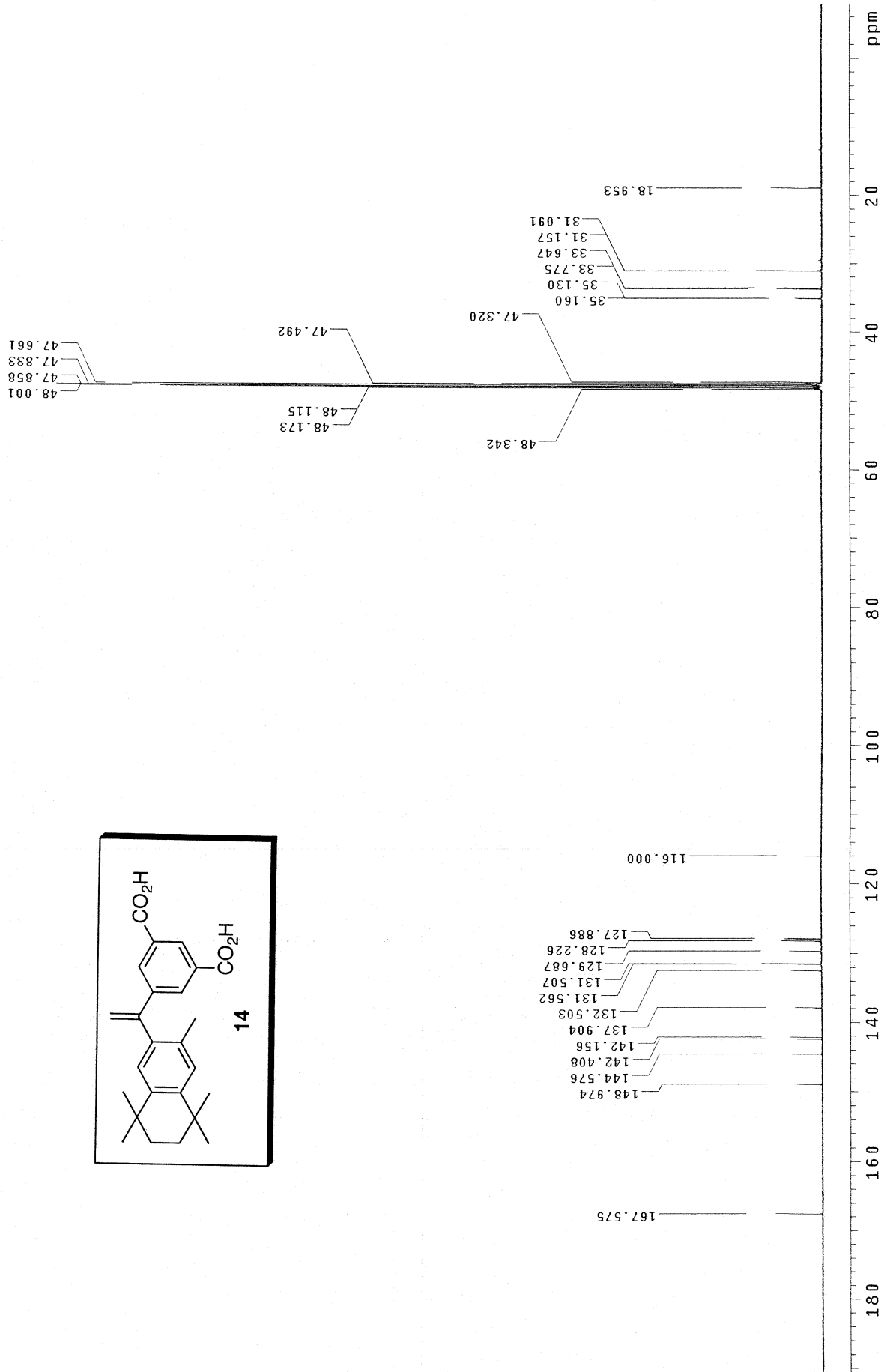
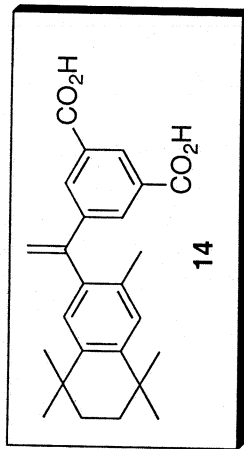




cwI-143

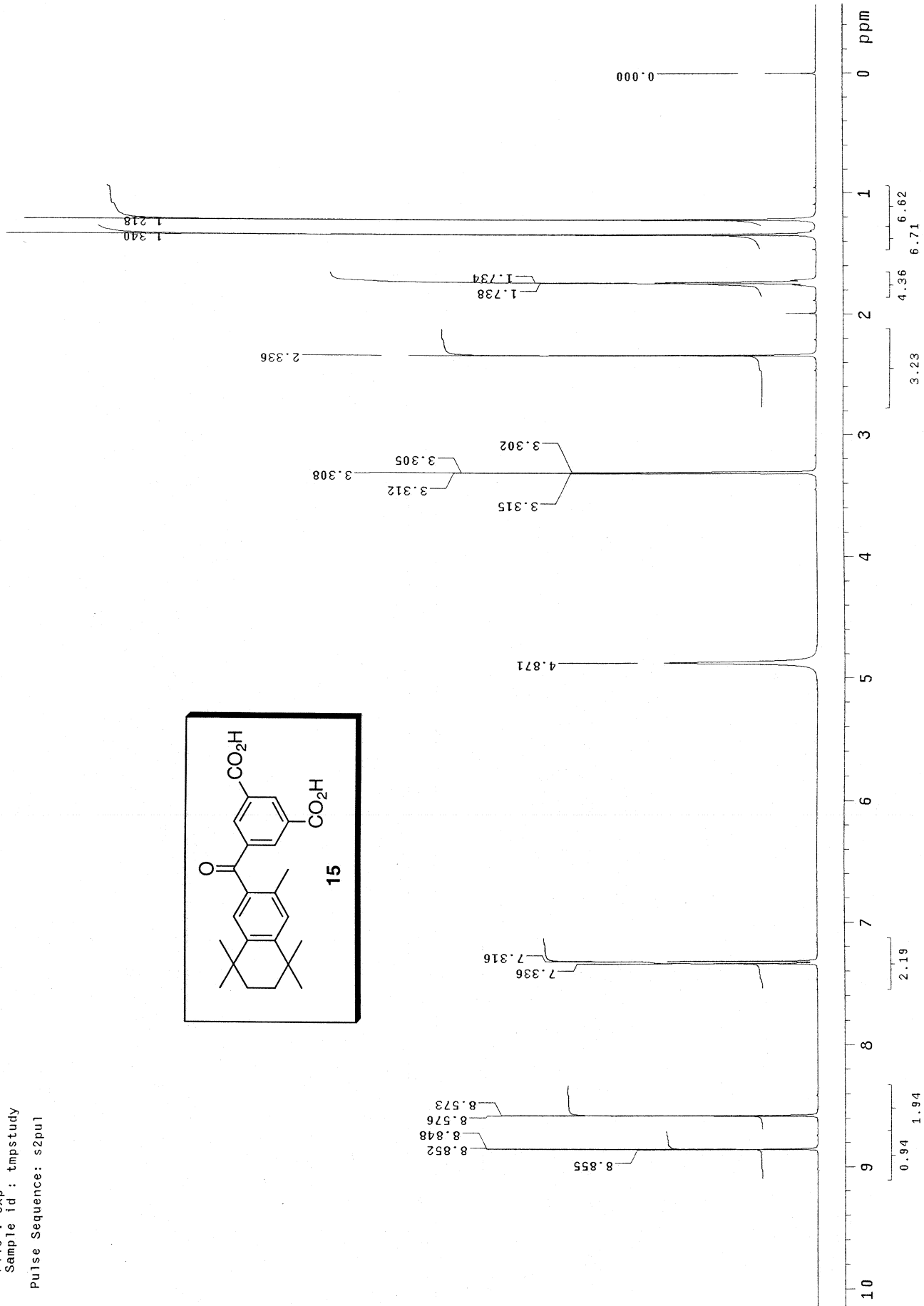
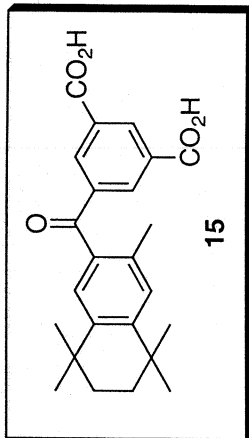
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Pulse Sequence: s2pu1



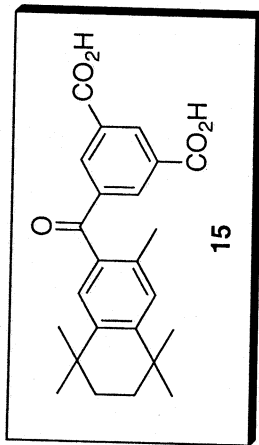
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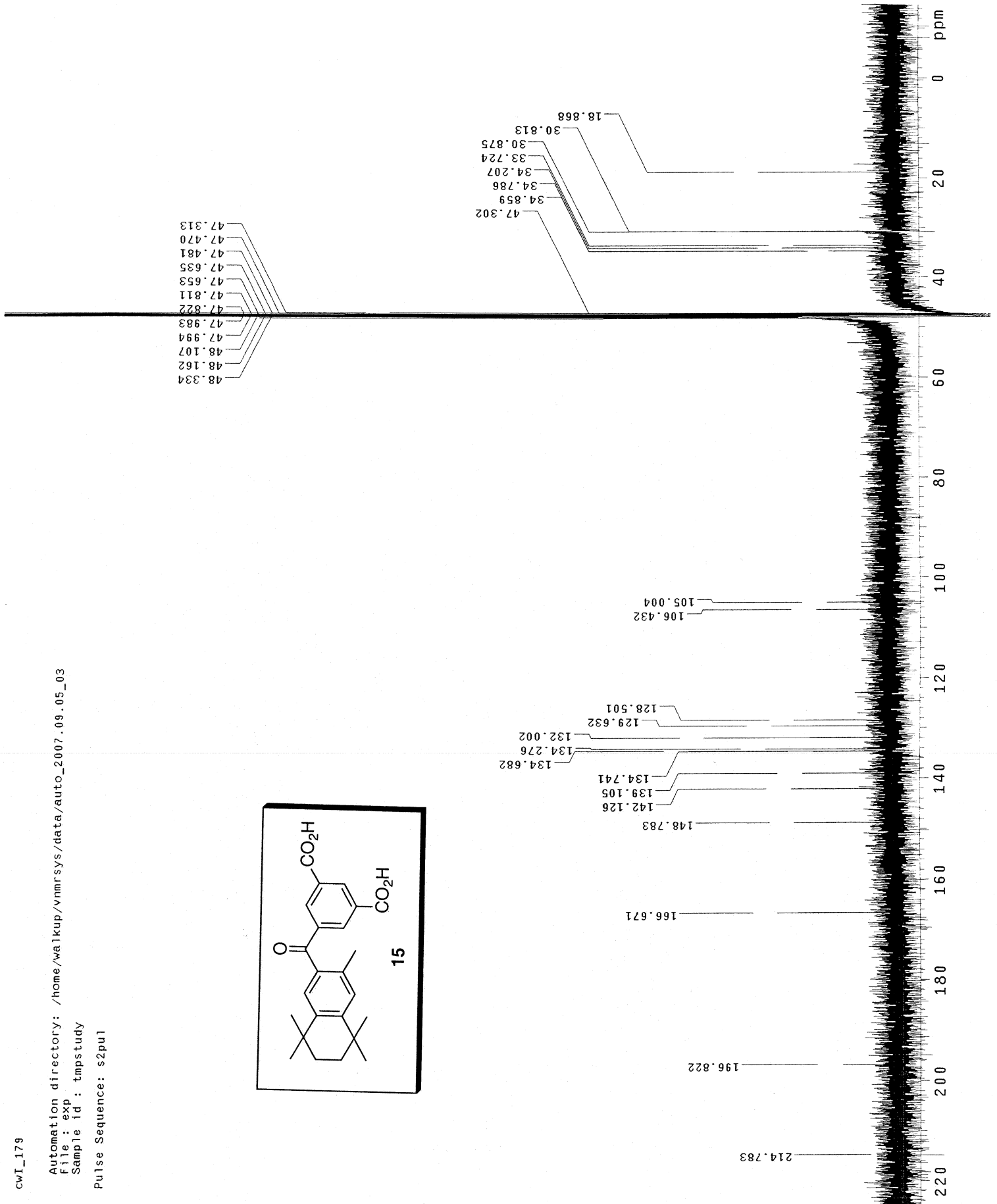


cwi\_179

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Pulse Sequence: s2pul

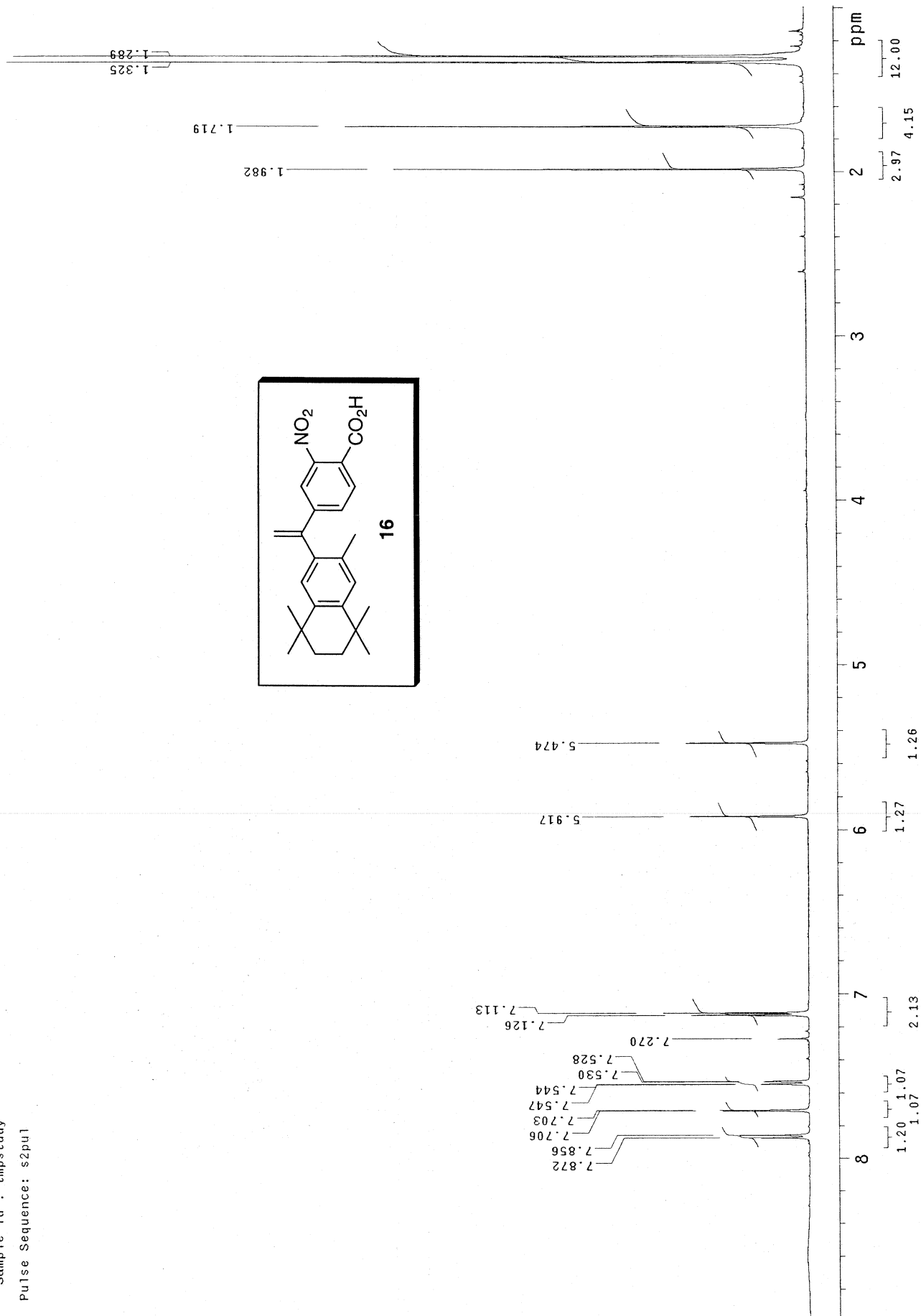
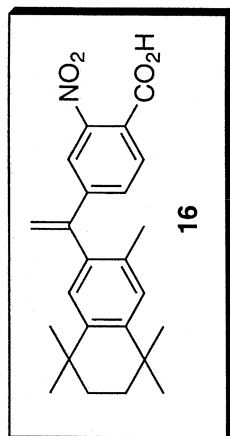


S11



CV-151

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Pulse Sequence: s2pu1



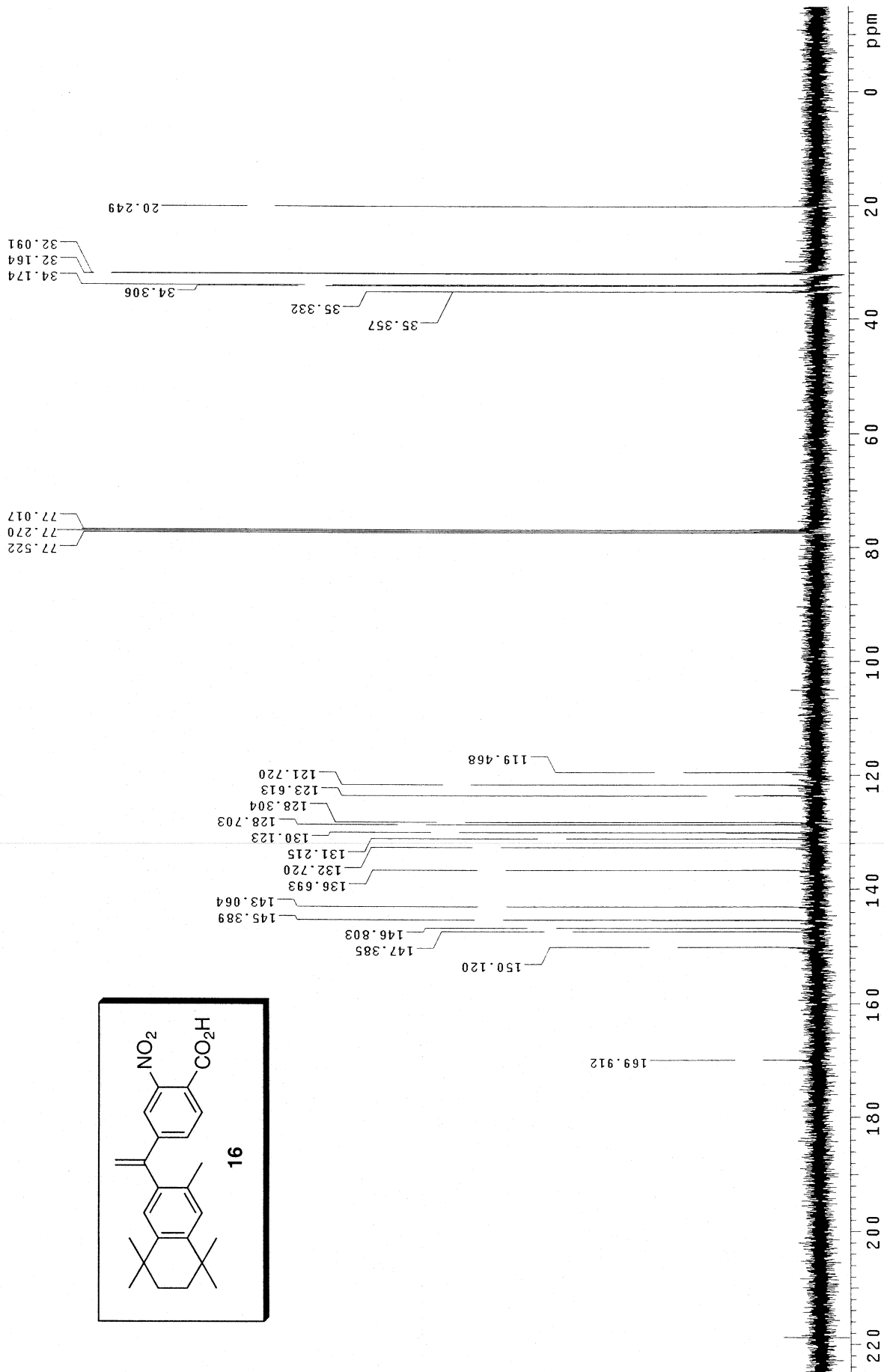
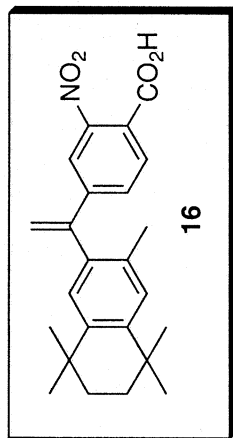
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File: exp

Sample id: tmpstudy

Pulse Sequence: s2pul



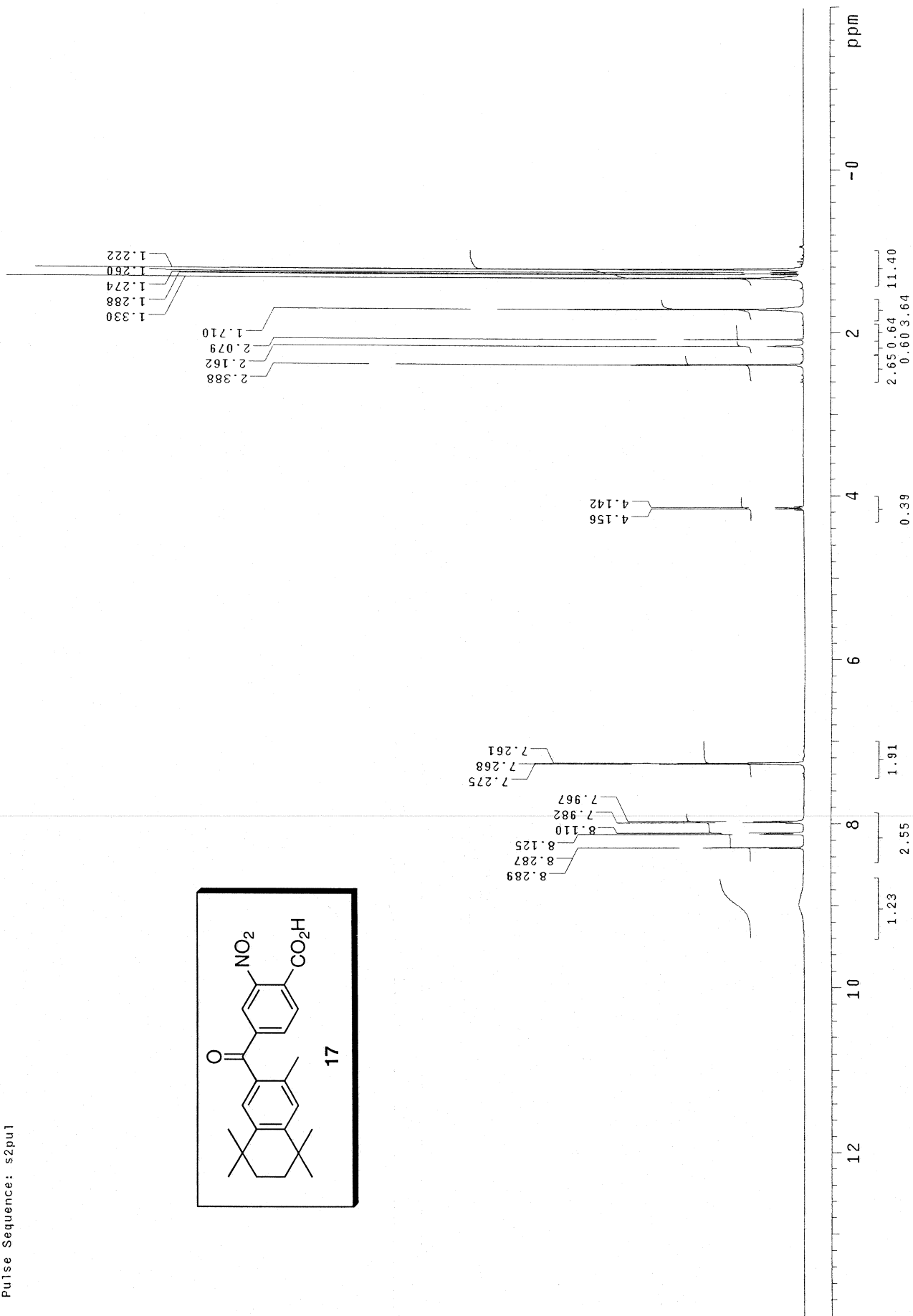
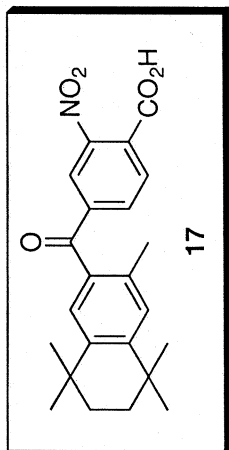
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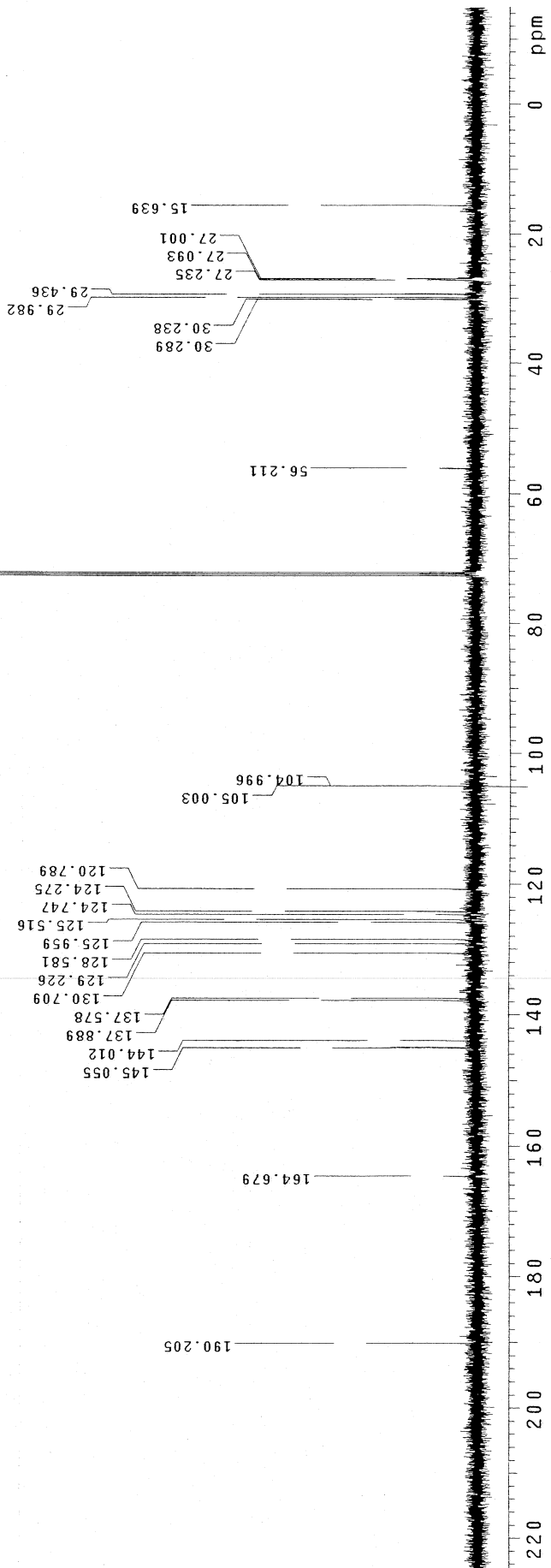
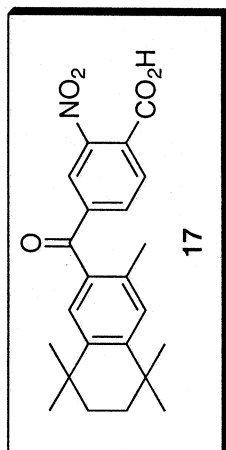
File: exp

Sample id: tmpstudy

Pulse Sequence: s2pul1



CWT-169  
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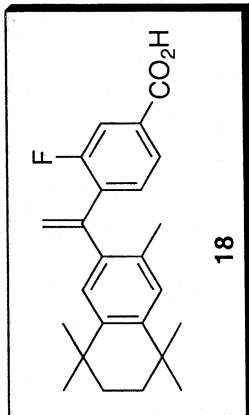


CWII-061 1 1 C:\Bruker\TOPSPIN wagner

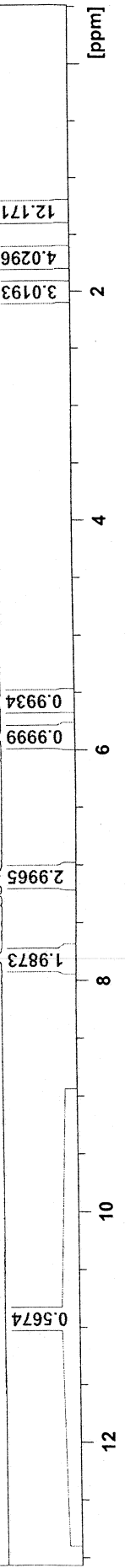
CWII-061

1H

7.8203  
7.7955  
7.7781  
7.2600  
7.1595  
7.1347  
7.1144  
7.0677  
5.8908  
5.5911  
3.0193  
4.0296  
12.1715  
1.9928  
1.7030  
1.3025  
1.2869



18





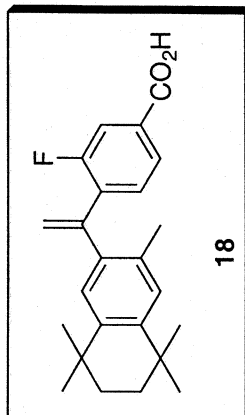
CWII-061 5 2 C:\Bruker\TOPSPIN wagner

CWII-061  
C13

171.0189  
170.9969  
161.0735  
158.5740  
144.4640  
143.4293  
142.4046  
138.2223  
134.8364  
134.7144  
132.3401  
130.7823  
130.7521  
129.5612  
129.4812  
128.1034  
127.8330  
125.6627  
125.6293  
121.7348  
121.6616  
117.8647  
117.6128

77.3204  
77.0023  
76.8851

35.1625  
33.9802  
33.8880  
31.9097  
31.8492  
19.7792



CW11-065 1 1 C:\Bruker\TOPSPIN wagner

CW11-065

<sup>1</sup>H

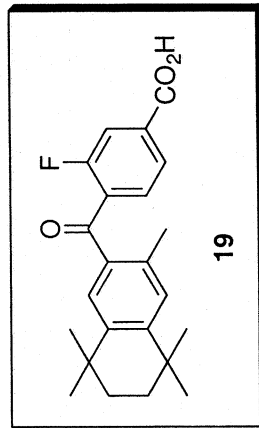
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7.8957  
7.8758  
7.7835  
7.7574  
7.6626  
7.6440  
7.6253  
7.3273  
7.2861

2.4998  
2.4014

1.6177

1.2624  
1.0918



818

0.9389

1.0000

0.9914

1.0524

2.0618

3.0764

4.1125

12.7242

[ppm]

0

2

4

6

8

10

12

CWII-065 2 1 C:\Bruker\TOPSPIN wagner

CWII-065

CT3

193.5564

165.6647

160.4420

157.9412

149.4128

141.9191

135.6482

135.5731

135.1088

133.9672

131.4939

131.3512

131.0163

129.7863

129.5833

125.3805

116.9217

116.6882

40.1343

39.9255

39.7166

39.5080

39.2991

39.0902

38.8820

34.2547

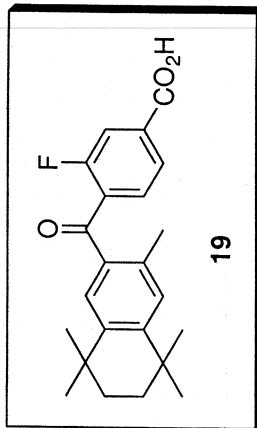
34.1418

33.4552

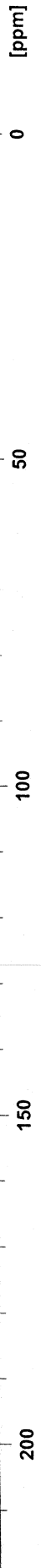
31.2729

31.1585

20.3164



S19

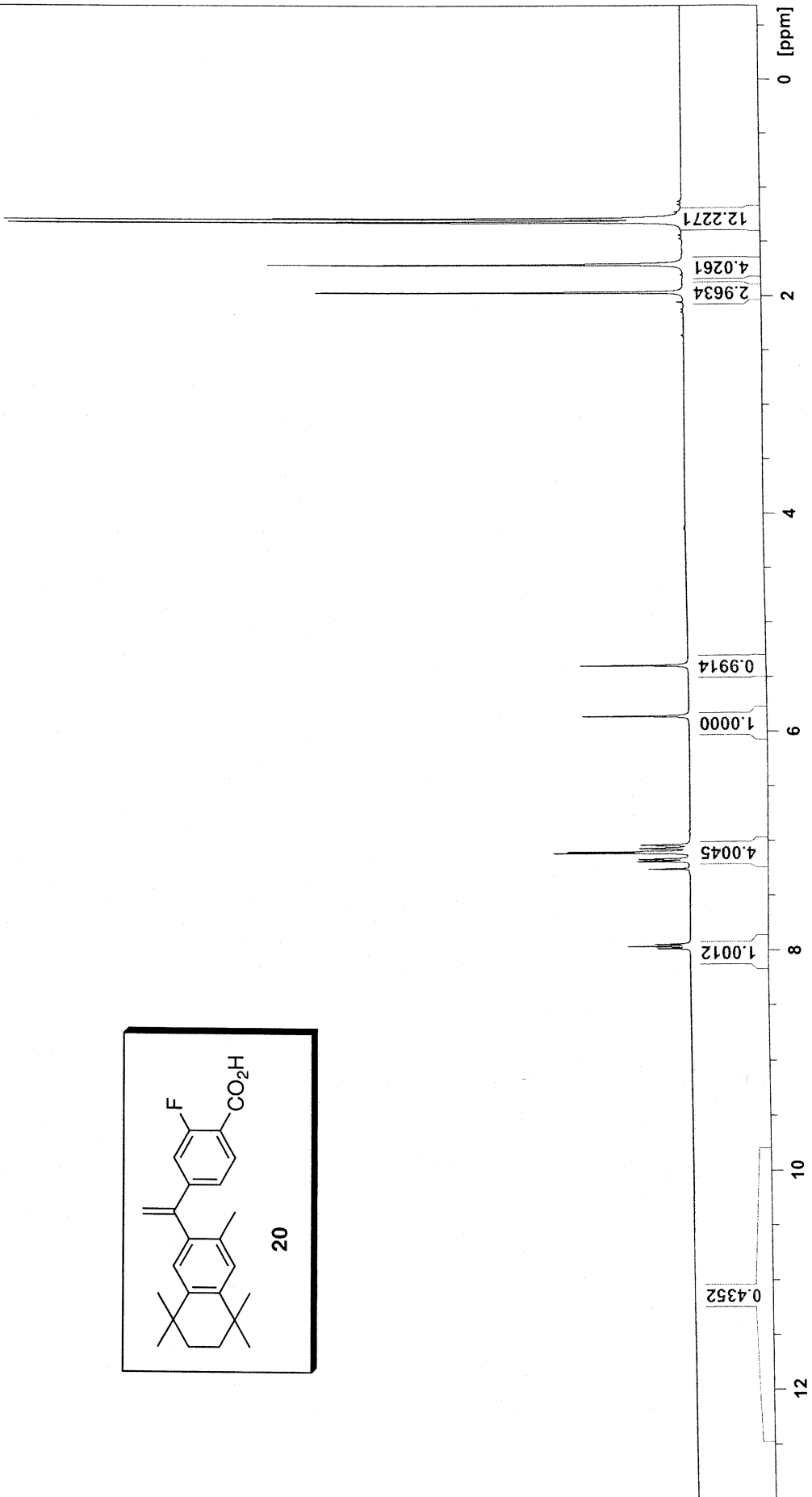
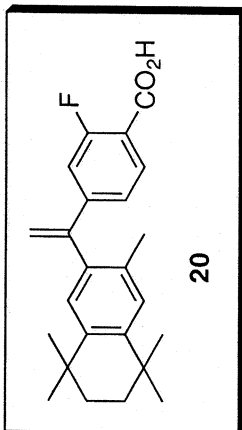


CWII-063 1 1 C:\Bruker\TOPSPIN wagner

CWII-063

<sup>1</sup>H

7.9863  
7.9665  
7.9467  
7.2600  
7.1905  
7.1697  
7.1139  
7.1019  
7.0721  
7.0412  
- 5.8624  
- 5.3977  
- 1.9692  
- 1.7106  
- 1.3166  
- 1.2856

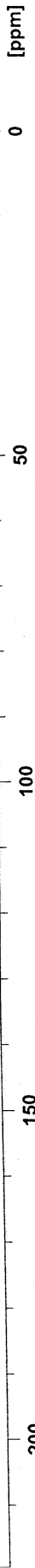
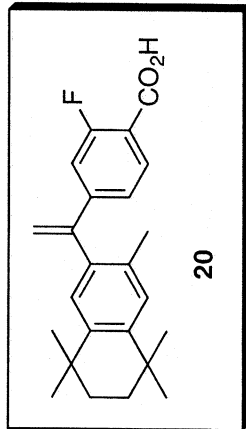


CWII-063 2 1 C:\Bruker\TOPSPIN wagner

CWII-063

C13

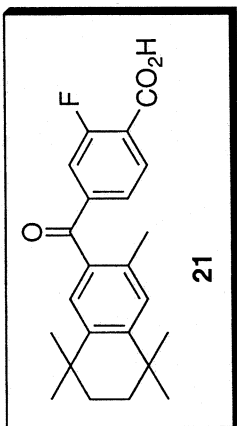
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169.4012  
164.0461  
161.4486  
149.0012  
148.9154  
148.0307  
144.7246  
142.5196  
137.1591  
132.6900  
132.6042  
128.1828  
128.0156  
122.1773  
122.1445  
118.1866  
115.9926  
115.8987  
115.1365  
114.9057  
77.3146  
76.9973  
76.6793  
35.1412  
35.1215  
34.0105  
33.8878  
31.9108  
31.8526  
19.8696



CWII-067 1 1 C:\Bruker\TOPSPIN wagner

CWII-067

<sup>1</sup>H



8.1454  
8.1267  
8.1081  
7.6491  
7.6262  
7.5955  
7.2736  
7.2602  
7.2286

2.3636

1.7022

1.3203  
1.2187

0.7171

0.9810

1.9680

2.2000

3.0000

4.1551

12.4282

[ppm]

0

2

4

6

8

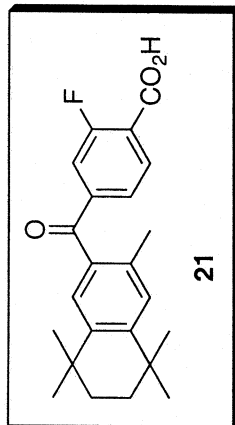
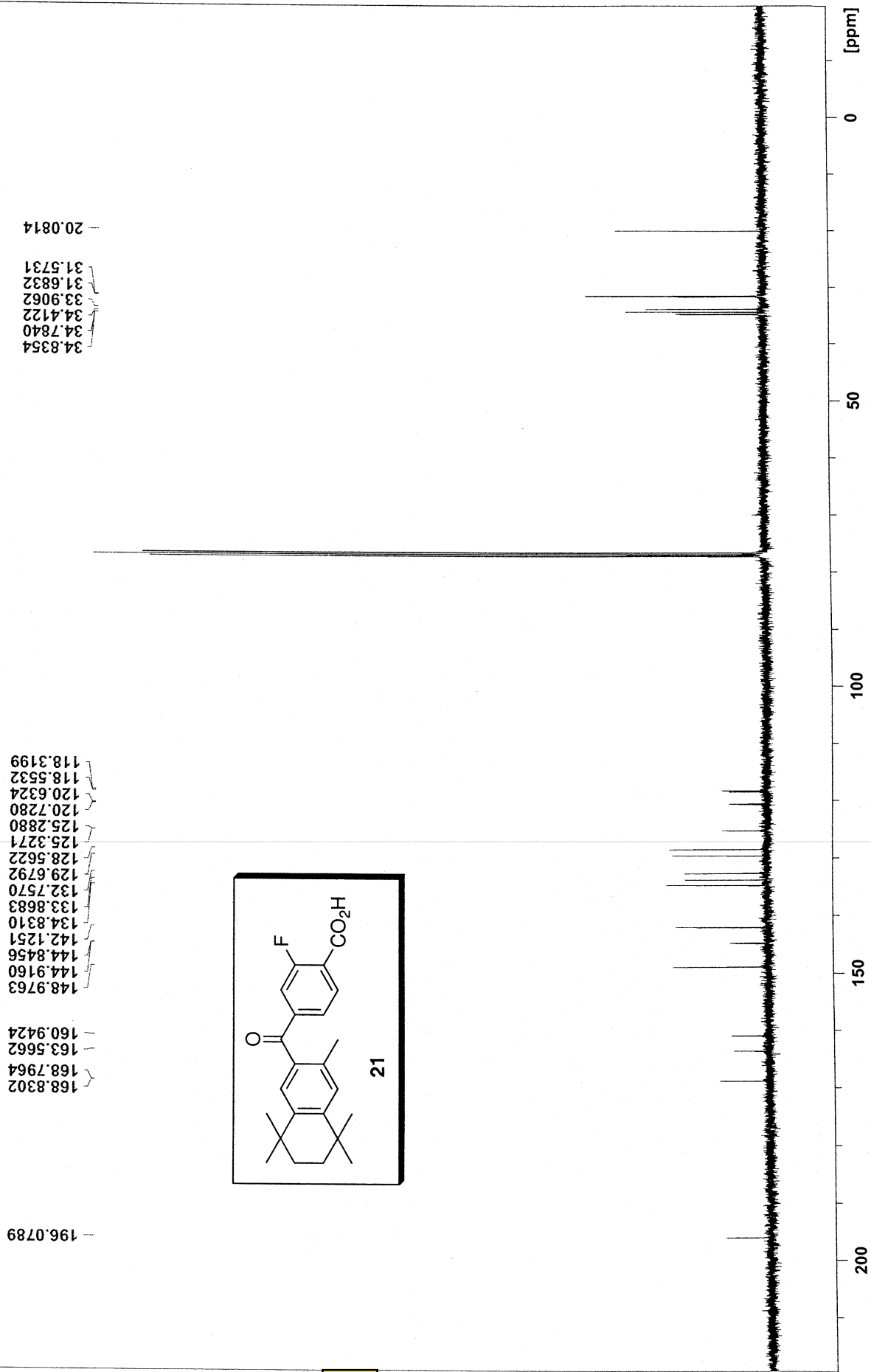
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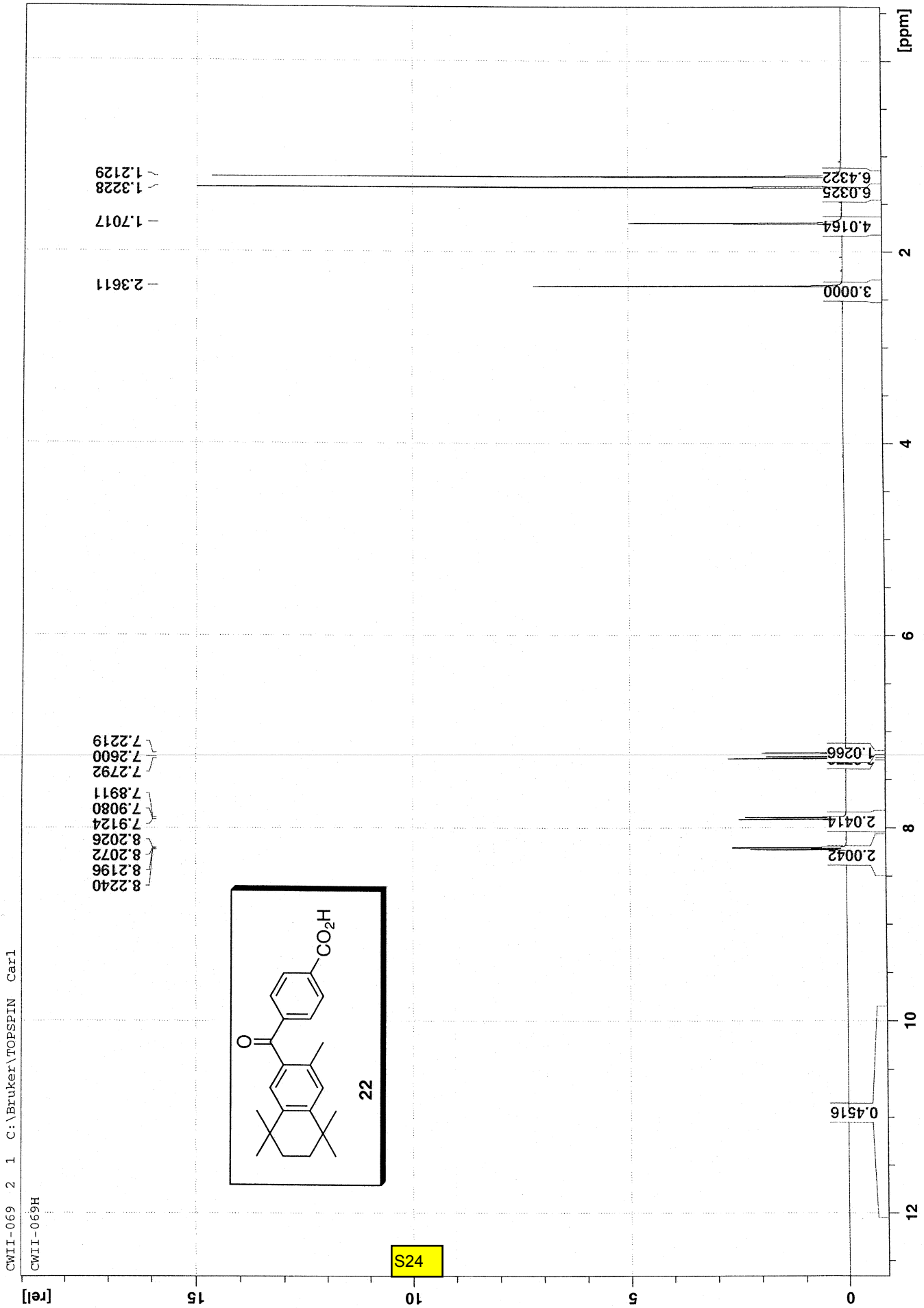
12

CWII-067 2 1 C:\Bruker\TOPSPIN wagner

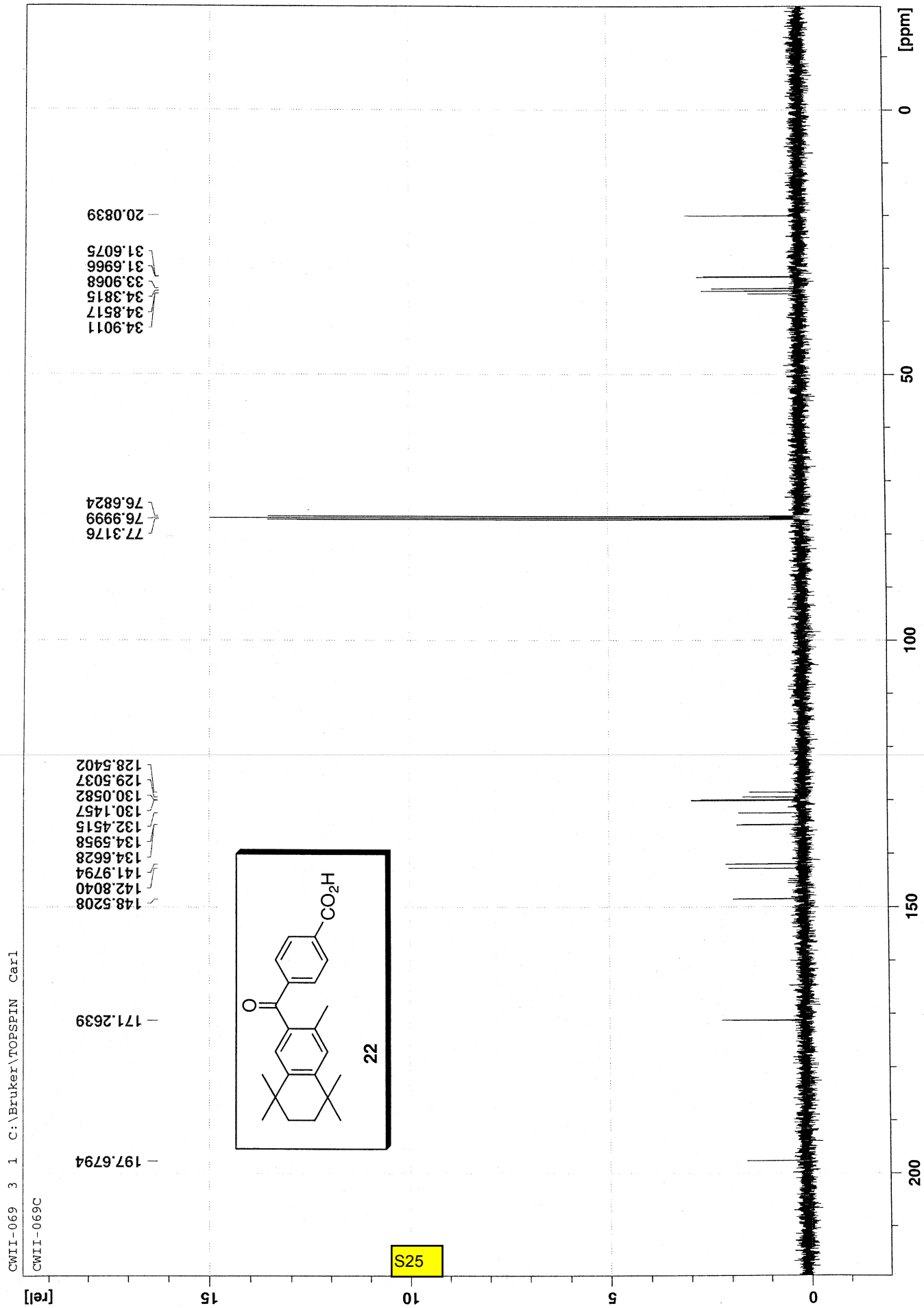
CWII-067

C13

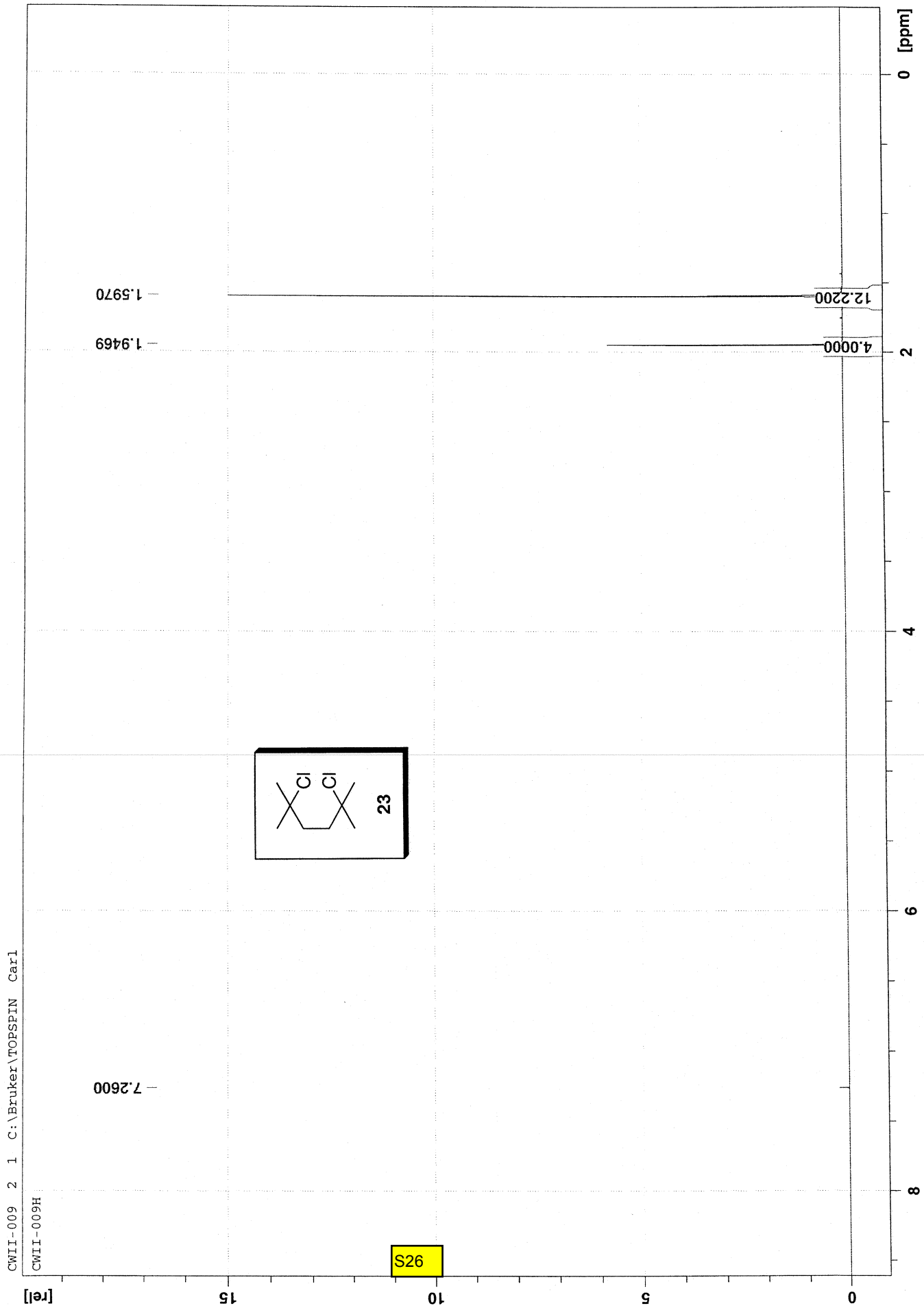








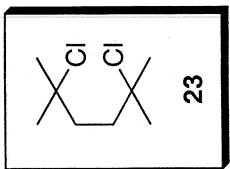
S25

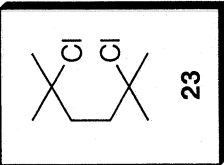
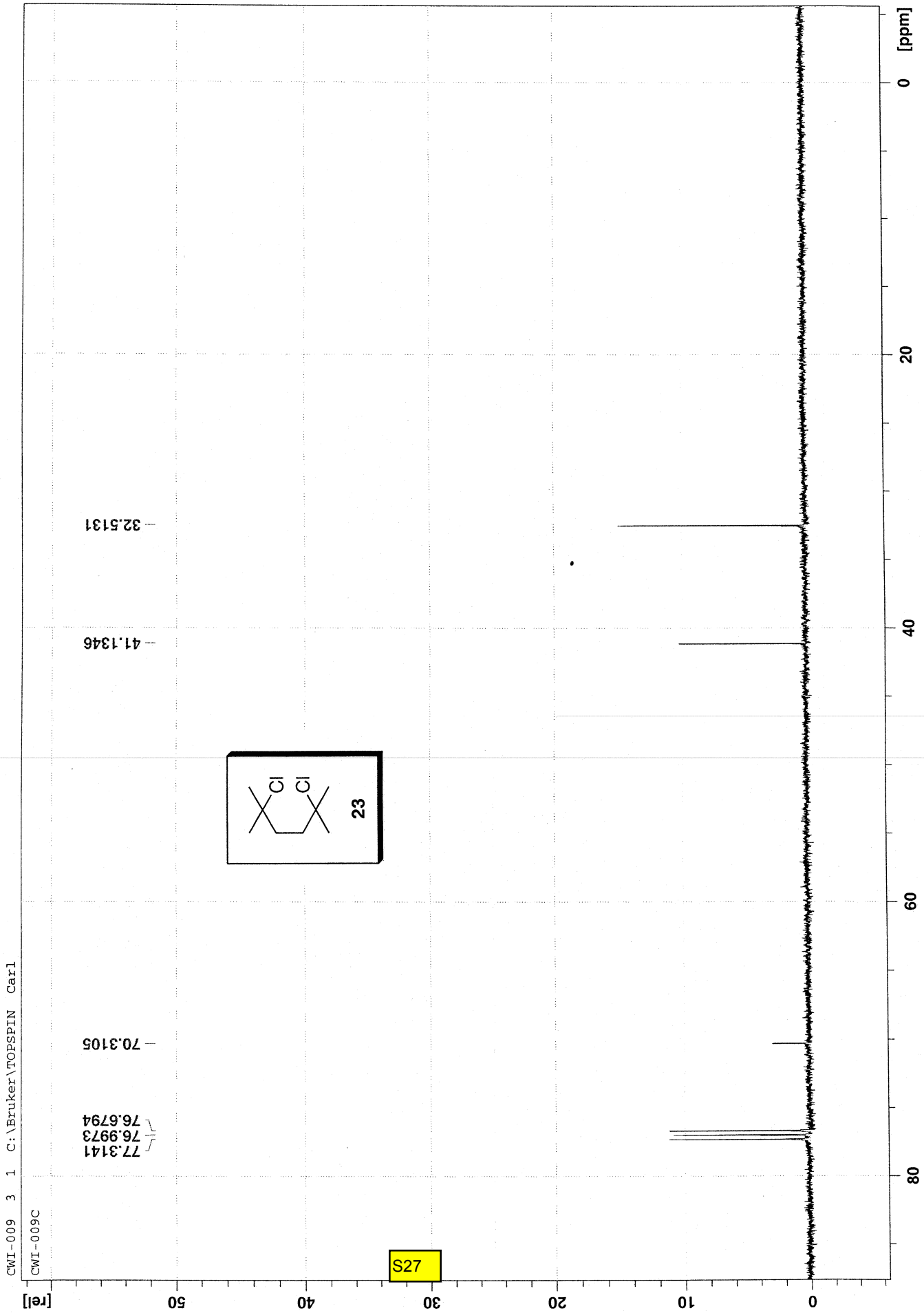


CWII-009 2 1 C:\Bruker\TOPSPIN Carl

CWII-009H

S26



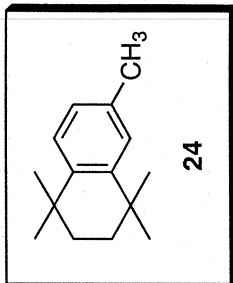


CWI-009 3 1 C:\Bruker\TOPSPIN Carl

CWI-009C

S27

S28



7.260  
7.229  
7.209  
7.127  
6.981  
6.960

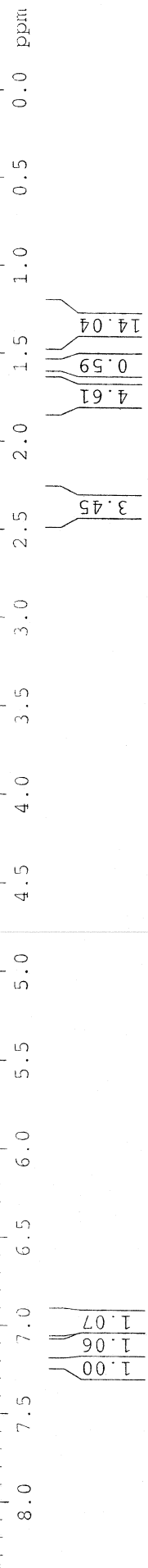
2.315  
1.688  
1.554  
1.291  
1.282

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 EXPNO 1  
 PROCNO 1  
 DU /u  
 USER cwagner

F2 - Acquisition Parameters  
 Date\_ 20050705  
 Time 13.07  
 INSTRUM AVB-400  
 PROBHD 5 mm PABBO BB-7C30  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SMH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9594243 sec  
 RG 101.6  
 DW 60.400 use  
 DE 6.00 use  
 TE 297.5 K  
 D1 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.20 use  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300177 MHz  
 IFTWV FM



144.62  
141.99  
134.72  
126.98  
126.51  
126.40

77.31  
76.99  
76.68

35.19  
35.13  
34.10  
33.87  
33.87  
31.91  
31.84

21.12

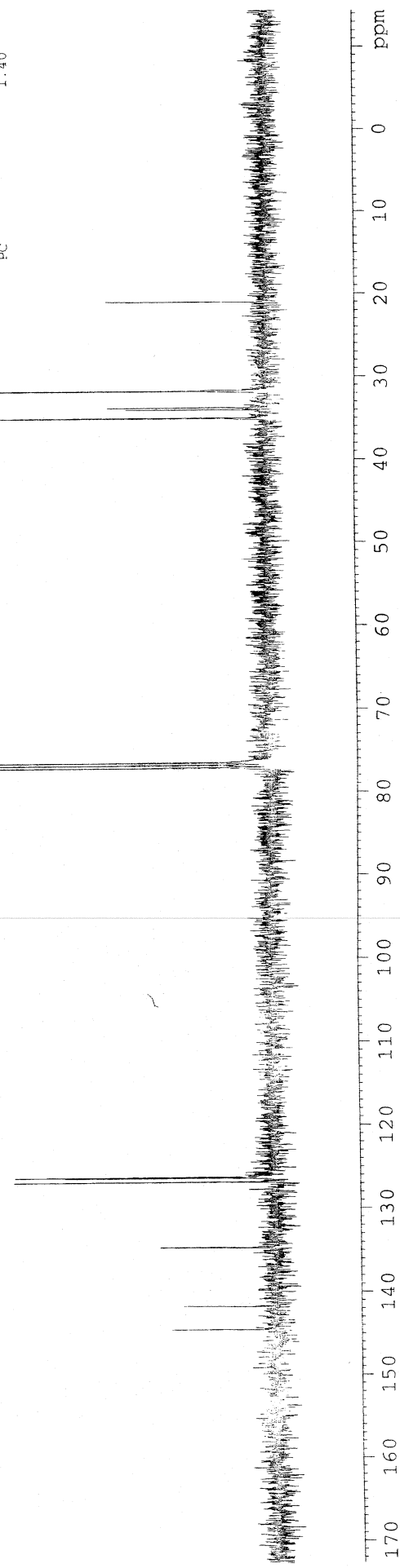
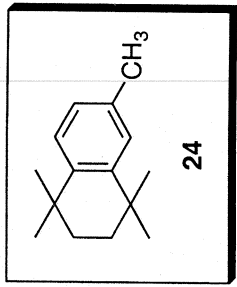
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 EXPNO 1  
 PROCNO 1  
 DU /u  
 USER cwagner

F2 - Acquisition Parameters  
 Date\_ 20060705  
 Time 17.59  
 INSTRUM AVB-400  
 PROBD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 64  
 DS 0  
 SMH 23980.814 Hz  
 FIDRES 0.385918 Hz  
 AQ 1.3664756 sec  
 RG 16384  
 DW 20.850 usec  
 DE 6.00 usec  
 TE 294.8 K  
 DI 1.5000000 sec  
 JLI 0.0300000 sec  
 DELTA 1.3999998 sec  
 MCREST 0.0000000 sec  
 MCWRK 0.0150000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 8.50 usec  
 PL1 -2.00 dB  
 SFO1 100.6228298 MHz

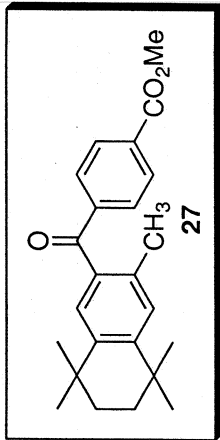
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 CPDPRG2 waltz16  
 NUC2 1H  
 P2 70.00 usec  
 PL2 -3.00 dB  
 PL13 16.00 dB  
 PL12 16.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127766 MHz  
 WDW EM  
 SSB 0  
 LB 1.50 Hz  
 GB 0  
 PC 1.40



8.175  
8.171  
8.159  
8.154  
7.913  
7.908  
7.896  
7.891  
7.303  
7.252

4.002  
2.389  
1.736  
1.645  
1.358  
1.243



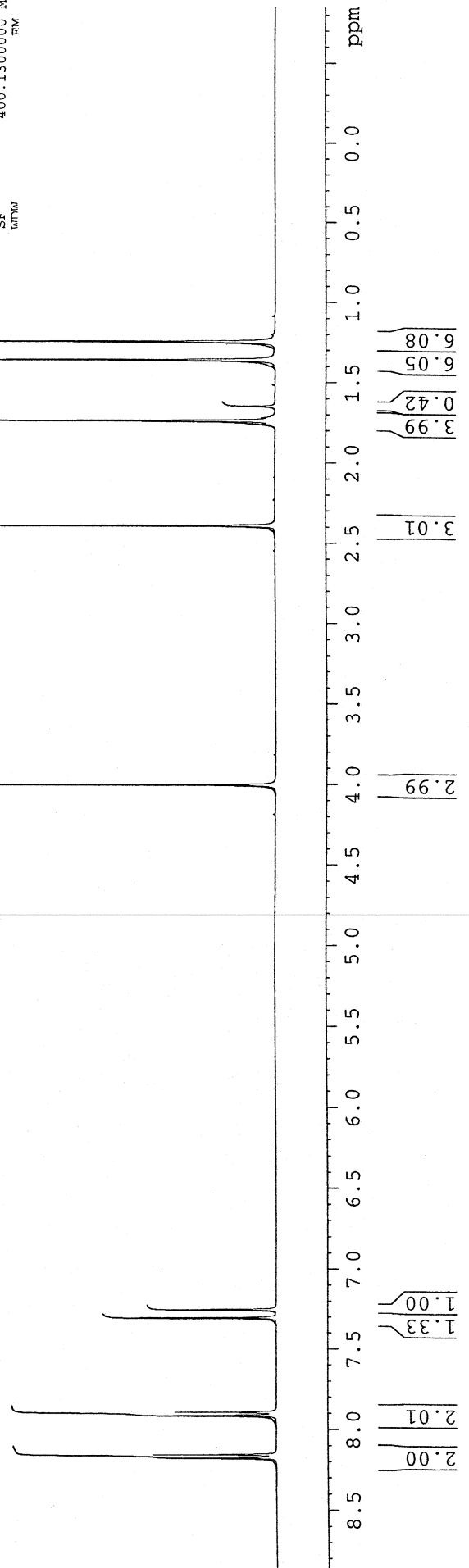
S30

Current Data Parameters  
 NAME cwi-019Ha  
 EXPNO 1  
 PROCNO 1  
 DU /u  
 USER cwagner

F2 - Acquisition Parameters  
 Date\_ 20060731  
 Time\_ 18.07  
 INSTRUM AVB-400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQAQ 3.9584243 sec  
 RG 143.7  
 DW 60.400 use  
 DE 6.00 use  
 TE 294.5 K  
 D1 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.20 use  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32788  
 SF 400.1300000 MHz  
 RM



AVB-400 ZBO Carbon Starting parameters 6/11/03 RN

197.72  
166.38  
148.35  
141.95  
141.89  
134.71  
134.57  
133.41  
129.98  
129.48  
129.43  
128.47

77.31  
76.99  
76.68

52.42

34.89  
34.84  
34.35  
33.88  
31.67

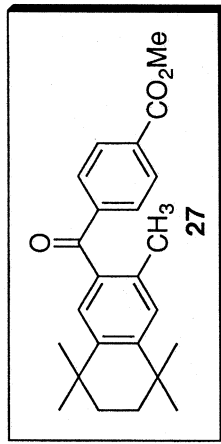
Current Data Parameters  
NAME CWI-019Cb  
EXPNO 1  
PROCNO 1  
DU /u  
USER cwagner

F2 - Acquisition Parameters  
Date\_ 20060731  
Time\_ 18.17  
INSTRUM AVB-400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 128  
DS 0  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 11585.2  
DW 20.850 usec  
DE 6.00 usec  
TE 295.4 K  
D1 1.5000000 sec  
d11 0.0300000 sec  
DELTA 1.3999998 sec  
MCREST 0.0000000 sec  
MCWRK 0.0150000 sec

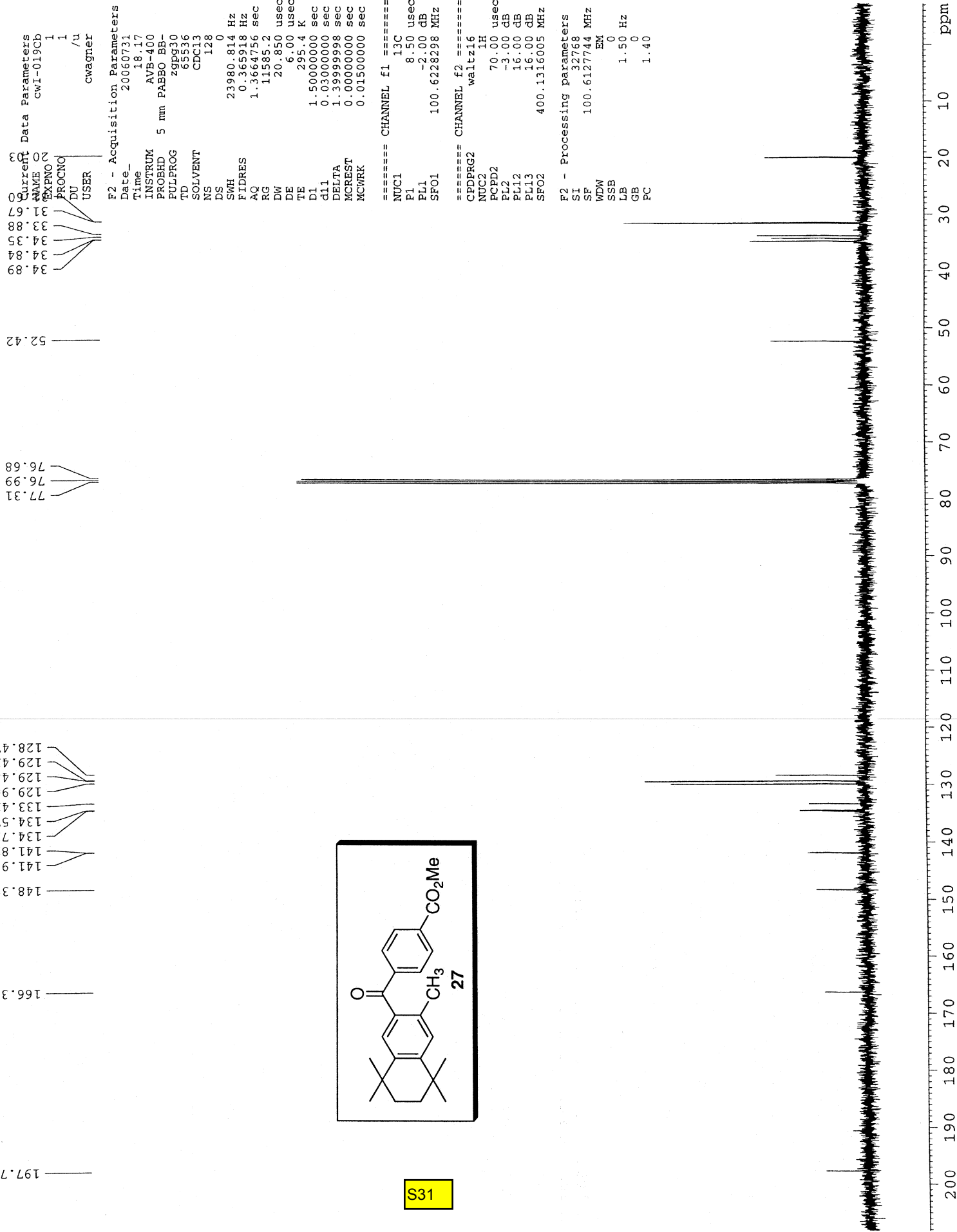
==== CHANNEL f1 =====  
NUC1 13C  
P1 8.50 usec  
PL1 -2.00 dB  
SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 70.00 usec  
PL2 -3.00 dB  
PL12 16.00 dB  
PL13 16.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127744 MHz  
WDW EM  
SSB 0  
LB 1.50 Hz  
GB 0  
PC 1.40



S31

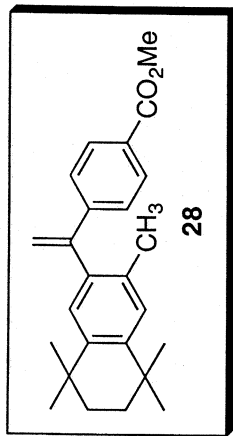


AVB-400 ZBO Proton starting parameters. 6/11/03 RN

7.973  
7.952  
7.360  
7.338  
7.260  
7.134  
7.083  
5.815  
5.812  
5.330  
5.327

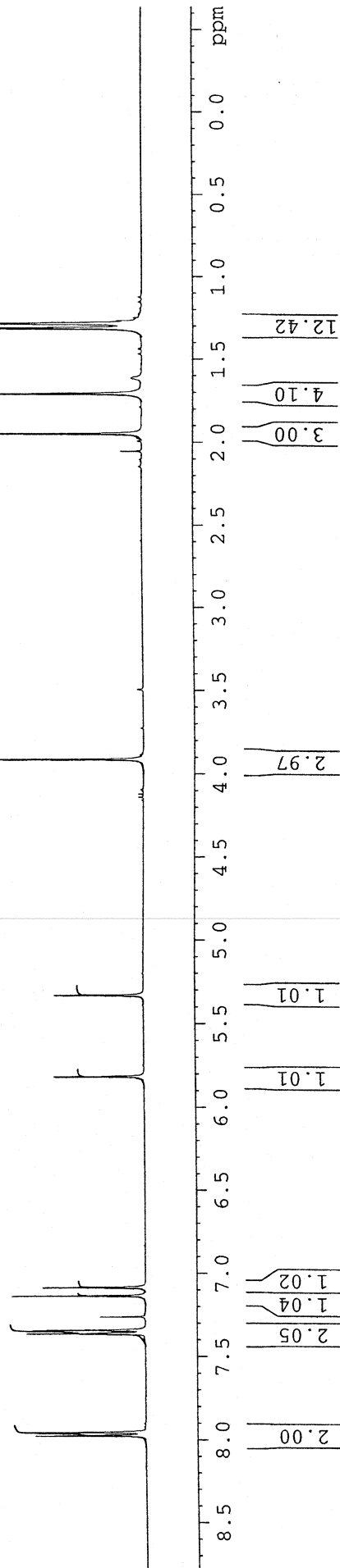
3.911

1.946  
1.706  
1.311  
1.281  
1.266



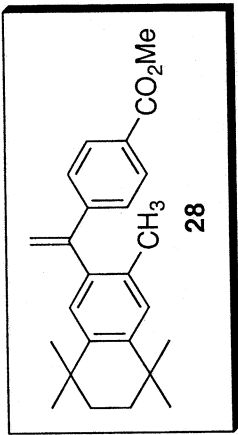
S32

Current Data Parameters  
 NAME CWI-027Ha  
 EXPNO 1  
 PROCNO 1  
 DU /u  
 USER cwagner  
 F2 - Acquisition Parameters  
 Date\_ 20060802  
 Time 18.06  
 INSTRUM AVB-400  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 8278.146 Hz  
 FIDRES 0.126314 Hz  
 AQ 3.9584243 sec  
 RG 90.5  
 DW 60.400 use  
 DE 6.00 use  
 TE 294.4 K  
 DI 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 8.20 use  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 400.1300180 MHz  
 WINDW RM





S33



```

Current Data Parameters
cNAME      cwi-027Ca
EXPNO      1
PROCNO     1
DU         /u
USER       cwagner

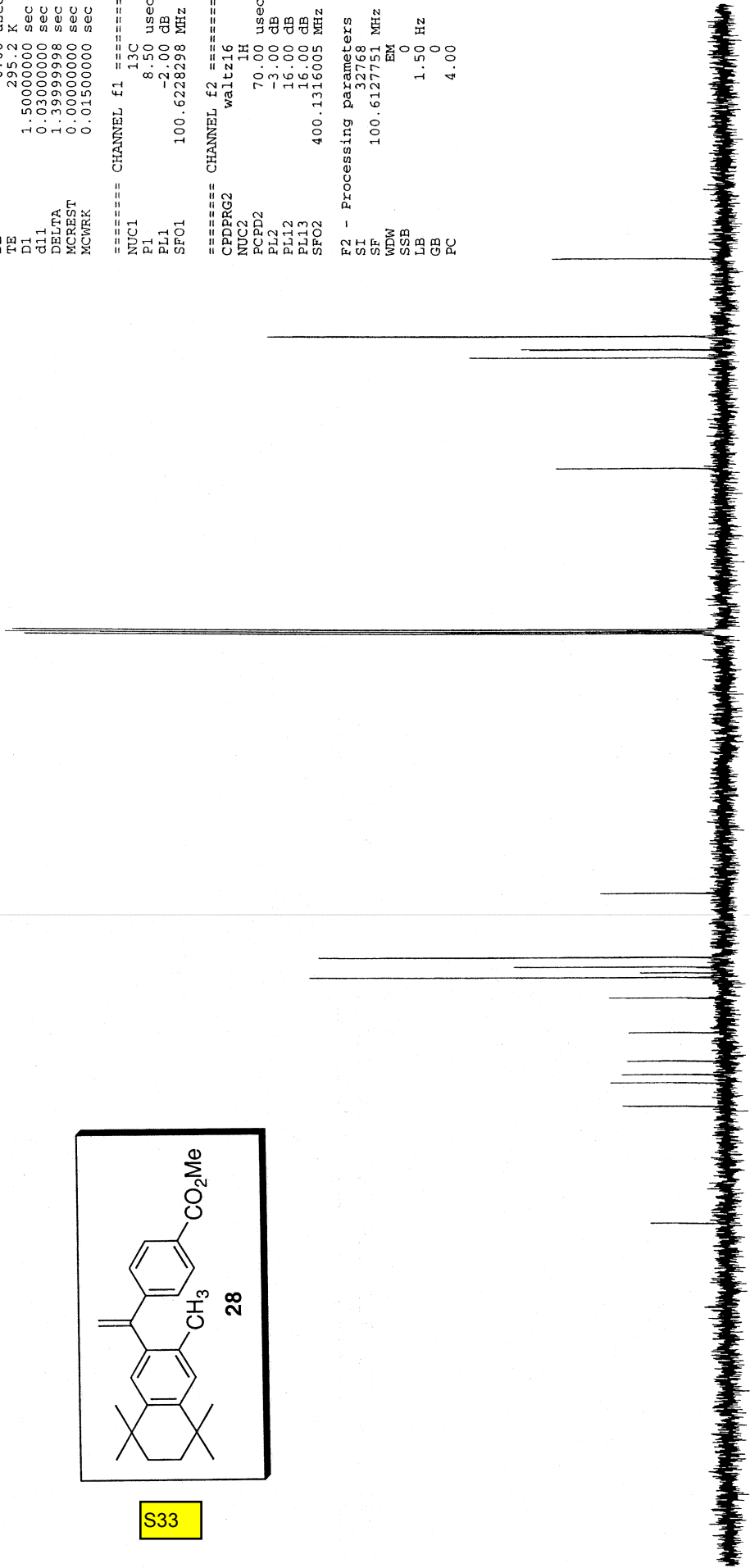
F2 - Acquisition Parameters
Date_      20060802
Time       18.13
INSTRUM    AVB-400
PROBHD     5 mm PABBO BB-
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         101
DS         0
SWH        23980.814 Hz
FIDRES     0.365918 Hz
AQ         1.3664756 sec
RG         13004
DW         20.850 usec
DE         6.00 usec
TE         295.2 K
D1         1.50000000 sec
d11        0.03000000 sec
DELTA      1.39999998 sec
MCREST     0.00000000 sec
MCWRK      0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         8.50 usec
PL1        -2.00 dB
SFO1       100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      70.00 usec
PL2        -3.00 dB
PL12       16.00 dB
PL13       16.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6127751 MHz
WDW        EM
SSB        0
LB         1.50 Hz
GB         0
PC         4.00
    
```

166.96  
149.14  
145.56  
144.32  
142.29  
137.99  
132.70  
129.61  
128.93  
128.05  
128.01  
126.55  
116.80  
77.32  
77.00  
76.68  
52.03  
35.16  
33.97  
33.87  
31.90  
31.86



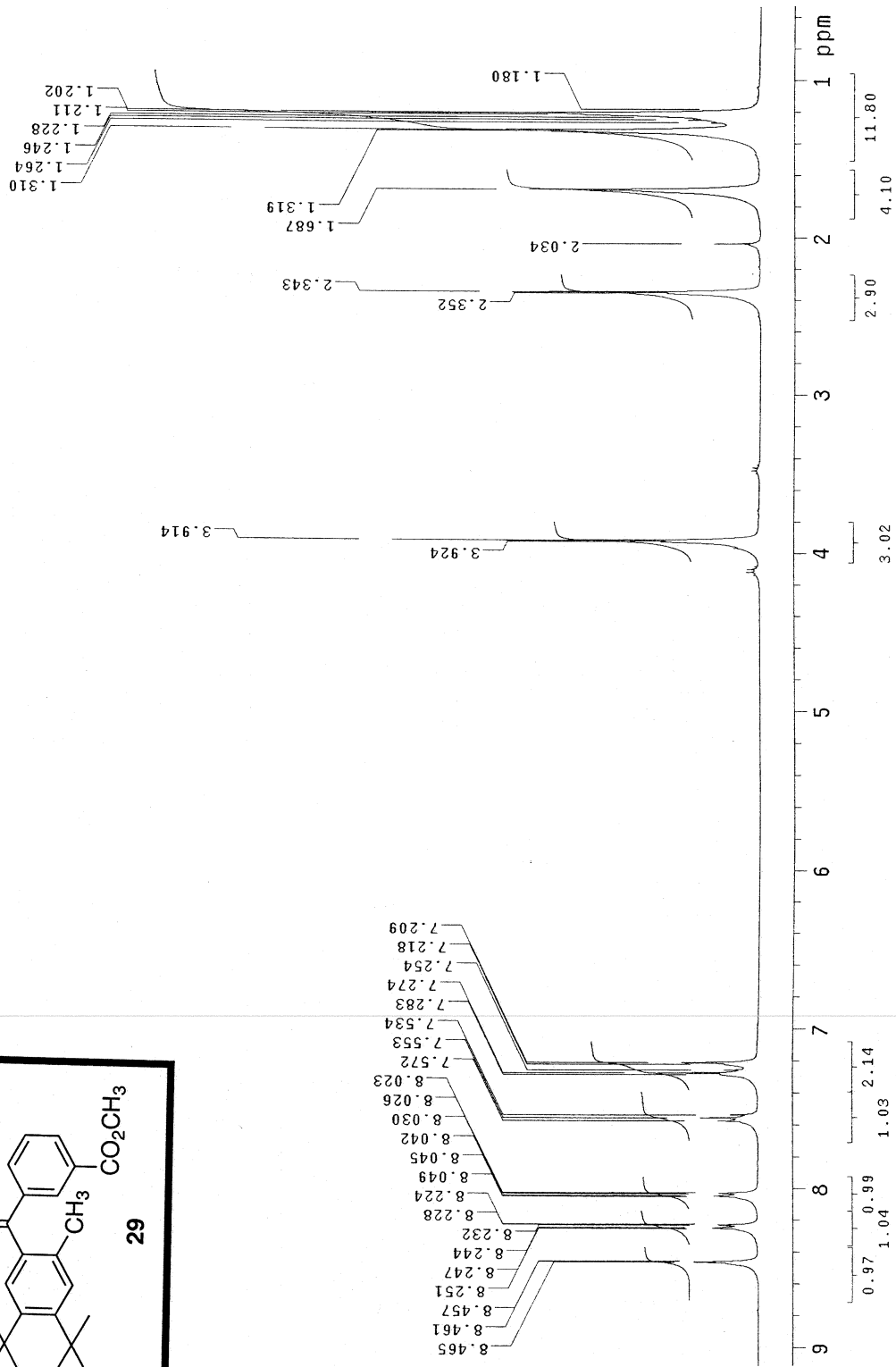
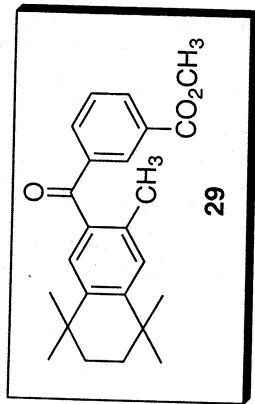
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

cwi-085

File : home/inova400/NMR\_User\_Data/wagner/cwi\_085H\_20july07.fid

Sample id : tmpstudy

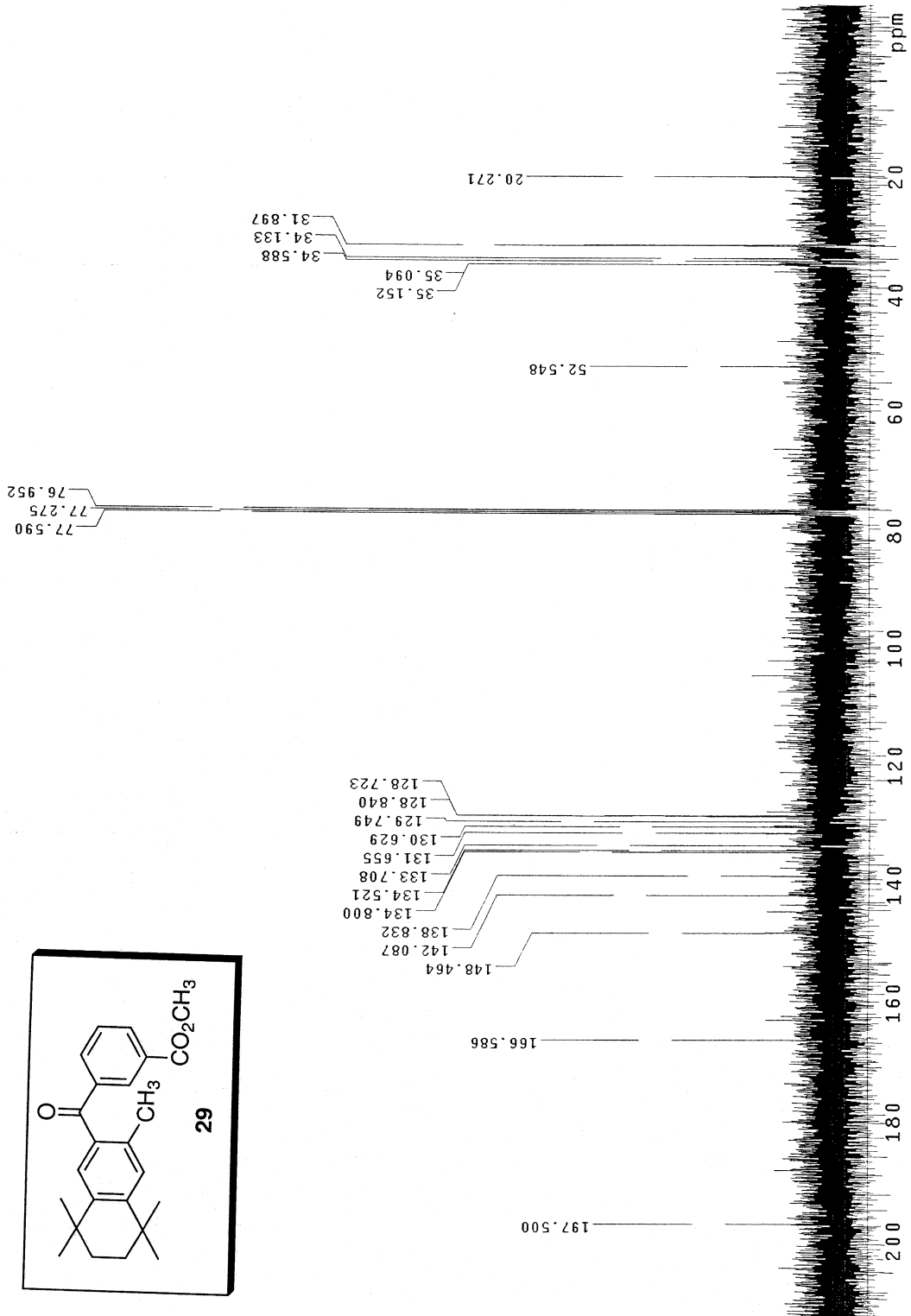
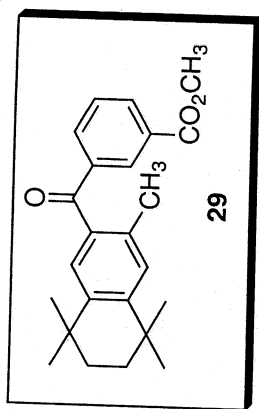
Pulse Sequence: s2pu1



cwI-085

File : home/inova400/NMR\_User\_Data/wagner/cwI\_085C\_20july07.fid  
Sample Id : tmpstudy

Pulse Sequence: s2pul

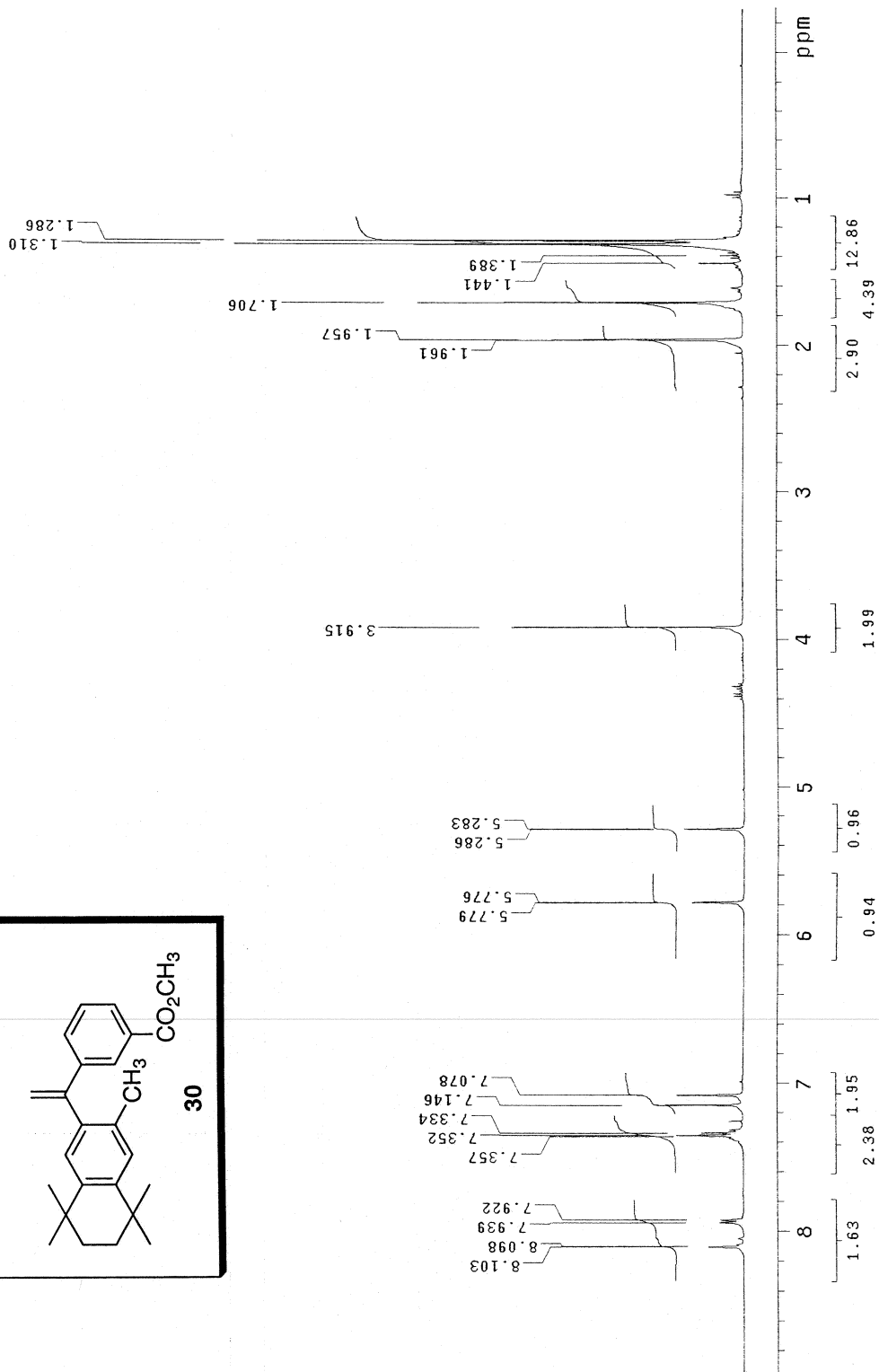
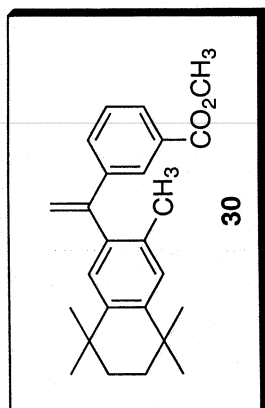


cwI-115

File : home/innov400/NMR\_User\_Data/wagner/cwI\_115H\_6august07.fid

Sample id : tmpstudy

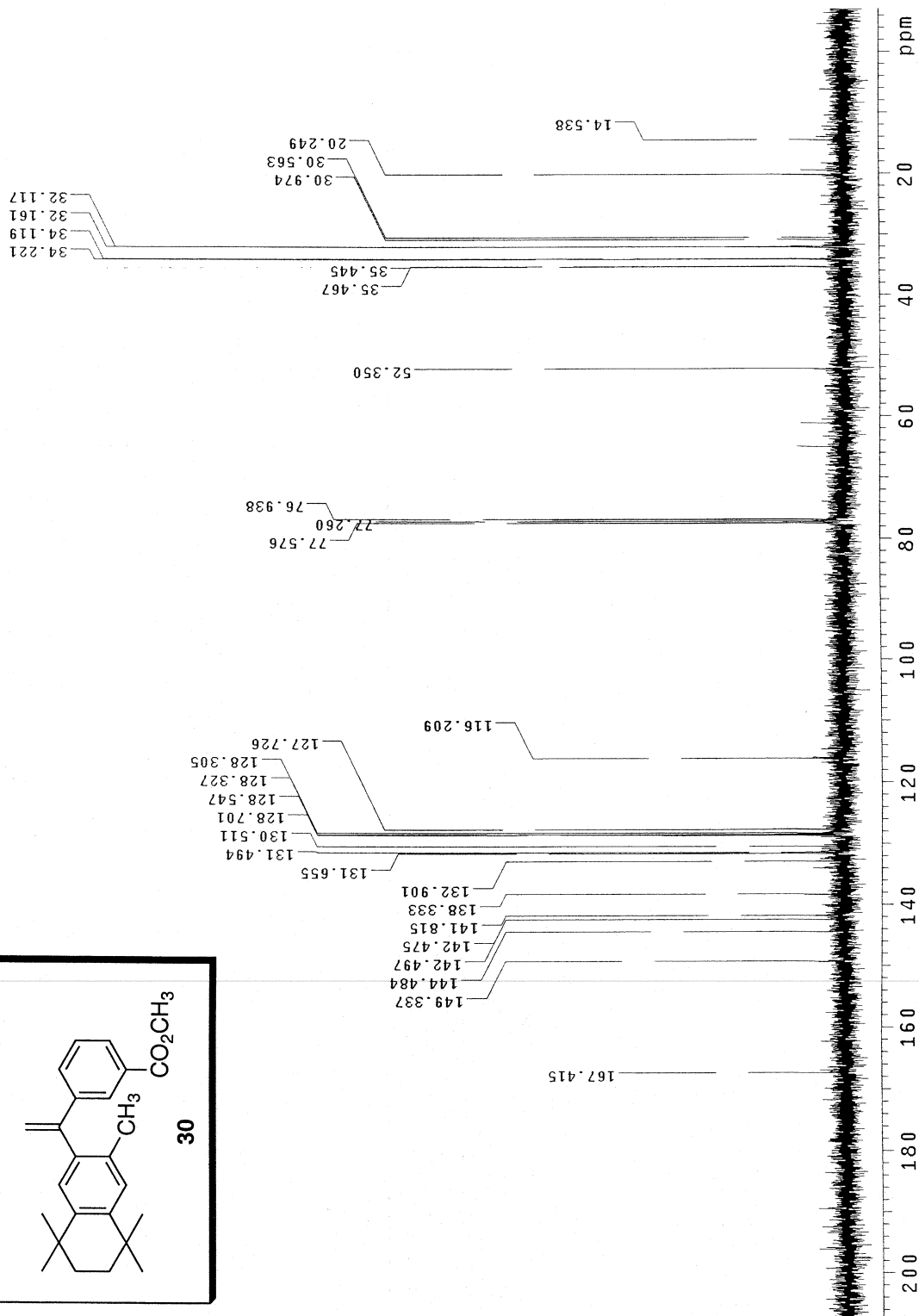
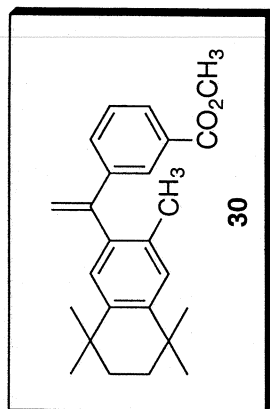
Pulse Sequence: s2pu1



cwI-115

File : home/inoVa400/NMR\_User\_Data/wagner/cwI\_115C\_6august07.fid  
Sample id : tmpstudy

Pulse Sequence: s2pul

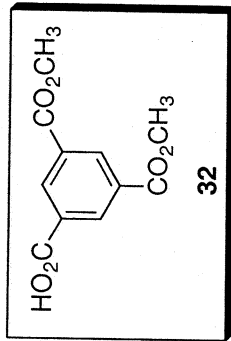


cwI-073

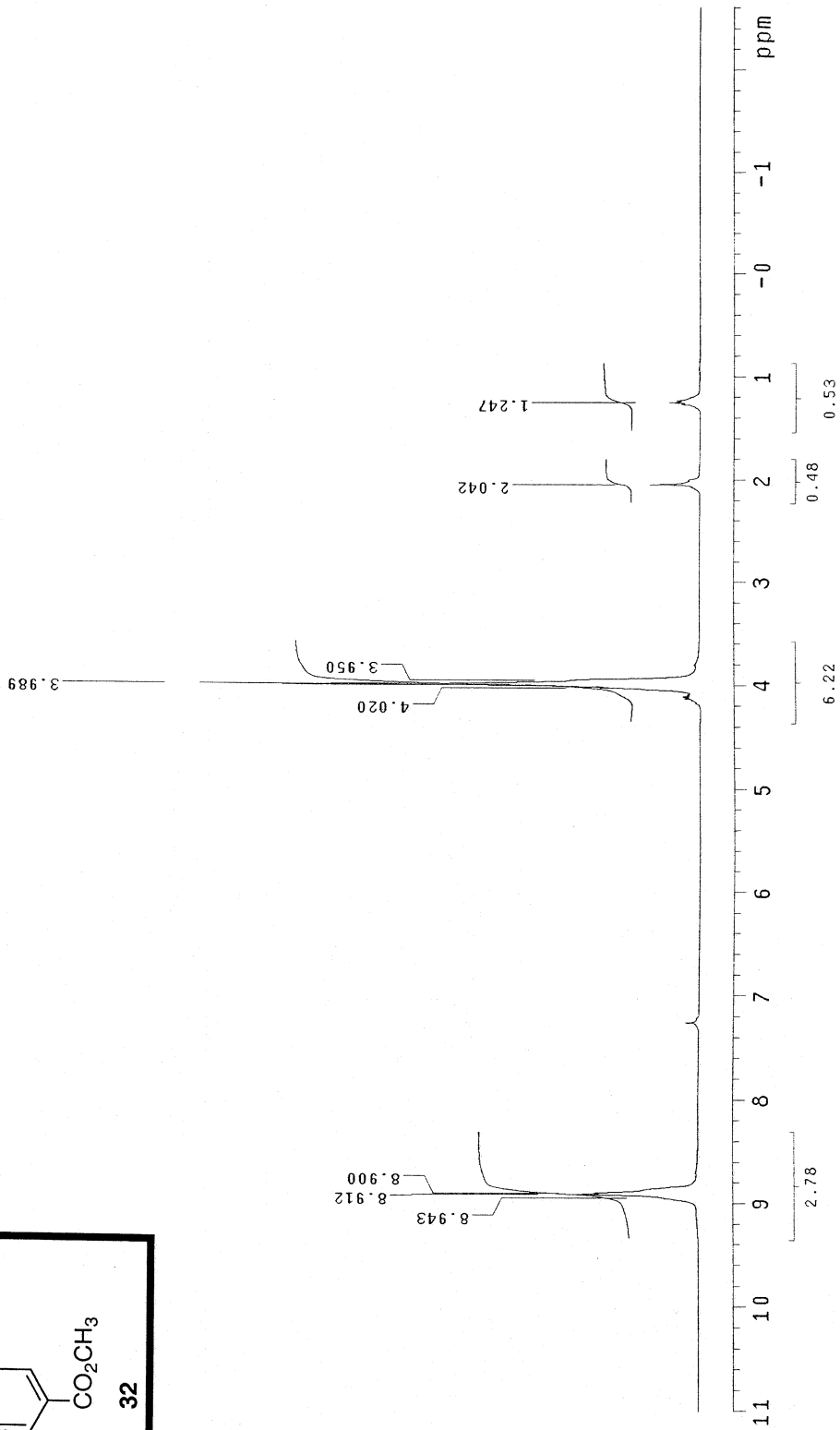
File : home/inova400/NMR\_User\_Data/wagner/cwI\_073H\_6august07.fid

Sample id : tmpstudy

Pulse Sequence: s2pu1



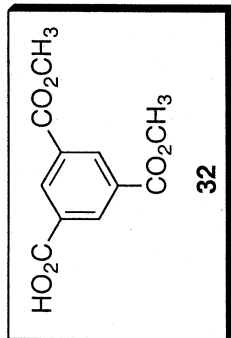
S38



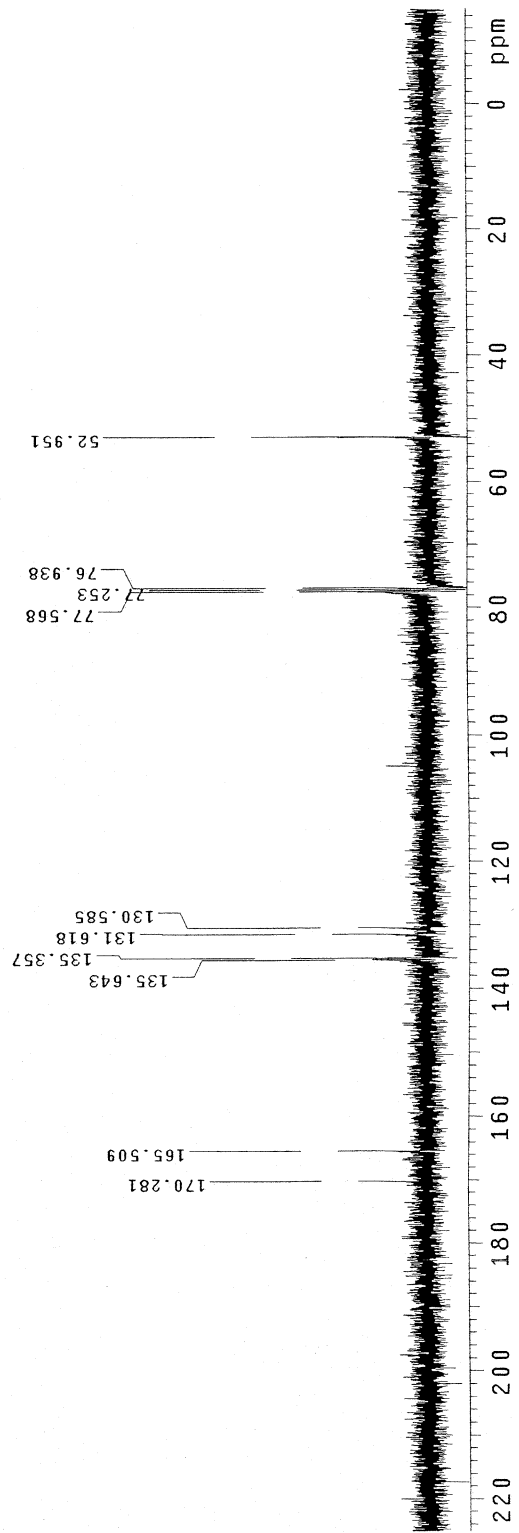
cwI-073

File : home/inova400/NMR\_User\_Data/wagner/cwI\_073C\_6august07.fid  
Sample id : tmpstudy

Pulse Sequence: s2pu1



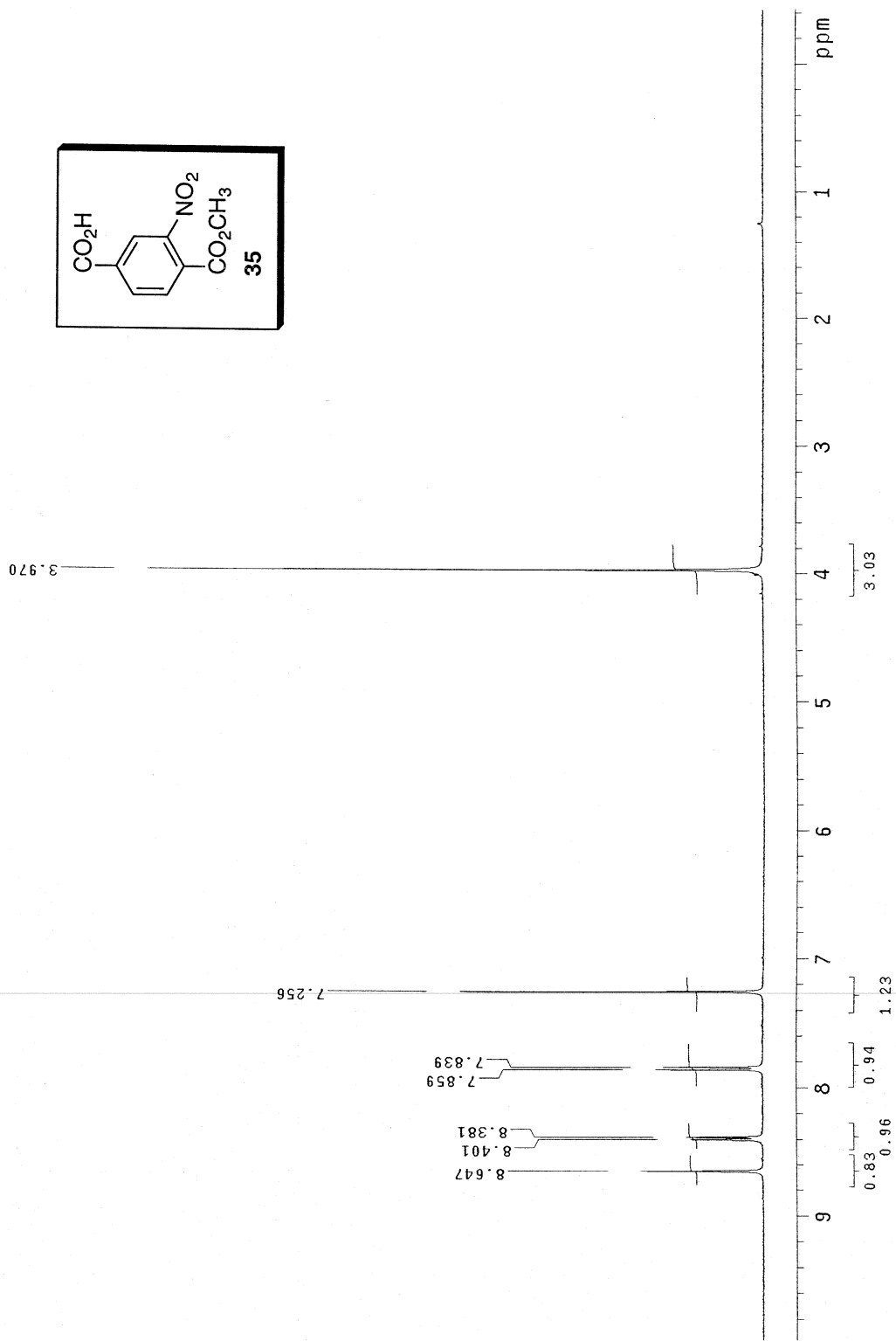
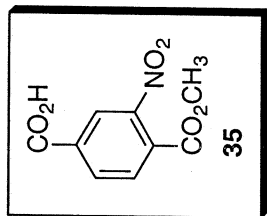
S39



cwI-055

File : home/innov400/NMR\_User\_Data/wagner/cwI\_055H.fid  
Sample id : tmpstudy

Pulse Sequence: s2pu1

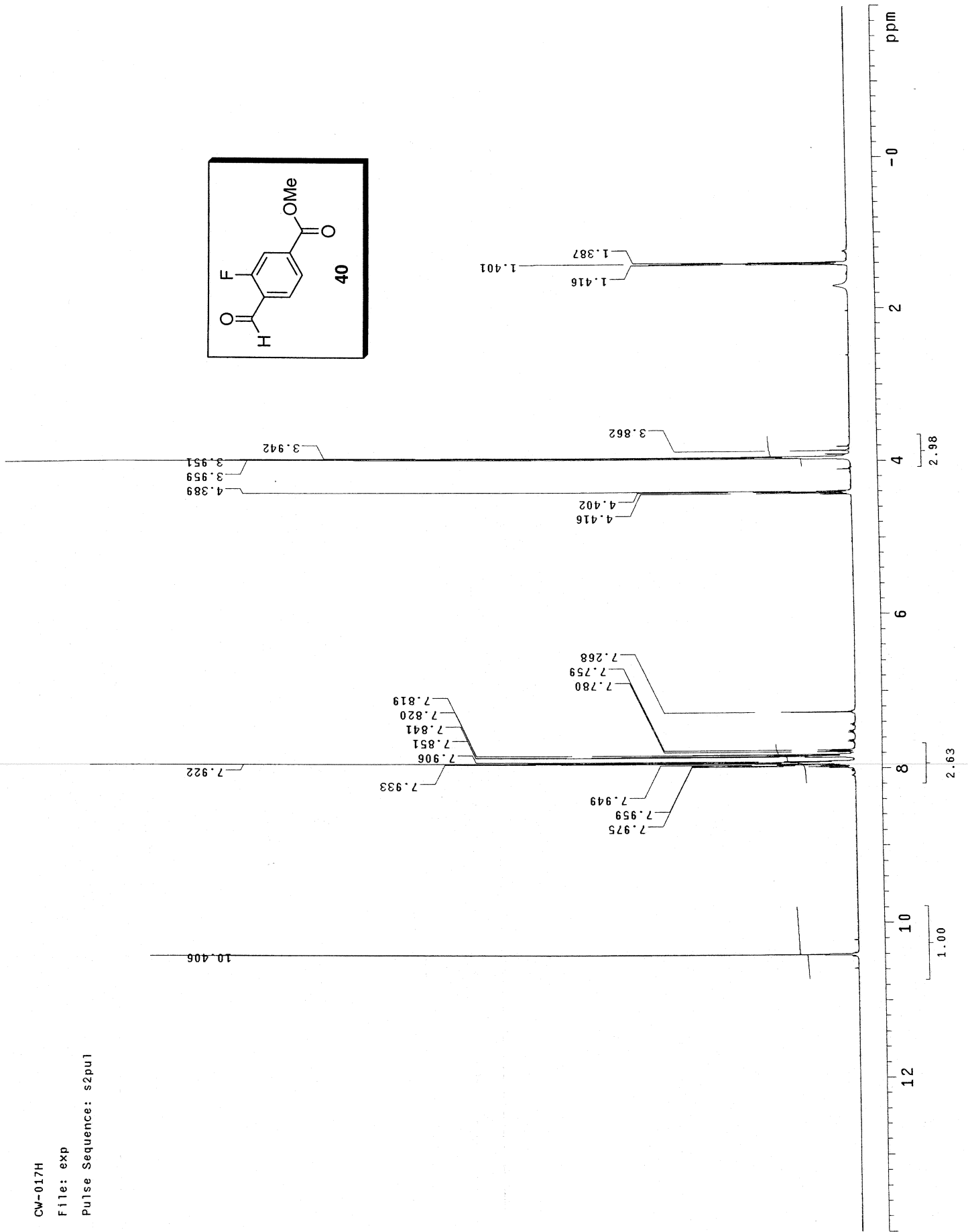
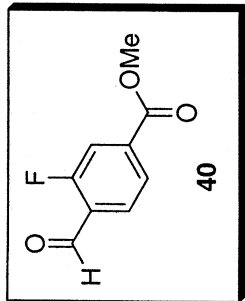




CW-017H

File: exp

Pulse Sequence: s2pu1

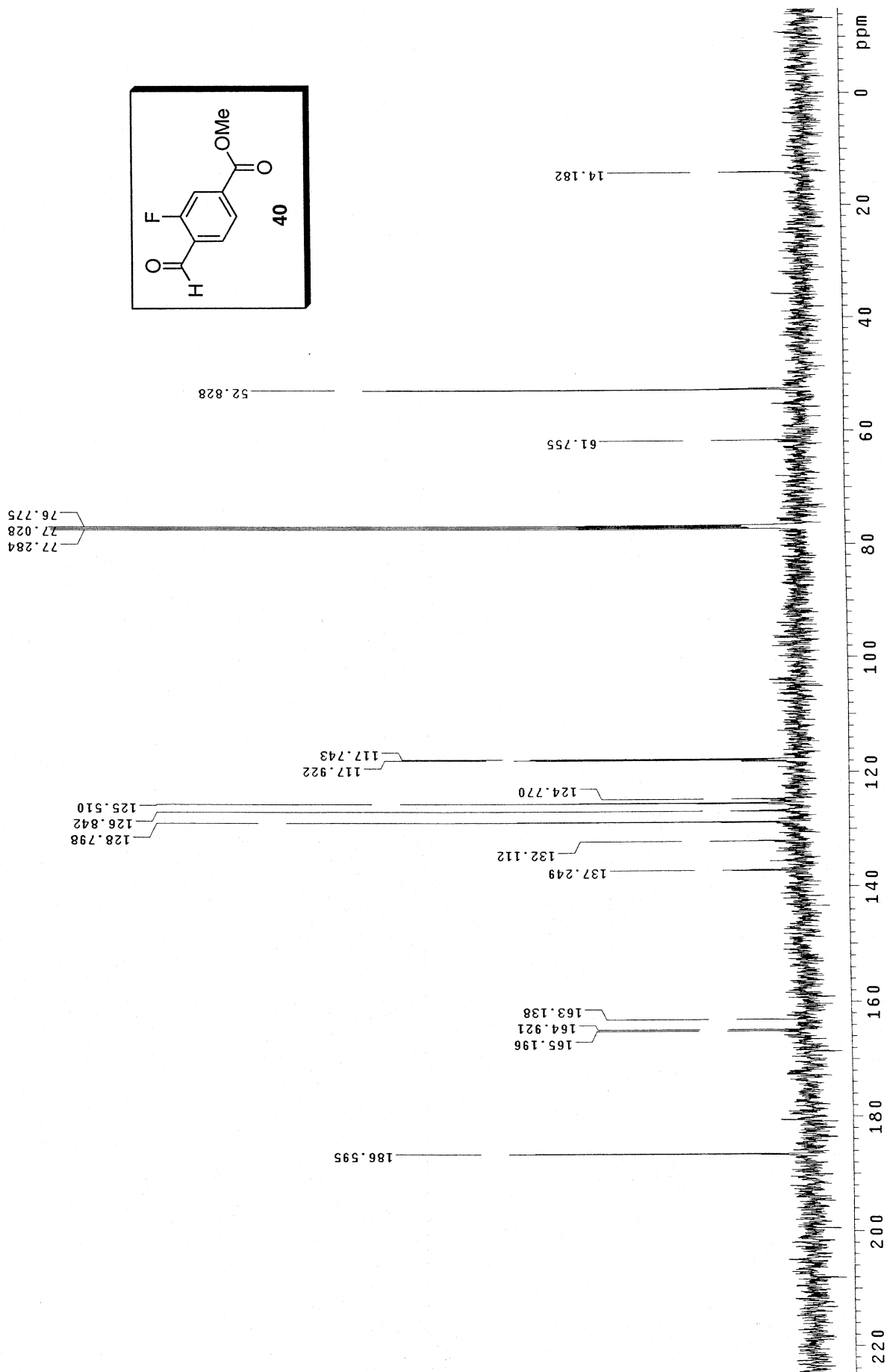
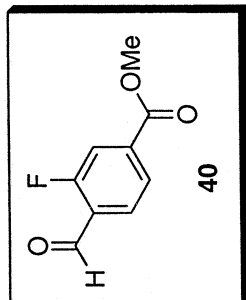


SODA091008

Sample: SODA091008

File: exp

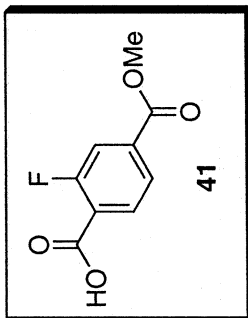
Pulse Sequence: s2pu1



CWII-039 1 1 C:\Bruker\TOPSPIN wagner

CWII-039

1H



8.1194  
8.1000  
8.0815  
7.9072  
7.8867  
7.8398  
7.8122  
7.2600

3.9666

3.0000

0.9694  
2.0229

0.8649

[ppm] 12 10 8 6 4 2

CWII-039 2 1 C:\Bruker\TOPSPIN wagner

CWII-039

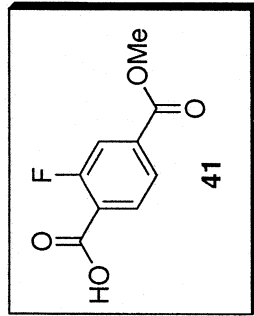
C13

168.5819  
168.5475  
165.0074  
164.9853  
163.4509  
160.8334

136.7489  
136.6650  
132.8283  
124.9280  
124.8866  
121.3188  
121.2242  
118.4185  
118.1759

77.3154  
76.9983  
76.6800

52.8191

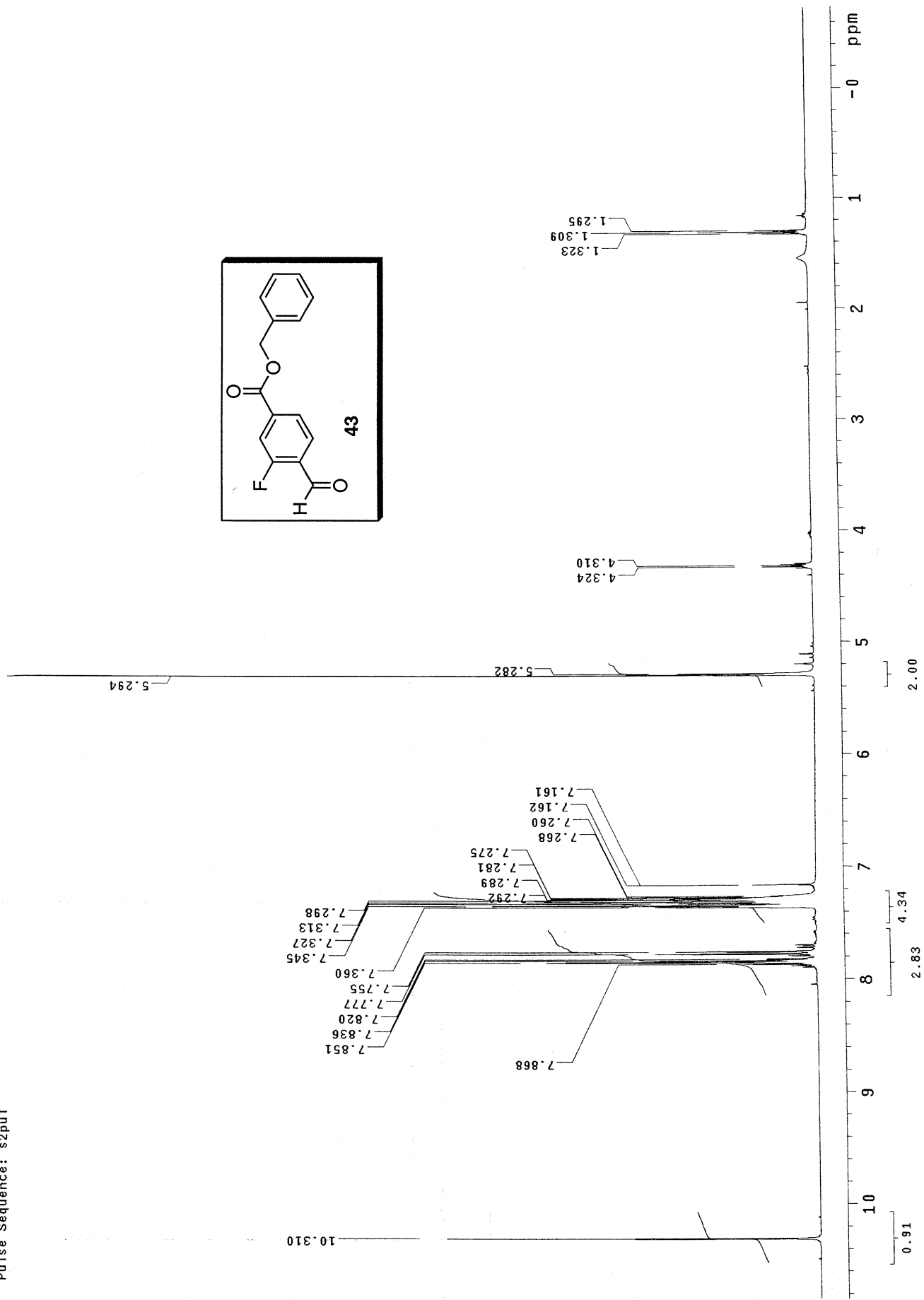
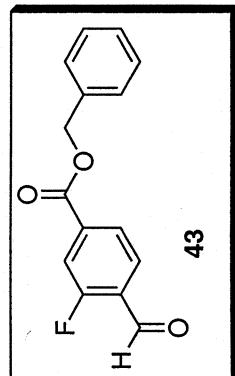


[ppm] 0 50 100 150 200

CWII-019H

File: exp

Pulse Sequence: s2pu1



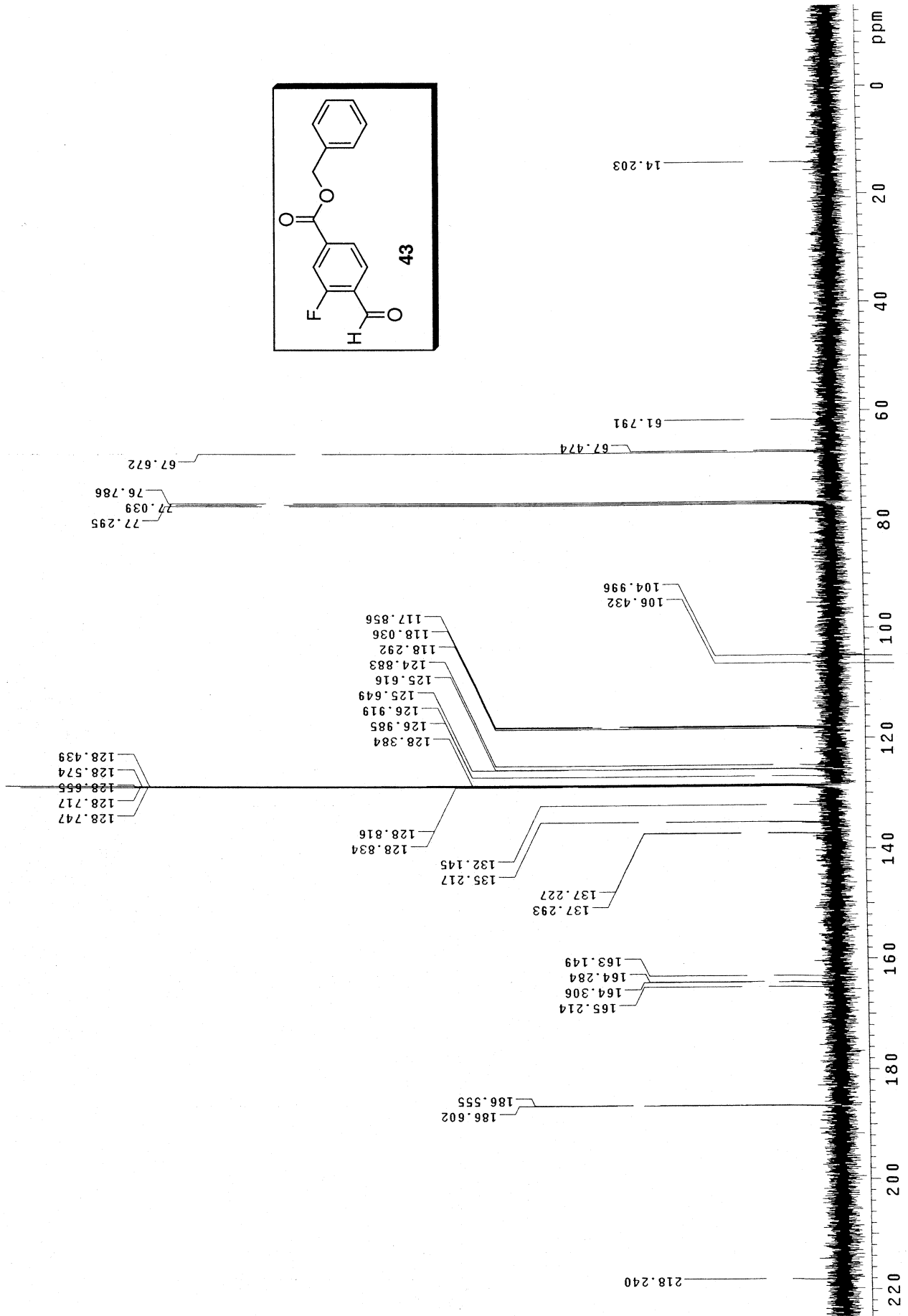
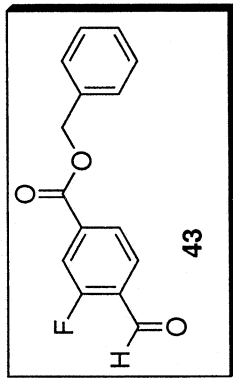
S45

SODA091008

Sample: SODA091008

File: exp

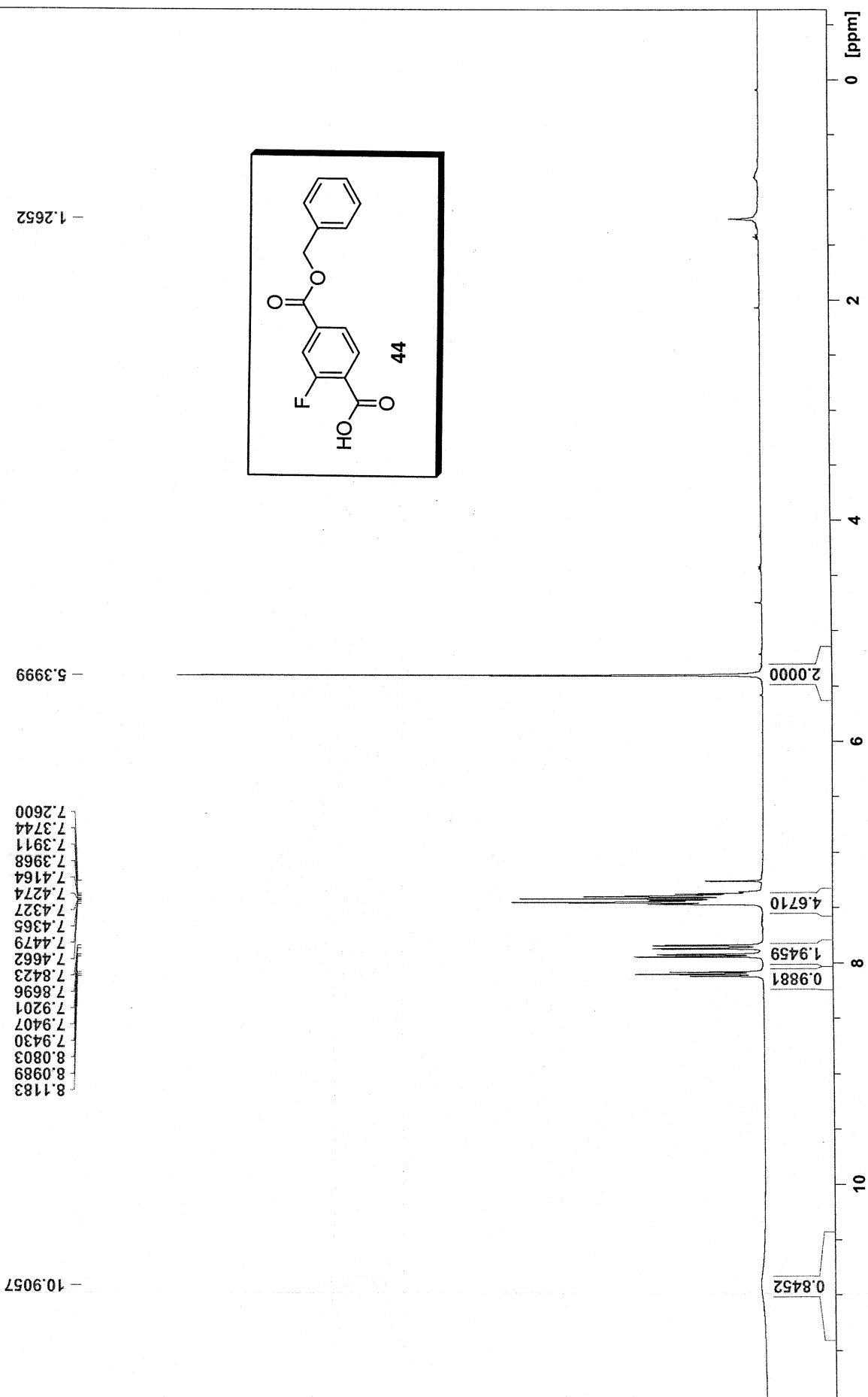
Pulse Sequence: s2pu1



CWII-033 1 1 C:\Bruker\TOPSPIN wagner

CWII-033

<sup>1</sup>H



CWII-033 2 1 C:\Bruker\TOPSPIN wagner

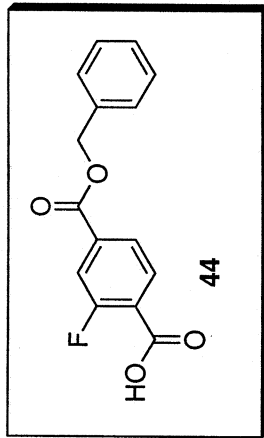
CWII-033

C13

168.7941  
168.7598  
164.3358  
164.3146  
163.4447  
160.8257

136.7701  
136.6857  
135.1887  
132.8234  
128.7022  
128.5980  
128.3803  
125.0183  
124.9796  
121.3710  
121.2764  
118.4850  
118.2439

77.3155  
76.9983  
76.6799  
-67.6099



0 [ppm] 50 100 150



CWII-041 1 1 C:\Bruker\TOPSPIN wagner

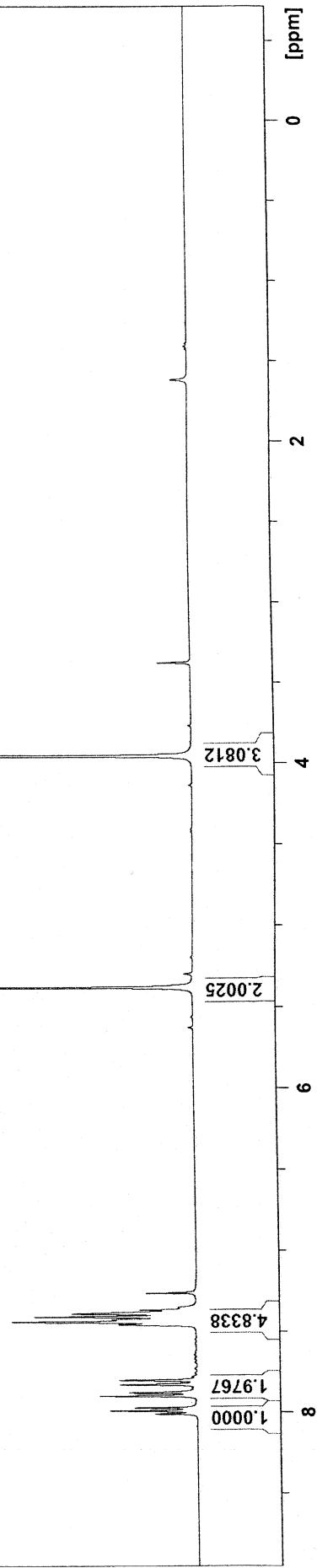
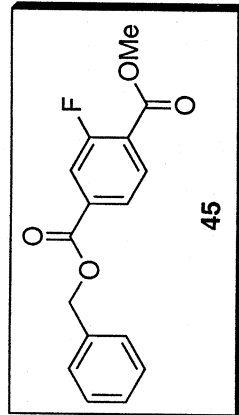
CWII-041

<sup>1</sup>H

8.0100  
7.9906  
7.9724  
7.8983  
7.8778  
7.8286  
7.8013  
7.4556  
7.4373  
7.4241  
7.4069  
7.3873  
7.3648  
7.3487  
7.2600

5.3799

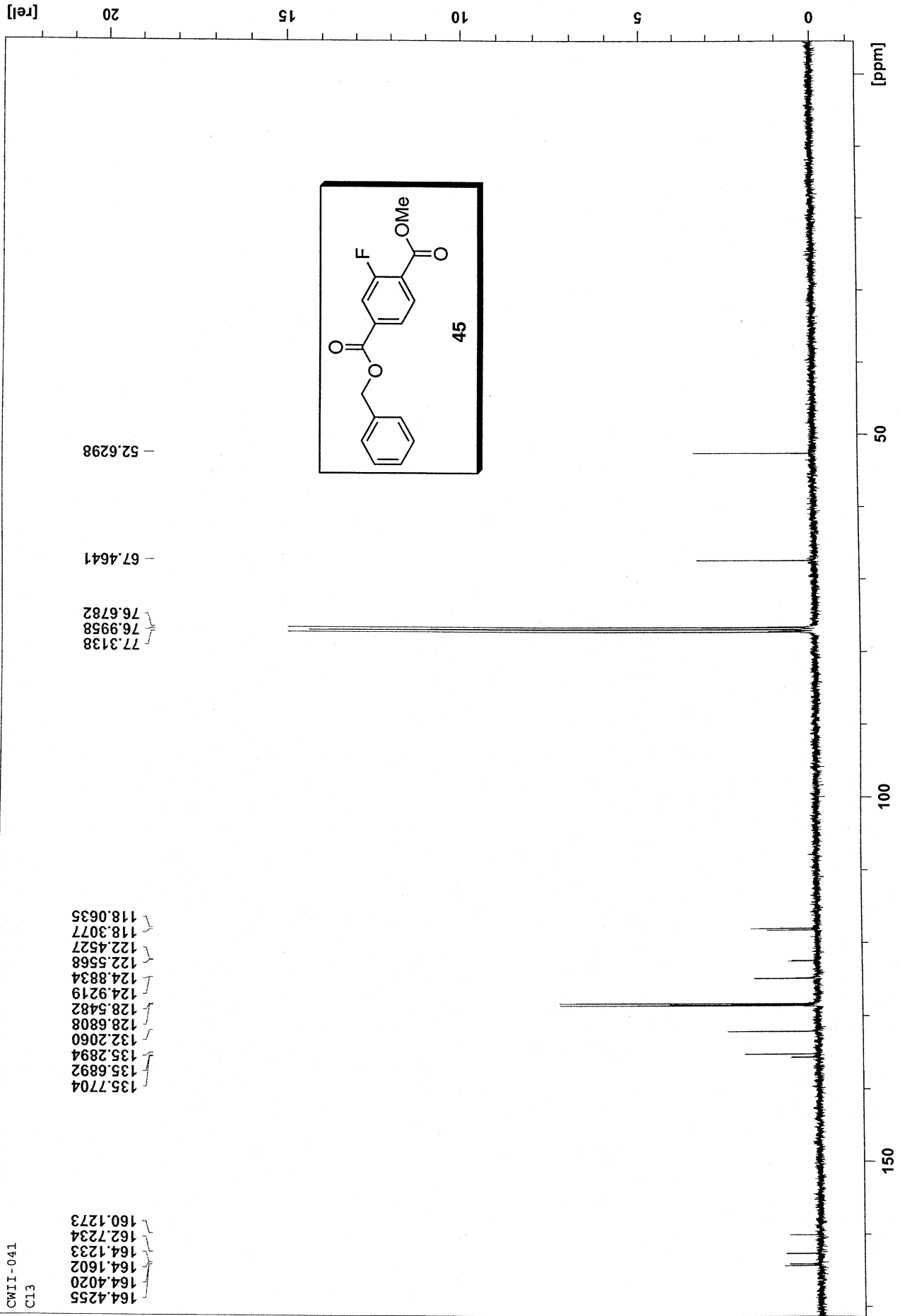
3.9532



CWII-041 2 1 C:\Bruker\TOPSPIN wagner

CWII-041

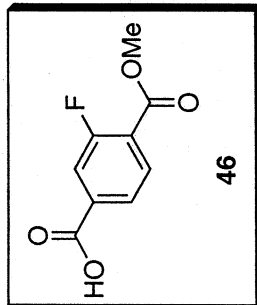
C13



CWII-047 1 1 C:\Bruker\TOPSPIN wagner

CWII-047

1H



7.9956  
7.9762  
7.9574  
7.8468  
7.8264  
7.7587  
7.7306

2.5000

3.8757

0.7663

1.000

0.9832

0.9568

2.8352

0 2 4 6 8 10 12 [ppm]

CWII-047 2 1 C:\Bruker\TOPSPIN wagner

CWII-047

C13

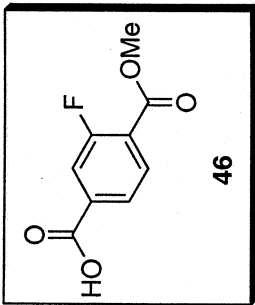
165.8926  
163.8718  
163.8616  
163.8259  
162.2341  
159.6650

137.4475  
137.3686  
- 132.5657

125.5487  
125.5119  
122.1749  
122.0688  
117.9908  
117.7562

- 53.0538

40.5240  
40.3149  
40.1061  
39.8974  
39.6883  
39.4798  
39.2713



[ppm]

50

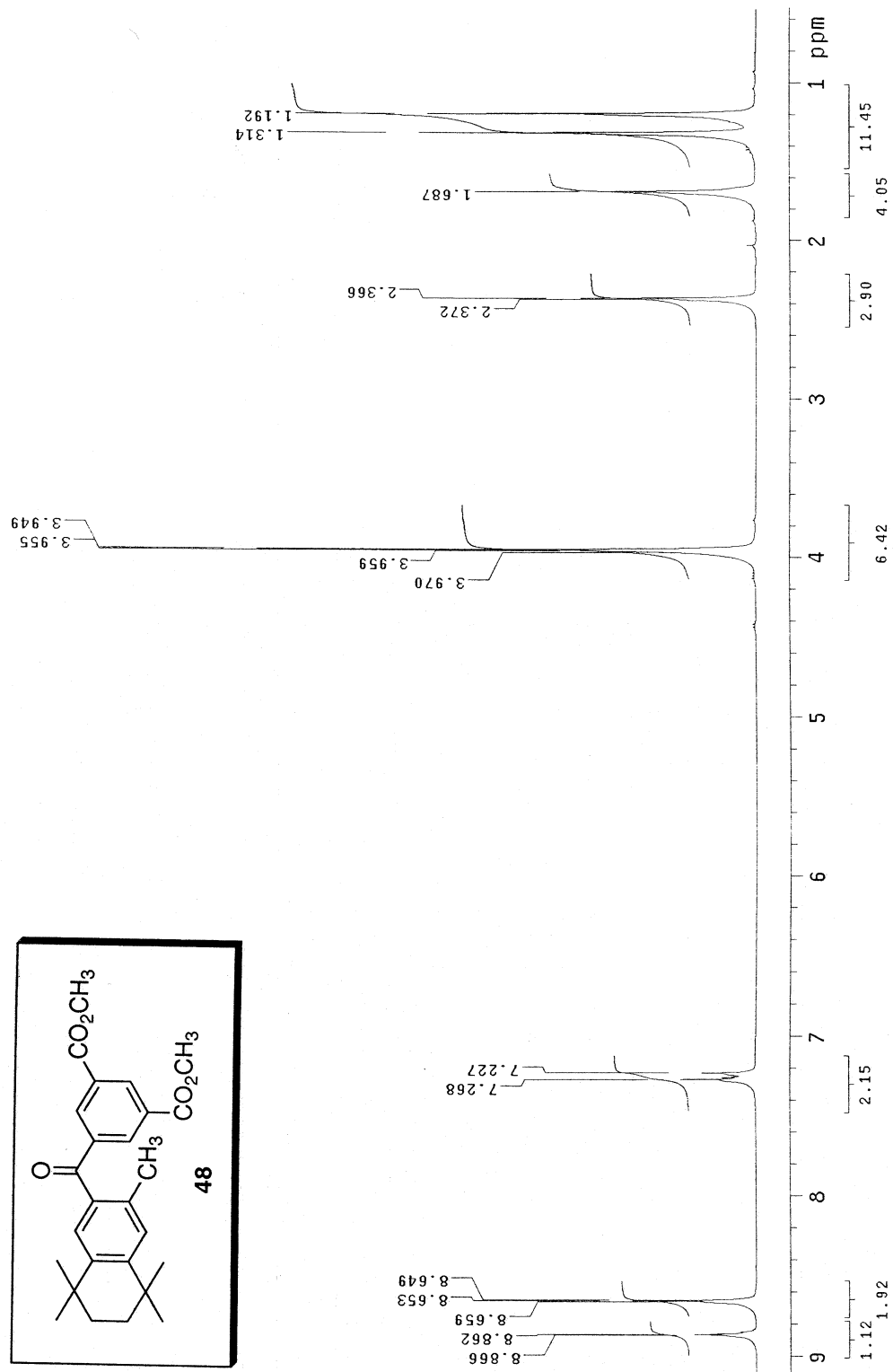
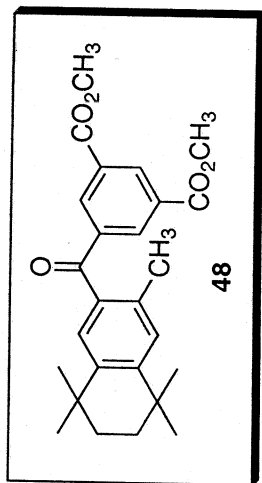
100

150

cwI-087

File : home/inova400/NMR\_User\_Data/wagner/cwI\_087H\_20july07.fid  
Sample Id : tmpstudy

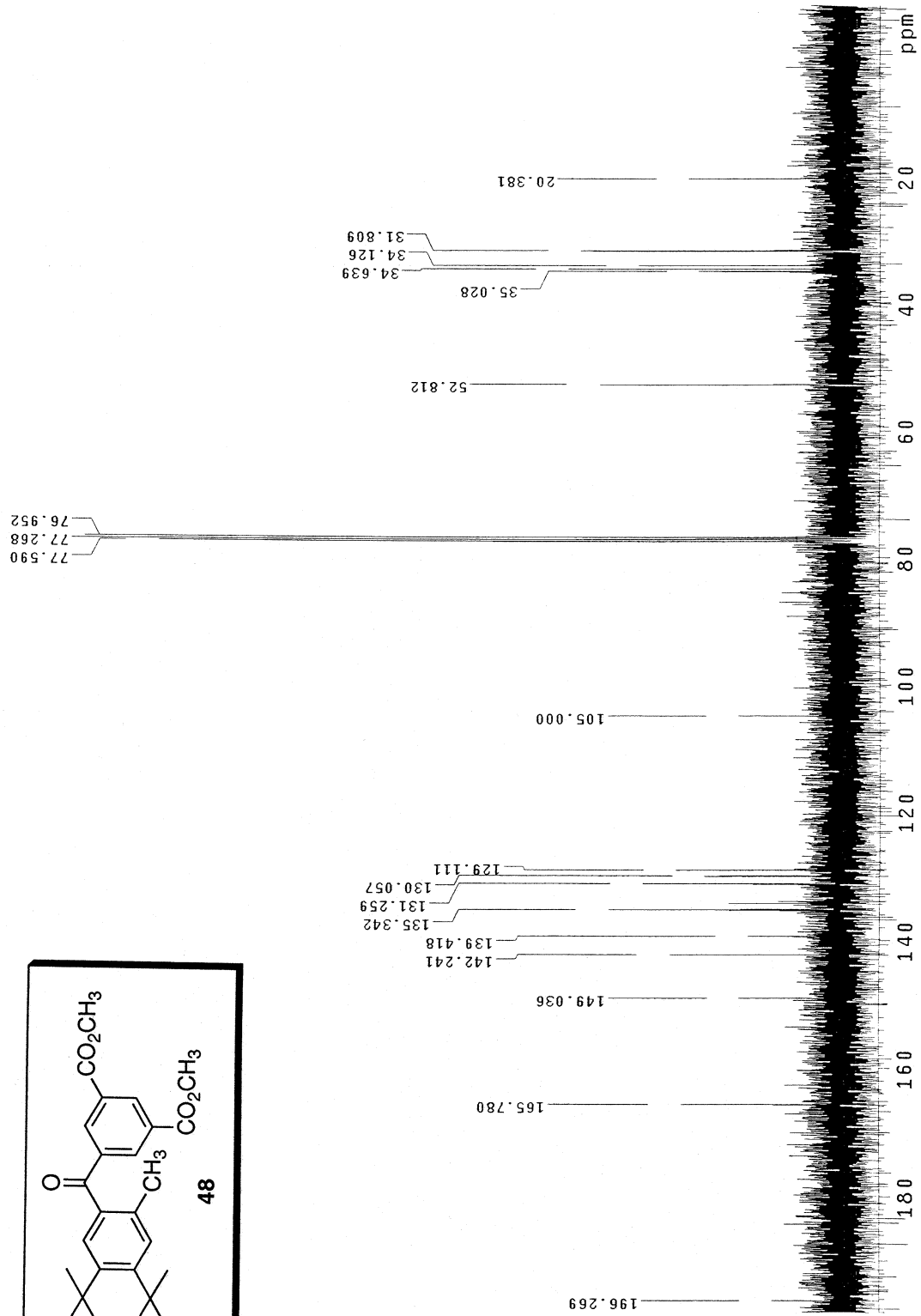
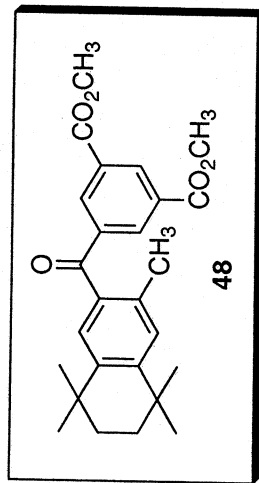
Pulse Sequence: s2pu1



cwI-087

File : home/inova400/NMR\_User\_Data/wagner/cwI\_087C\_20july07.fid  
Sample id : tmpstudy

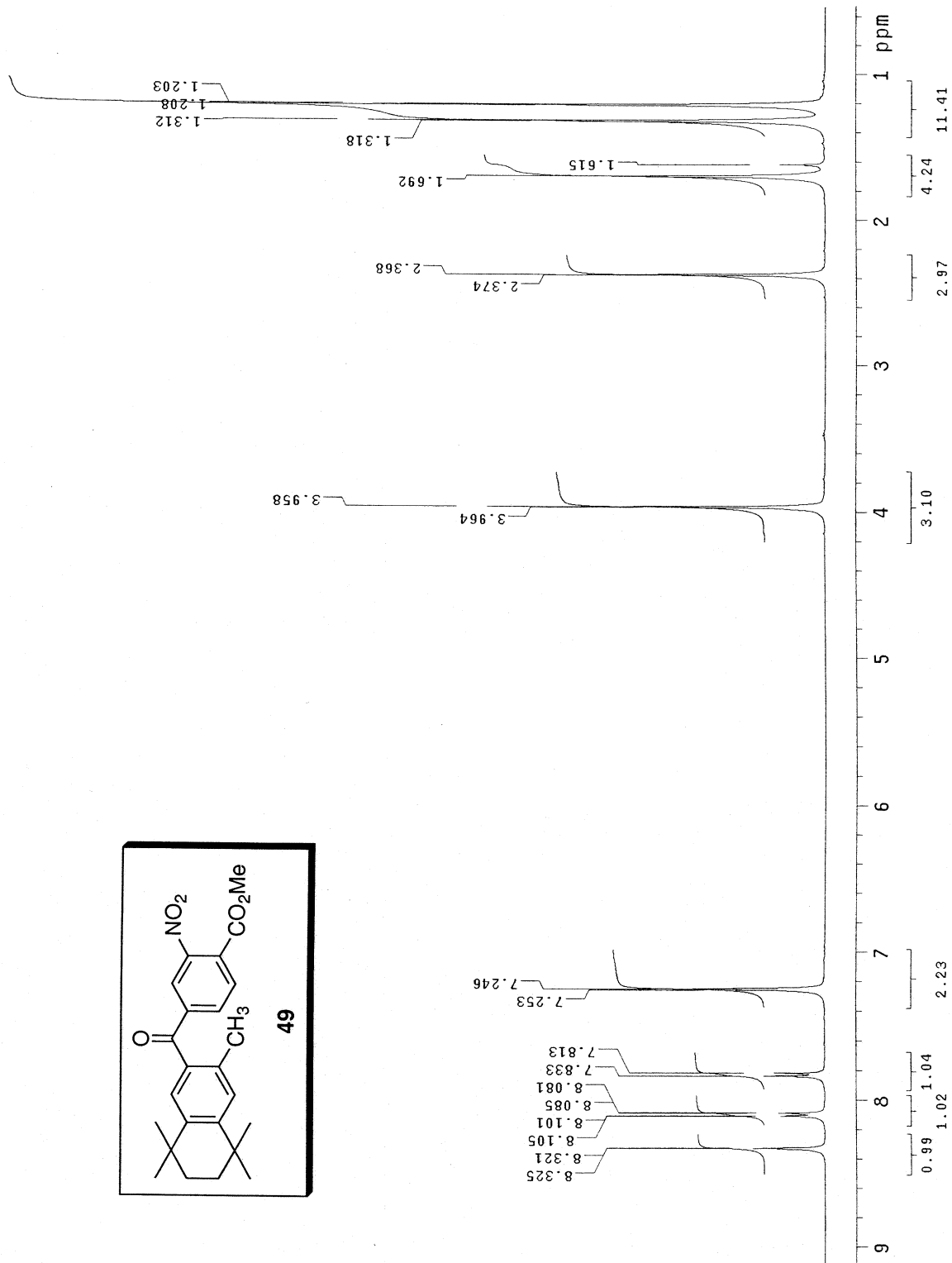
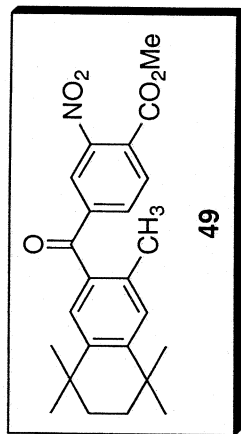
Pulse Sequence: s2pu1



cwI-067

File : home/invova400/NMR\_User\_Data/wagner/cwI\_067H\_20july07.fid  
Sample id : tmpstudy

Pulse Sequence: s2pu1

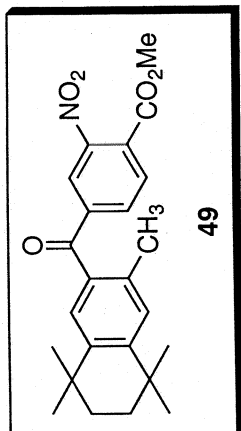


cwI-067

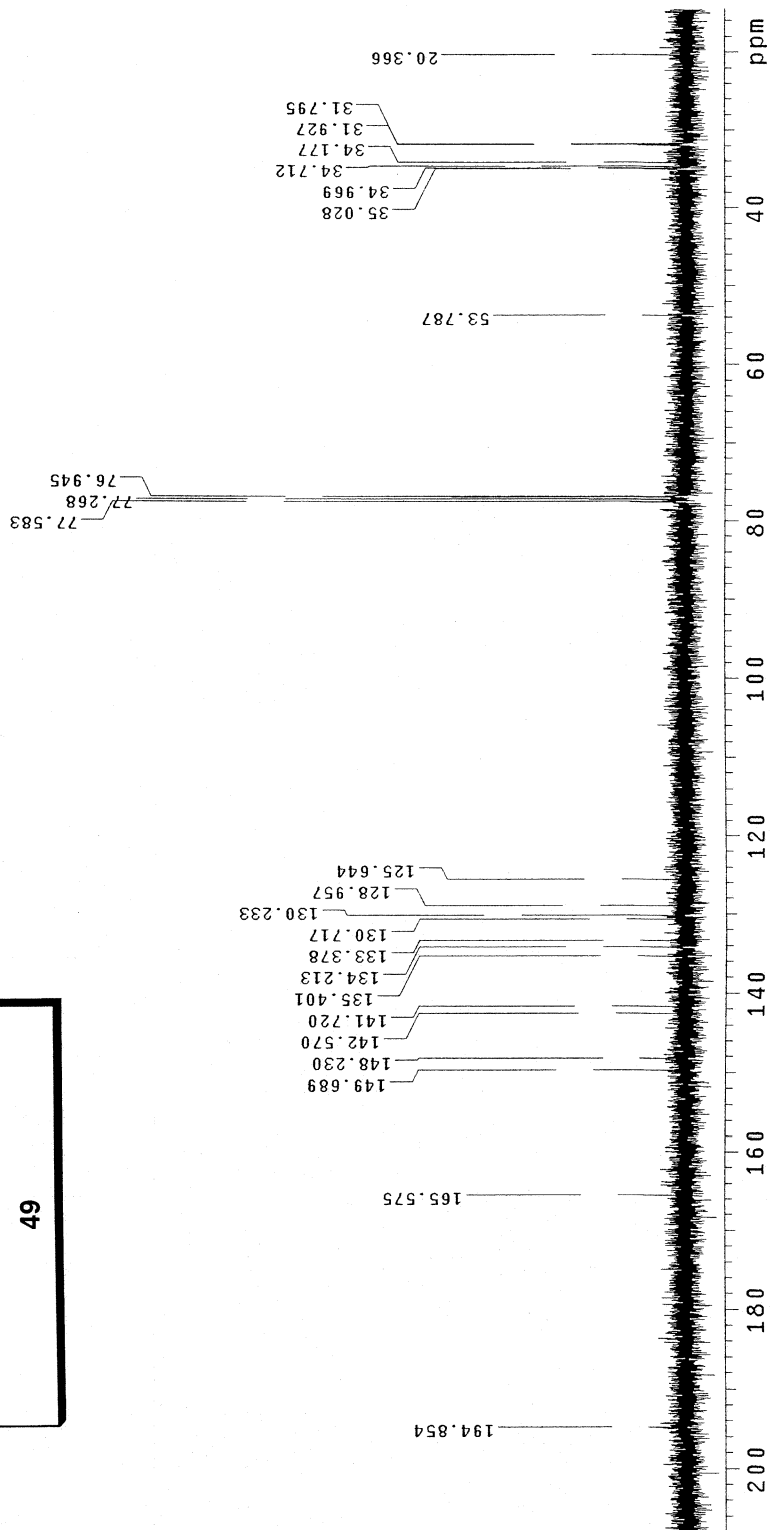
File : home/innov400/NMR\_User\_Data/wagner/cwI\_067C\_20july07.fid

Sample id : tmpstudy

Pulse Sequence: s2pu1



S56



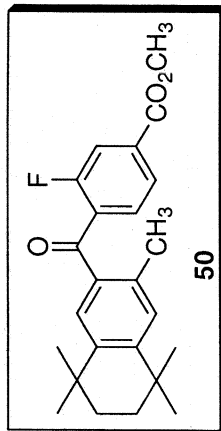


CWII-055 3 1 C:\Bruker\TOPSPIN wagner

CWII-055

<sup>1</sup>H

7.9191  
7.8992  
7.8110  
7.7856  
7.6245  
7.6060  
7.5877  
7.3199  
7.2600  
7.2047



3.9647  
2.5079  
1.6664  
1.2997  
1.1415

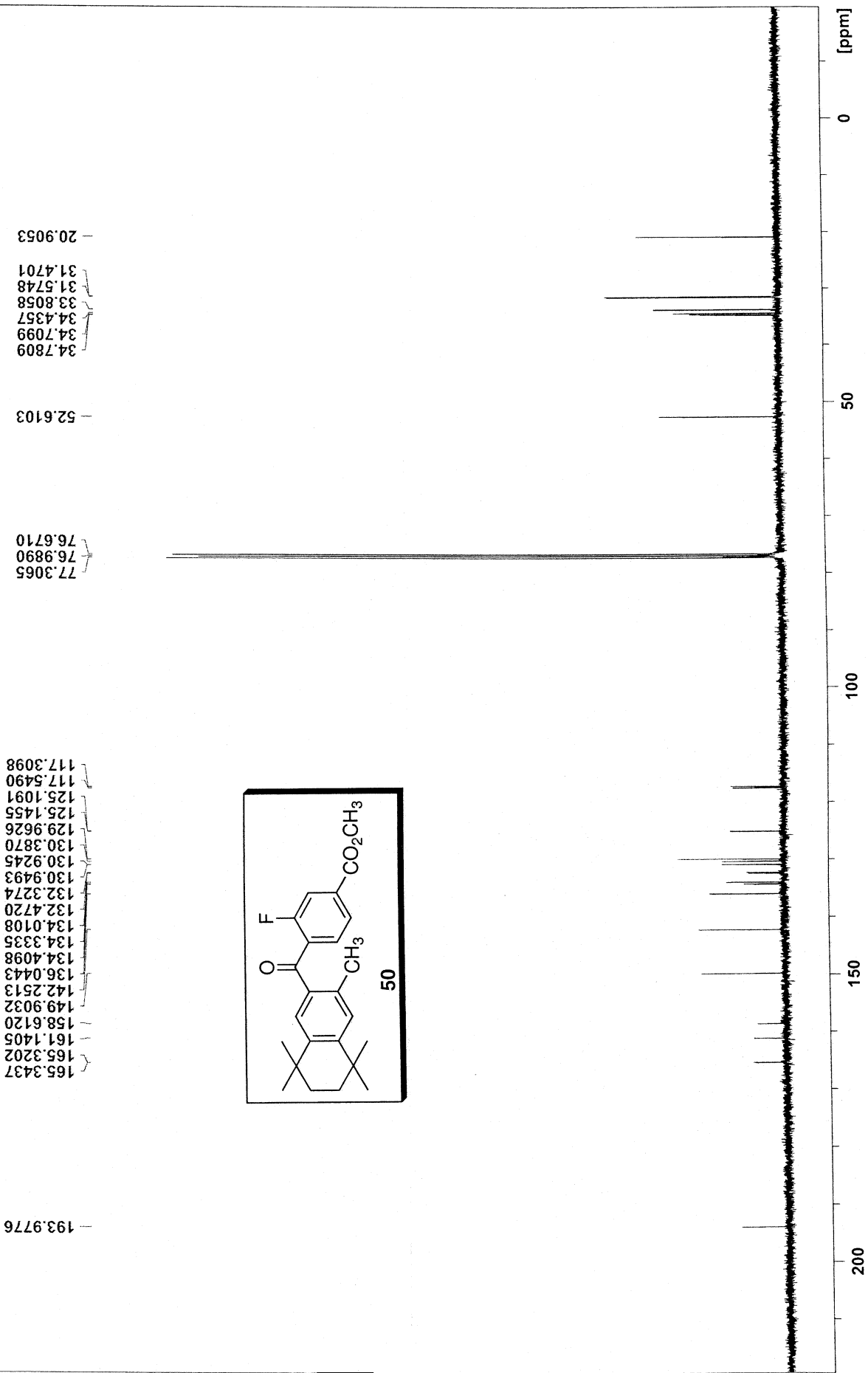
0.9999  
0.9737  
0.9391  
0.9372  
0.9411

2.9482  
2.8571  
4.0998  
5.9585  
5.8520



CWII-055 2 1 C:\Bruker\TOPSPIN wagner

CWII-055  
C13



CWII-053 1 1 C:\Bruker\TOPSPIN wagner

CWII-053

<sup>1</sup>H

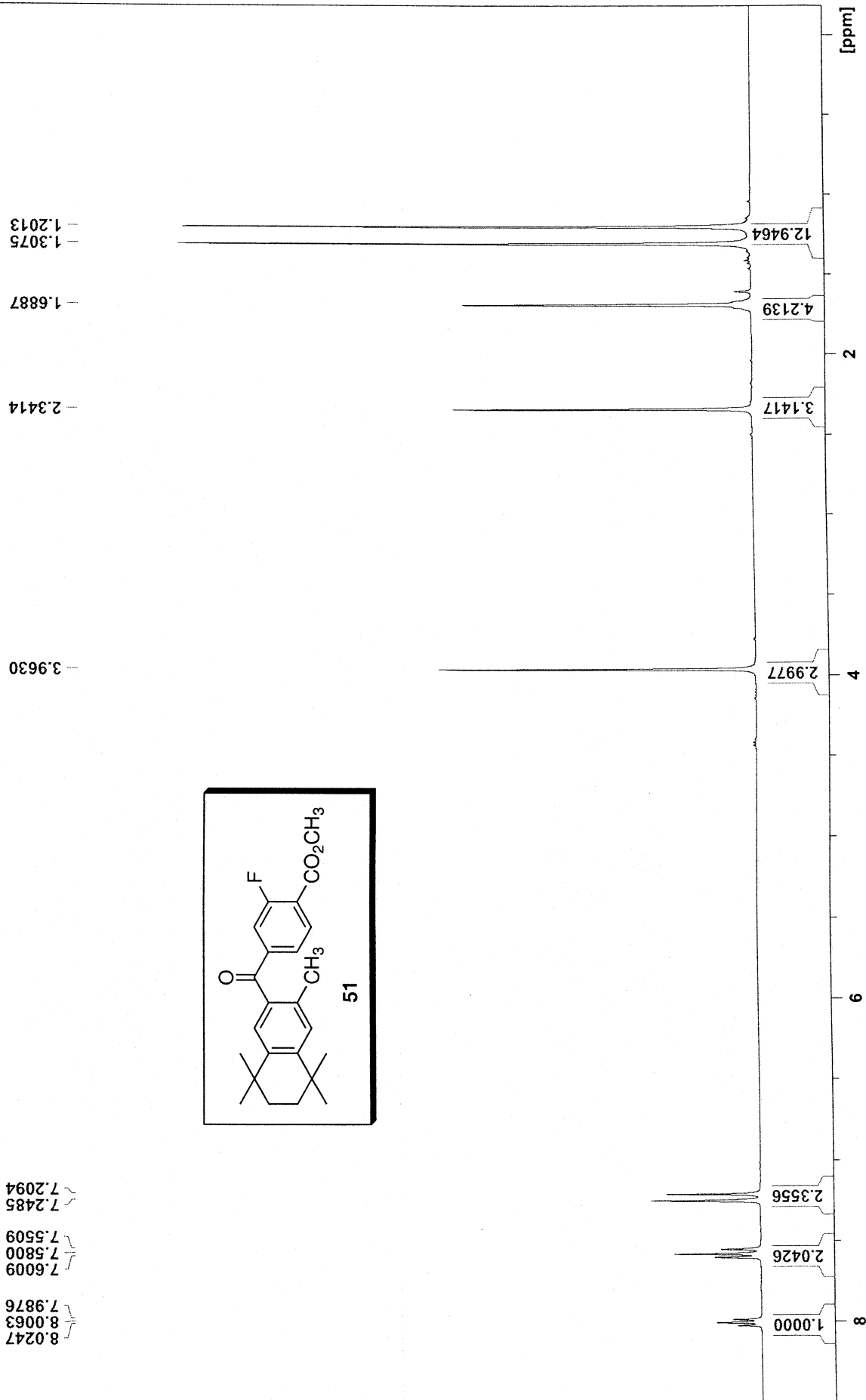
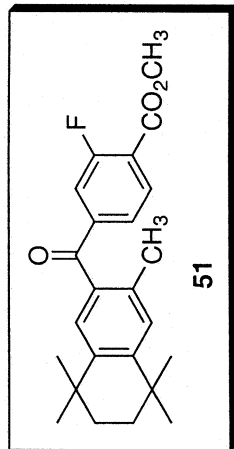
8.0247  
8.0063  
7.9876  
7.6009  
7.5800  
7.5509  
7.2485  
7.2094

3.9630

2.3414

1.6887

1.3075  
1.2013



CWII-053 2 1 C:\Bruker\TOPSPIN wagner

CWII-053

Cl3

196.0975

164.3066  
162.8174  
160.2148

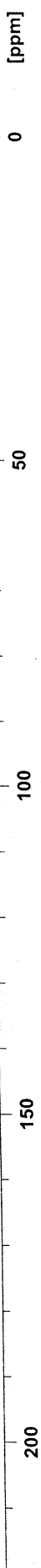
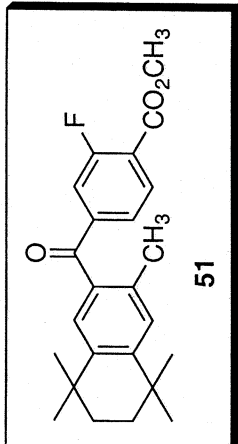
148.7664  
143.8833  
143.8123  
142.0273  
134.7124  
134.0125  
132.0975  
129.5912  
128.4601  
125.2466  
125.2075  
121.9348  
121.8281  
118.3880  
118.1510

77.3040  
76.9858  
76.6682

52.6235

34.8284  
34.7753  
34.3708  
33.8723  
31.6536  
31.5579

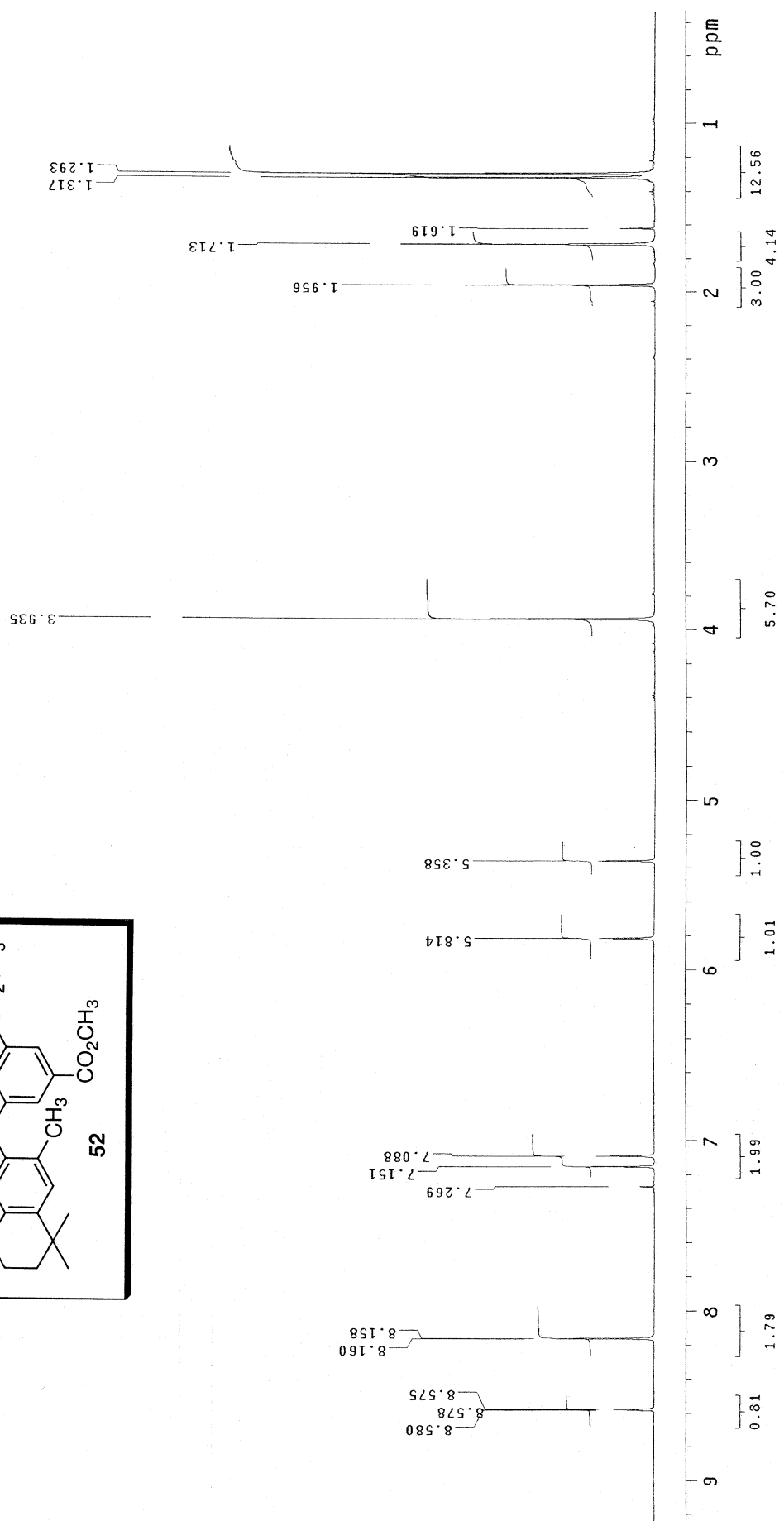
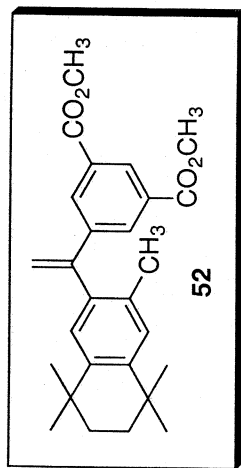
20.0094



CW-139

File : home/inova400/NMR\_User\_Data/wagner/CW\_139H.fid  
Sample id : tmpstudy

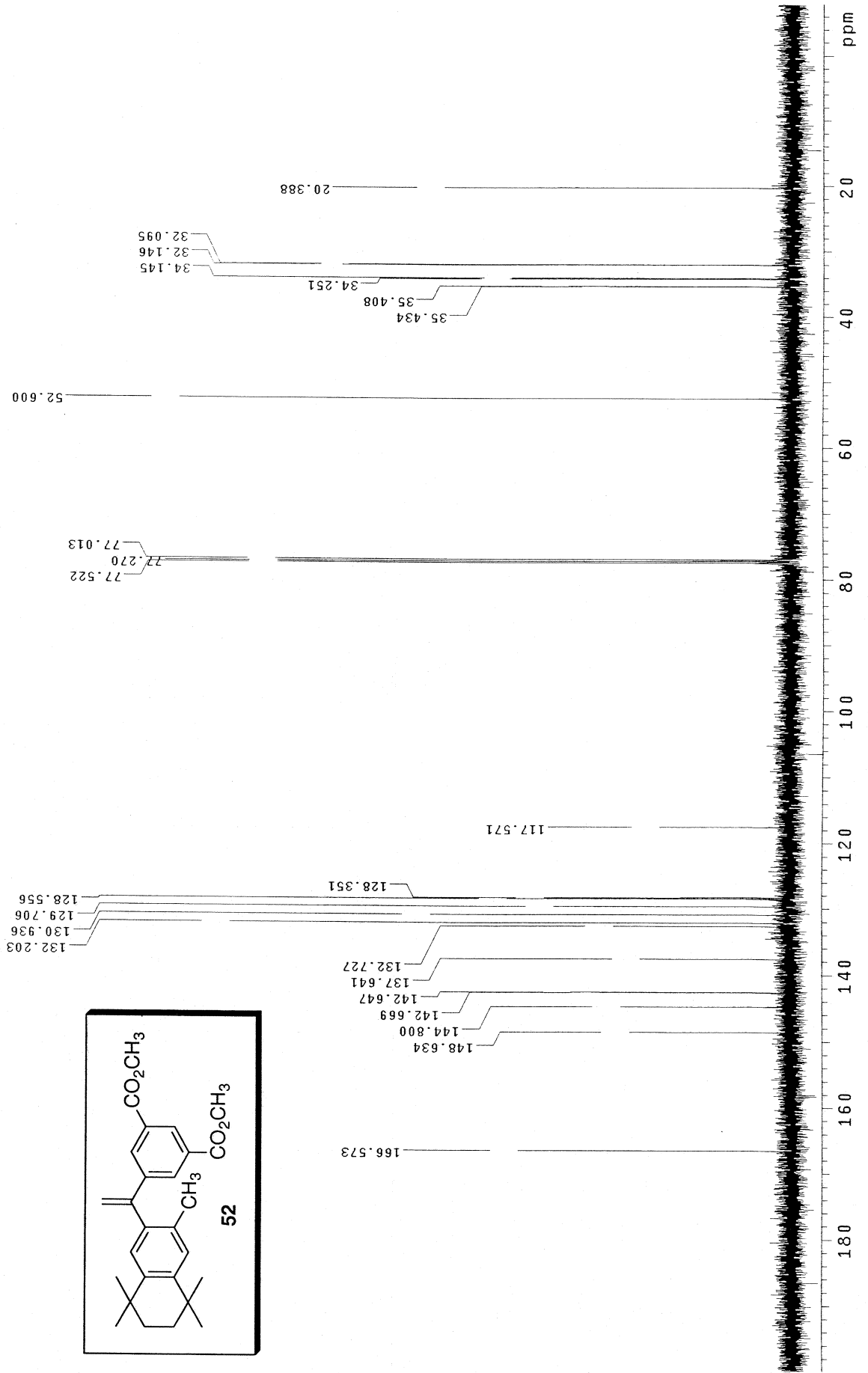
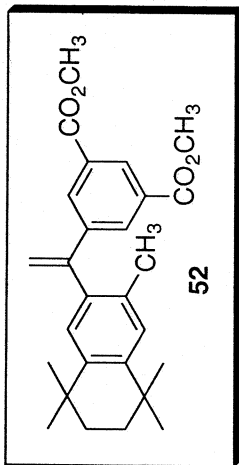
Pulse Sequence: s2pu1



cwi-139

File : home/inova400/NMR\_User\_Data/wagner/CW\_139C.fid  
Sample id : tmpstudy

Pulse Sequence: s2pu1

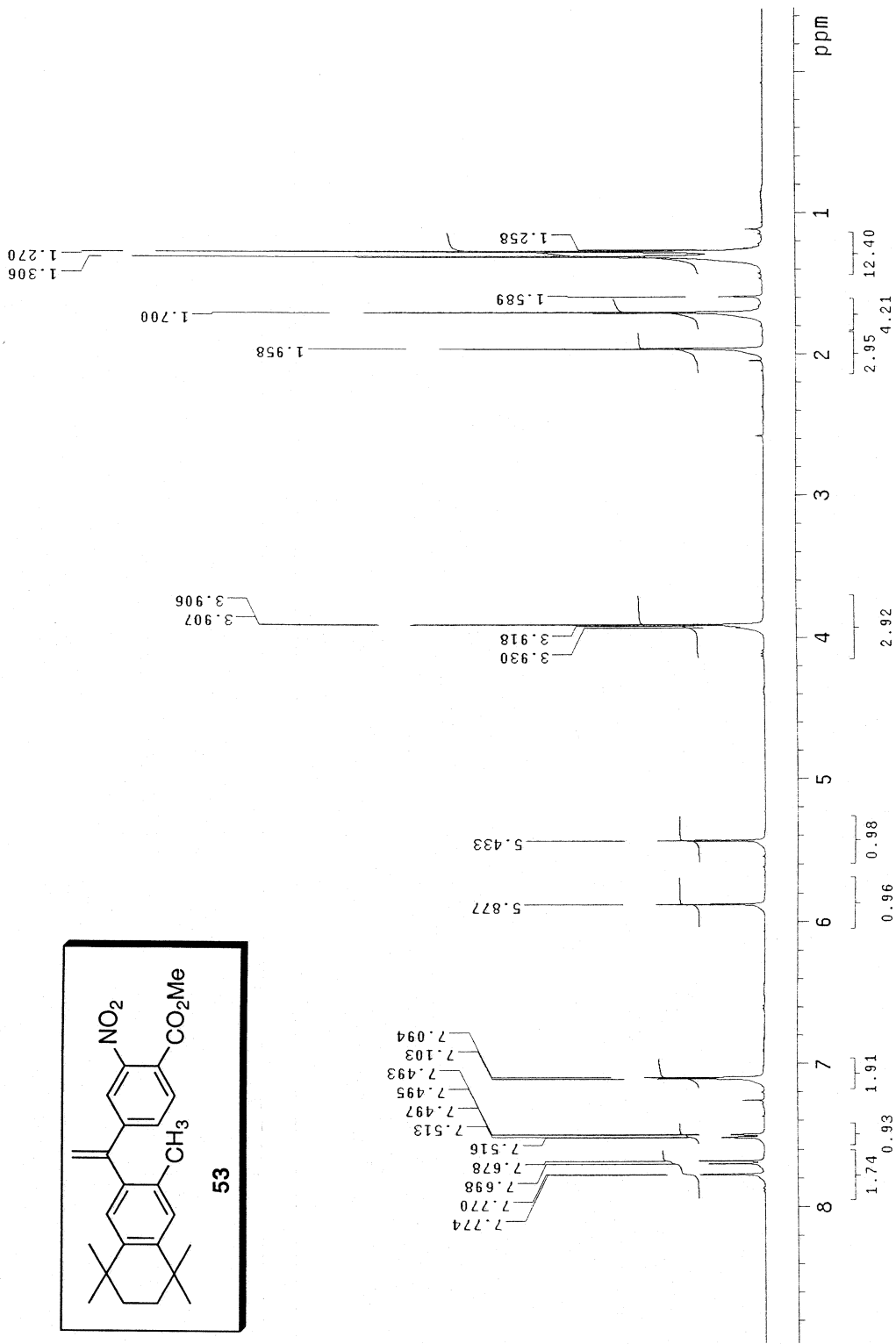
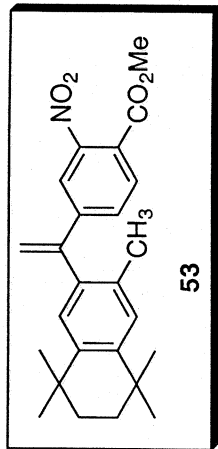


S62

cwI-113

File : home/inoval400/NMR\_User\_Data/wagner/cwI\_113H\_6august07.fid  
Sample id : tmpstudy

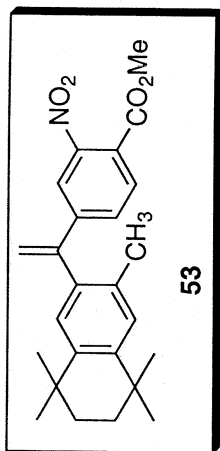
Pulse Sequence: s2pu1



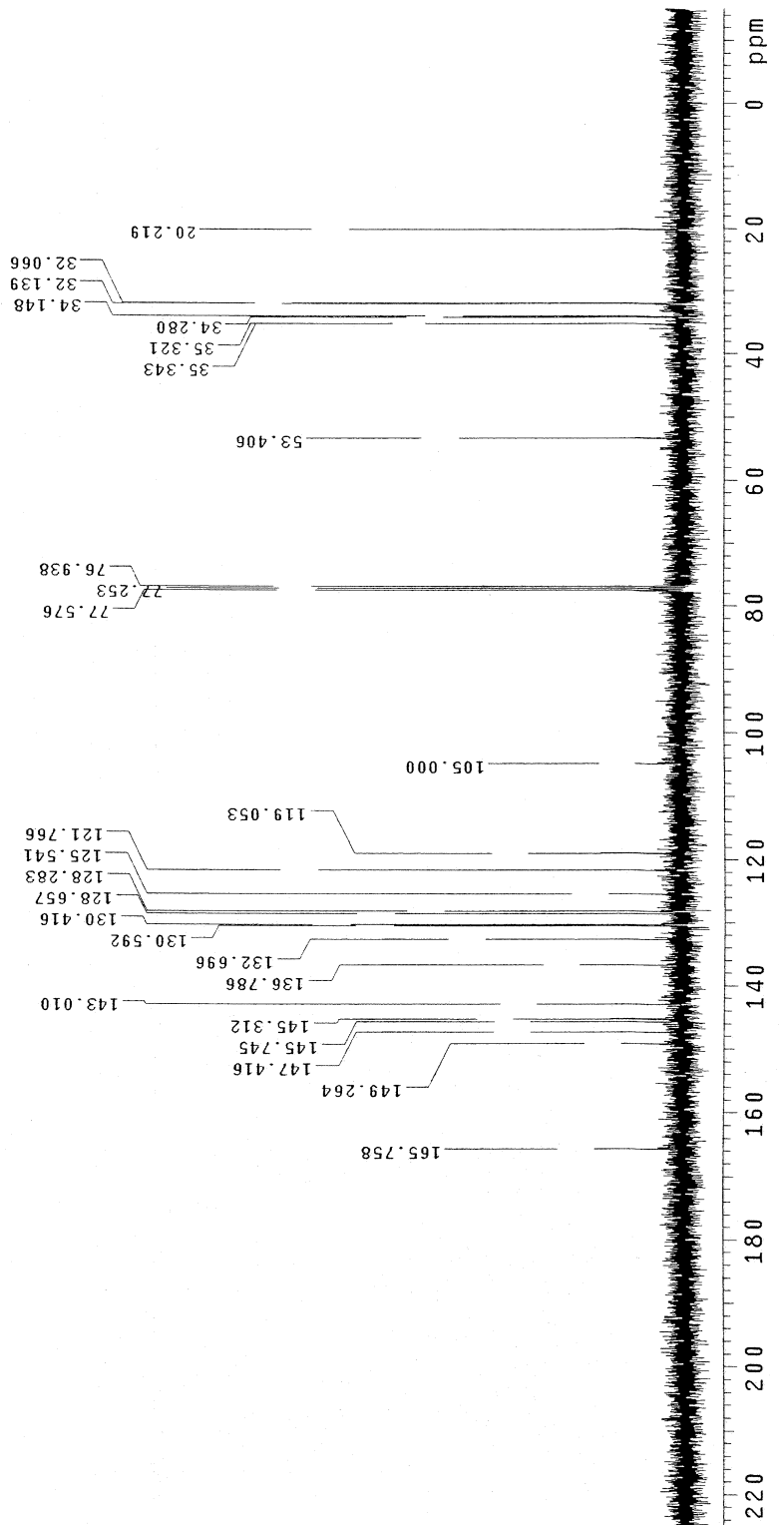
cwI-113

File : home/inova400/NMR\_User\_Data/wagner/cwI\_113C\_6august07.fid  
Sample id : tmpstudy

Pulse Sequence: s2pu1



S64





CWII-059 1 1 C:\Bruker\TOPSPIN wagner

CWII-059  
1H

7.7409  
7.7138  
7.6944  
7.2600  
7.1459  
7.1101  
7.0903  
7.0704  
7.0536

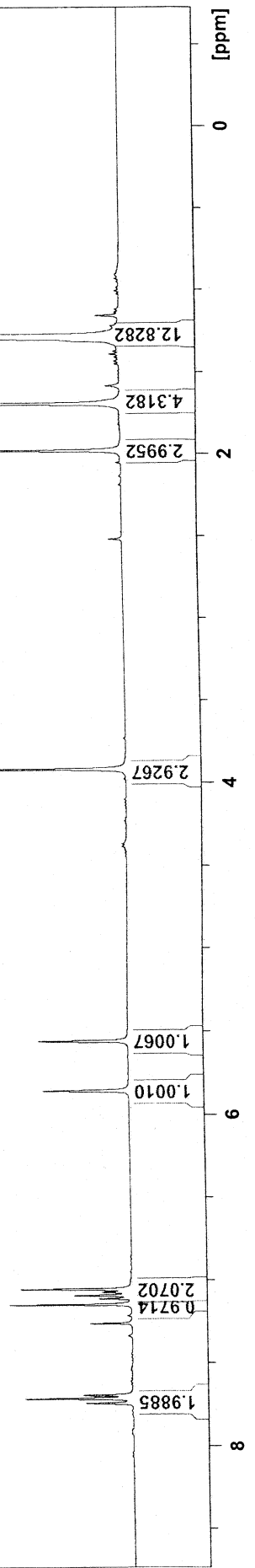
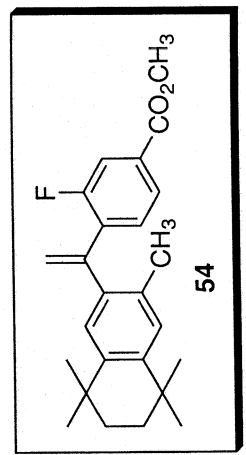
5.8551  
5.5570

3.9165

1.9776

1.6940

1.2941  
1.2756



CWII-059 2 1 C:\Bruker\TOPSPIN wagner

CWII-059

C13

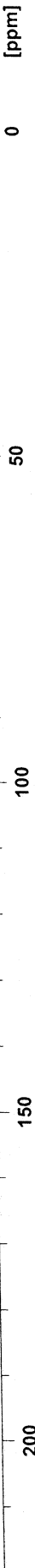
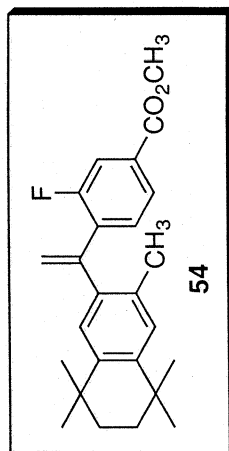
165.9000  
165.8744  
161.0434  
158.5498  
144.3661  
143.4969  
142.3369  
138.3183  
133.8239  
133.7022  
132.3348  
130.6126  
130.5802  
130.5177  
130.4378  
128.0565  
127.8020  
124.9737  
124.9398  
121.3639  
121.2909  
117.2652  
117.0138

77.3156  
76.9984  
76.6800

52.2925

35.1559  
35.1412  
33.9558  
33.8656  
31.8894  
31.8350

19.7565



CWII-057 1 1 C:\Bruker\TOPSPIN wagner

CWII-057

1H

7.8870  
7.8671  
7.8474  
7.2600  
7.1524  
7.1319  
7.1056  
7.0906  
7.0347  
7.0038

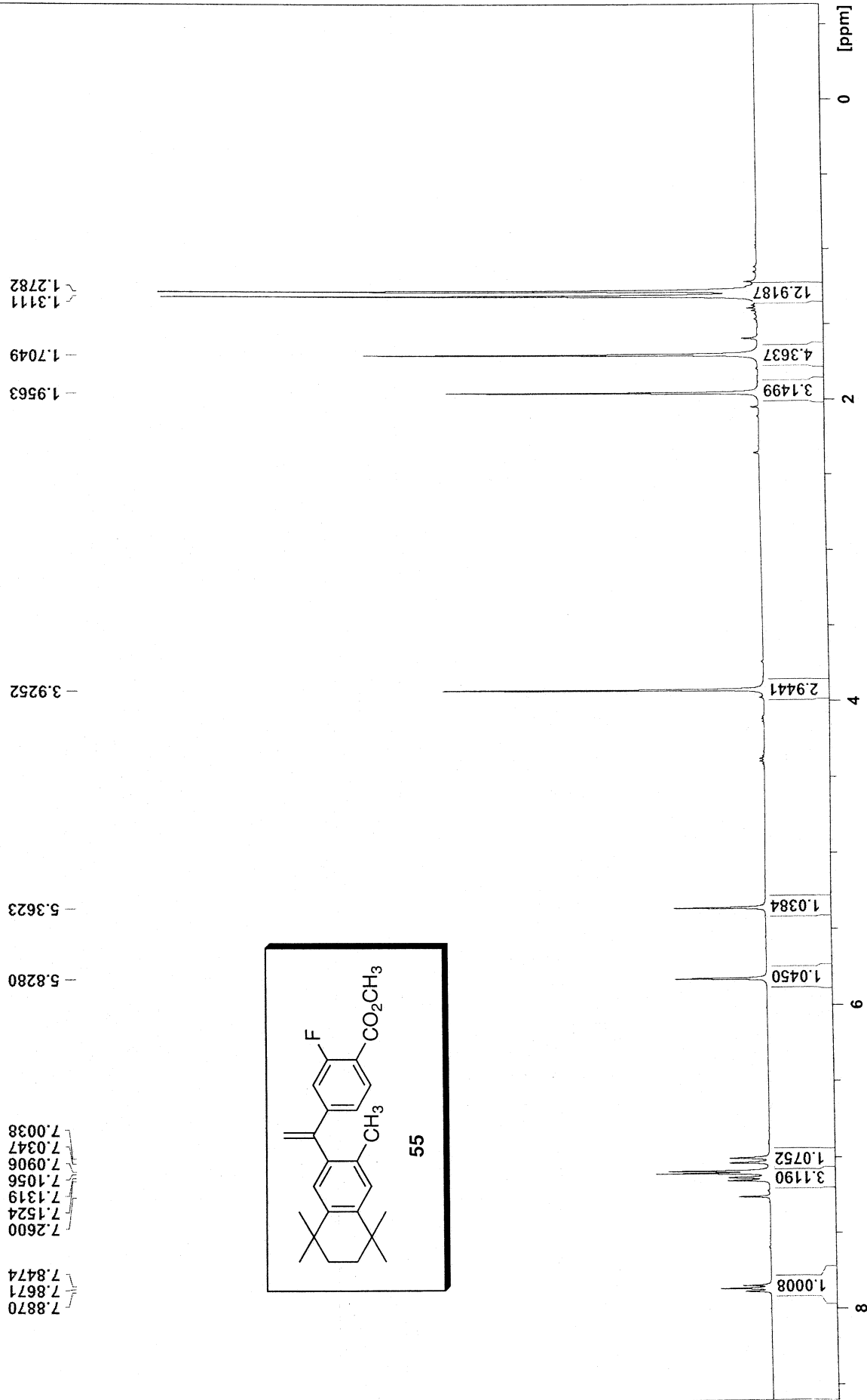
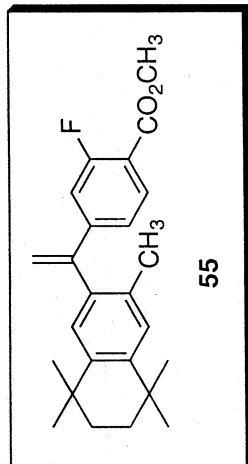
5.8280  
5.3623

3.9252

1.9563

1.7049

1.3111  
1.2782



CWII-057 2 1 C:\Bruker\TOPSPIN wagner

CWII-057

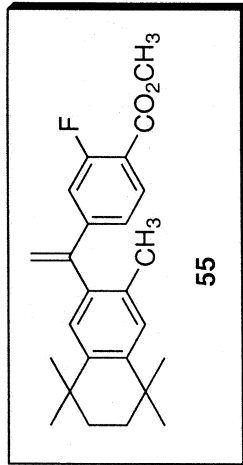
C13

164.8012  
164.7615  
163.3093  
160.7321  
148.1082  
147.8754  
147.7905  
144.6372  
142.4587  
137.2910  
132.6184  
132.0483  
128.1417  
128.0127  
122.0391  
122.0047  
117.7428  
117.1082  
117.0063  
115.0090  
114.7764

77.3206  
77.0025  
76.6852

52.2402

35.1449  
35.1244  
33.9959  
33.8763  
31.9015  
31.8496  
19.8547



[ppm] 0 50 100 150 200