

# **Synthesis and characterization of bis-cyclopropanated 1,3,5-tricarbonyl compounds. A combined synthetic, spectroscopic and theoretical study**

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## **Supporting Information**

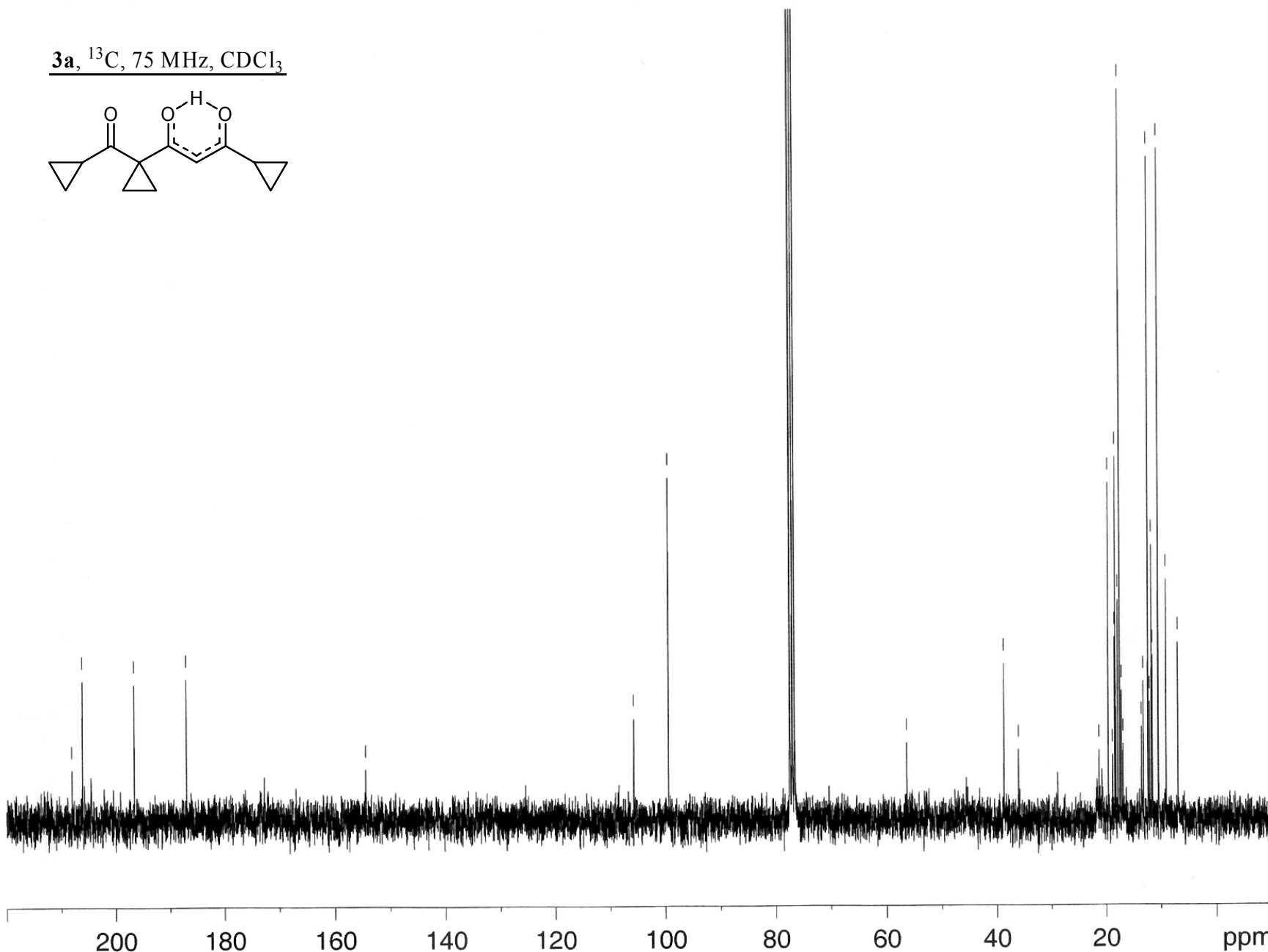
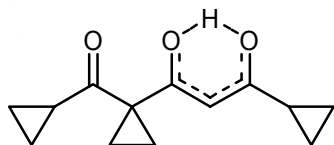
**Content:** Copies of NMR spectra



h1h1h1  
Aul3C CDC13 /opt/topspin 0702 20

208.08  
206.14  
196.61  
187.02  
154.48  
105.73  
99.44  
56.35  
38.66  
35.99  
21.27  
19.58  
18.80  
18.39  
18.27  
18.21  
17.82  
17.47  
17.16  
16.87  
13.55  
13.20  
12.32  
12.05  
11.69

**3a**,  $^{13}\text{C}$ , 75 MHz,  $\text{CDCl}_3$



Current Data Parameters  
NAME 070207.320  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20070208  
Time 10.02  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 297.4 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



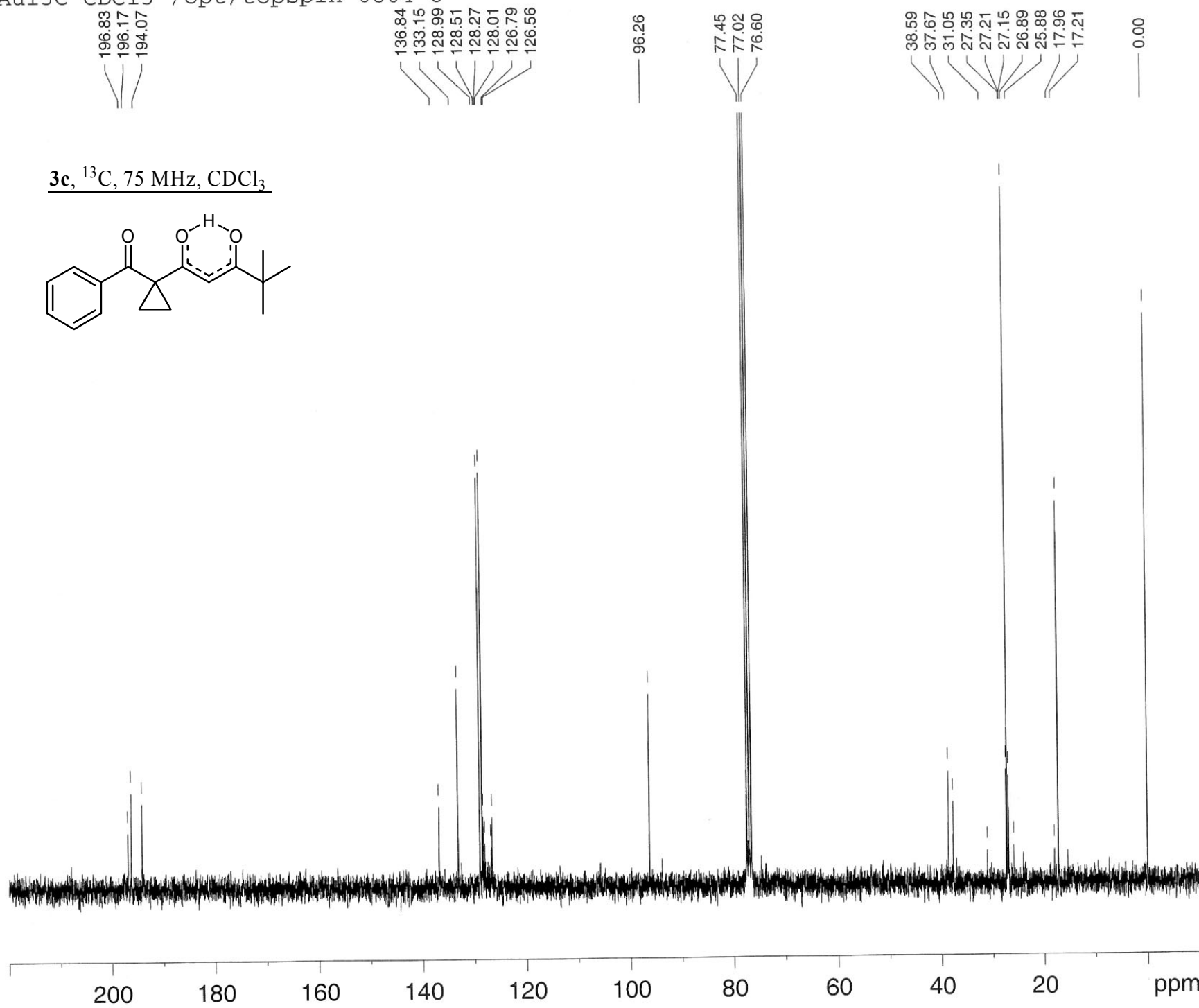
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EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080501  
Time 9.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
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TE 295.3 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

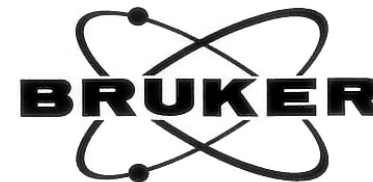
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NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677515 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



200 180 160 140 120 100 80 60 40 20 ppm



Current Data Parameters  
NAME 070810.307  
EXPNO 11  
PROCNO 1

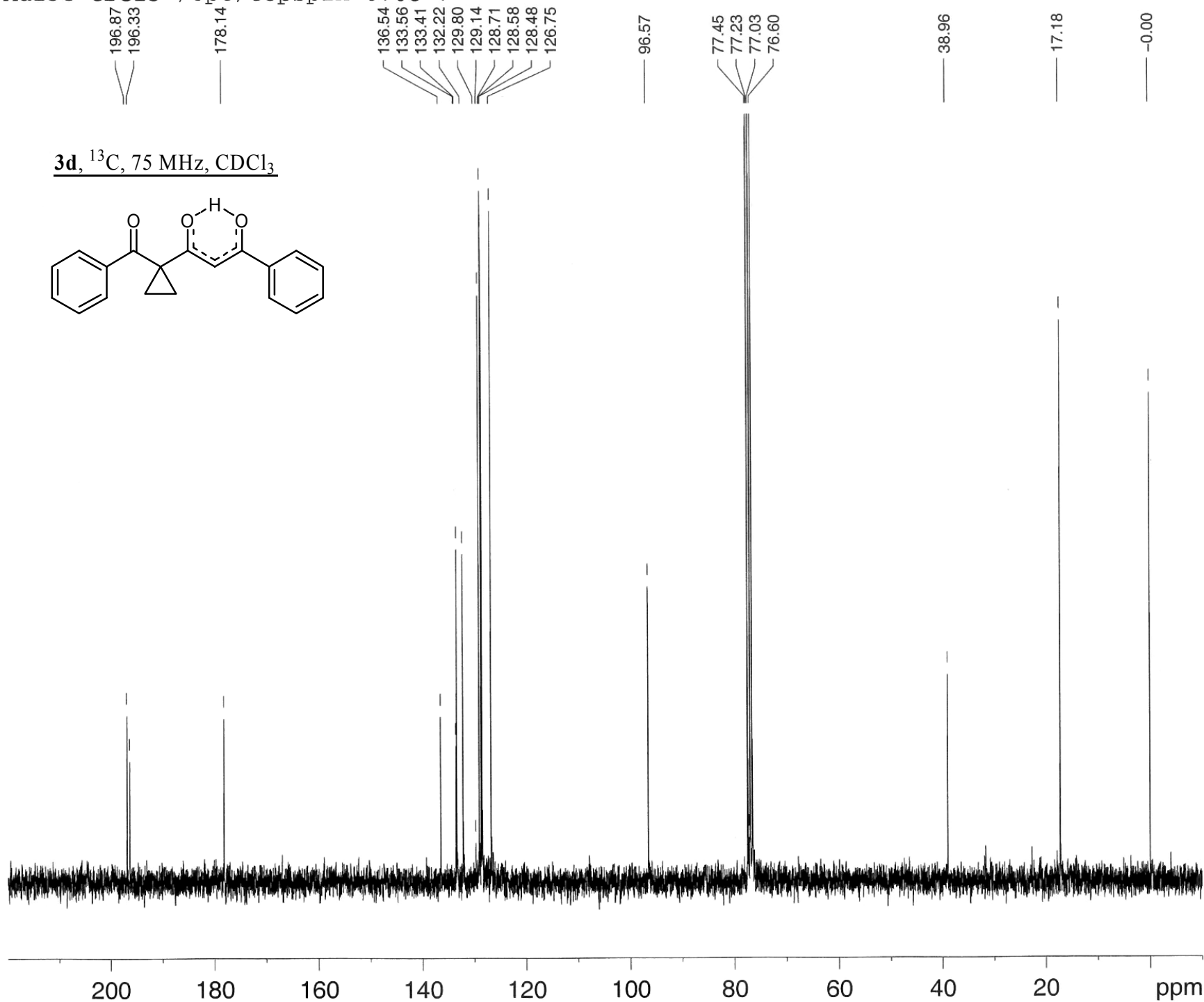
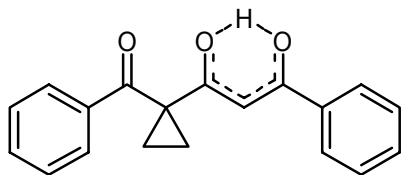
F2 - Acquisition Parameters  
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Time 20.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.6 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

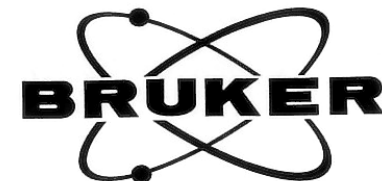
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677520 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3d, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>





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EXPNO 11  
PROCNO 1

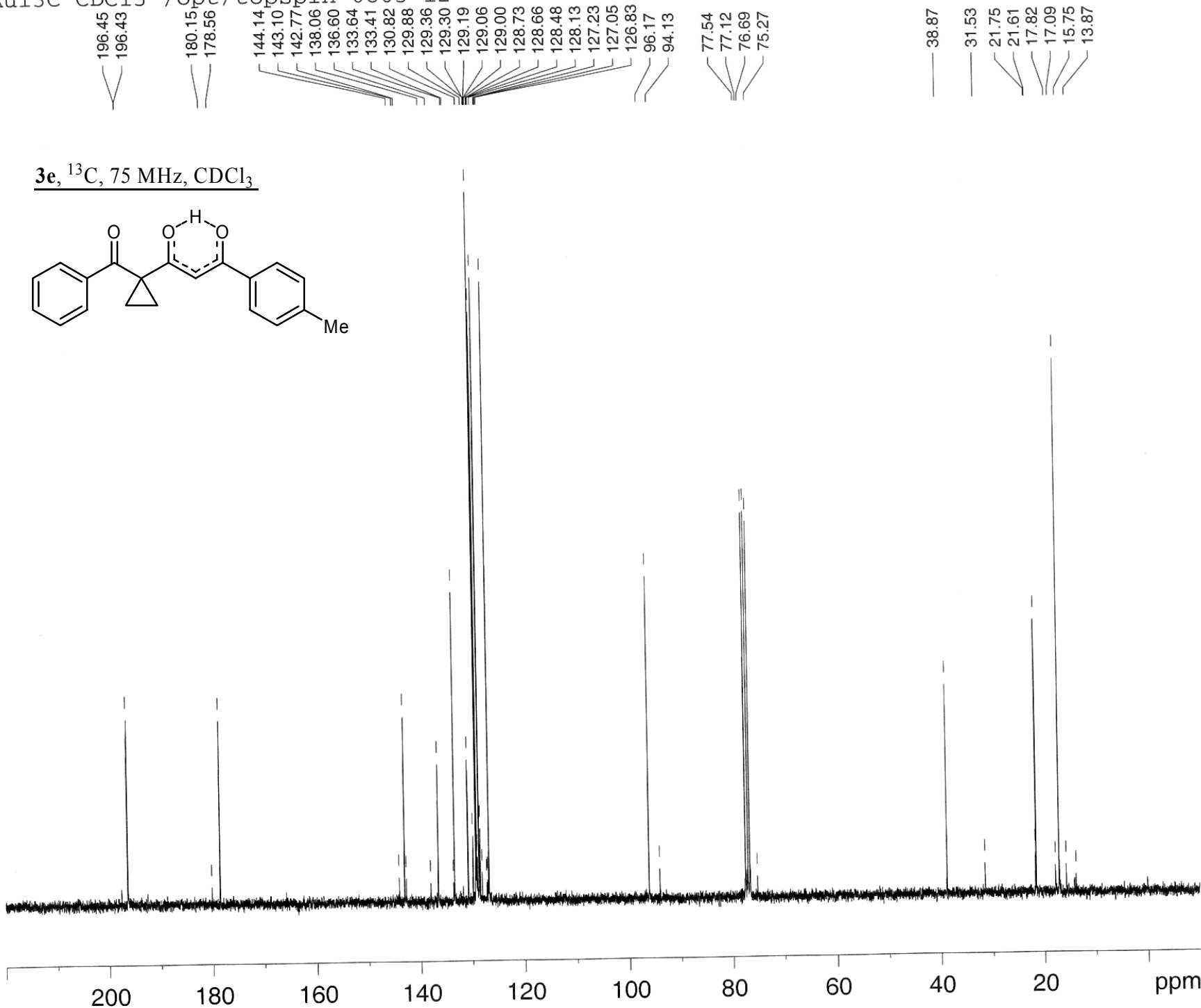
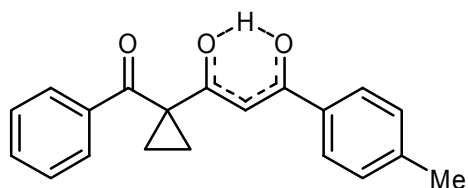
F2 - Acquisition Parameters  
Date\_ 20080526  
Time 17.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

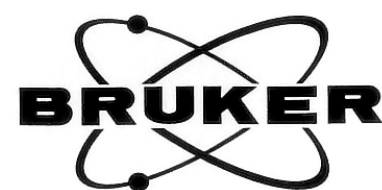
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

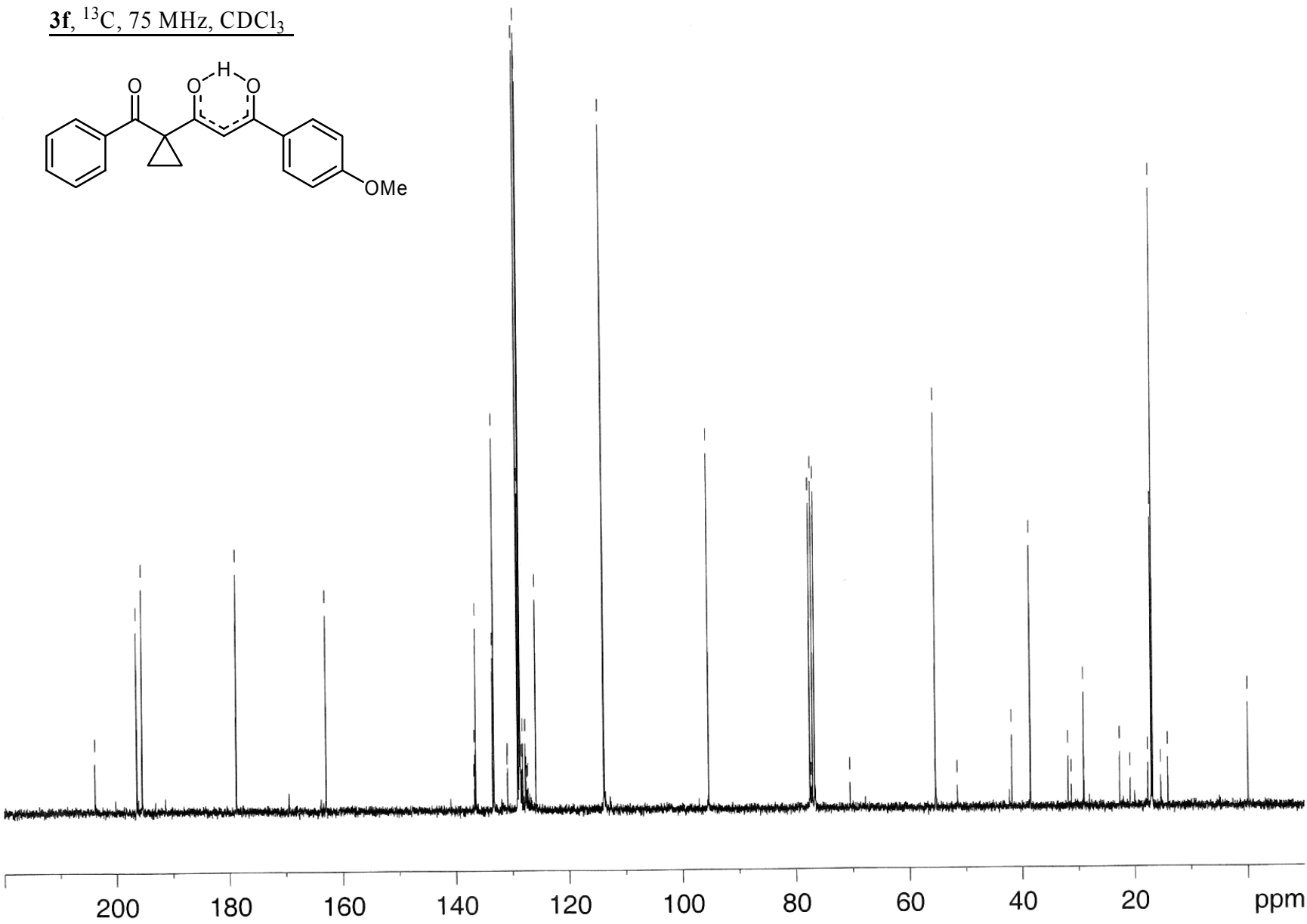
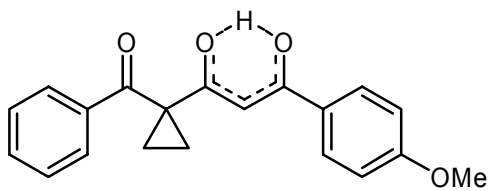
3e, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>





203.82  
196.39  
196.35  
195.43  
178.74  
163.01  
136.82  
136.71  
136.51  
133.50  
133.31  
130.92  
130.87  
129.12  
128.95  
128.90  
128.79  
128.75  
128.64  
128.40  
128.22  
127.74  
127.64  
127.45  
127.29  
125.88  
113.91  
113.81  
95.44  
77.55  
77.32  
77.12  
76.70  
70.46  
55.45  
55.36  
51.57  
41.84  
38.55  
31.86  
31.27  
29.09  
29.00  
22.68  
20.80  
17.65  
17.05  
16.85  
15.37  
14.12  
0.00

**3f**, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>



Current Data Parameters  
NAME 080414.335  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080415  
Time 2.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 295.7 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

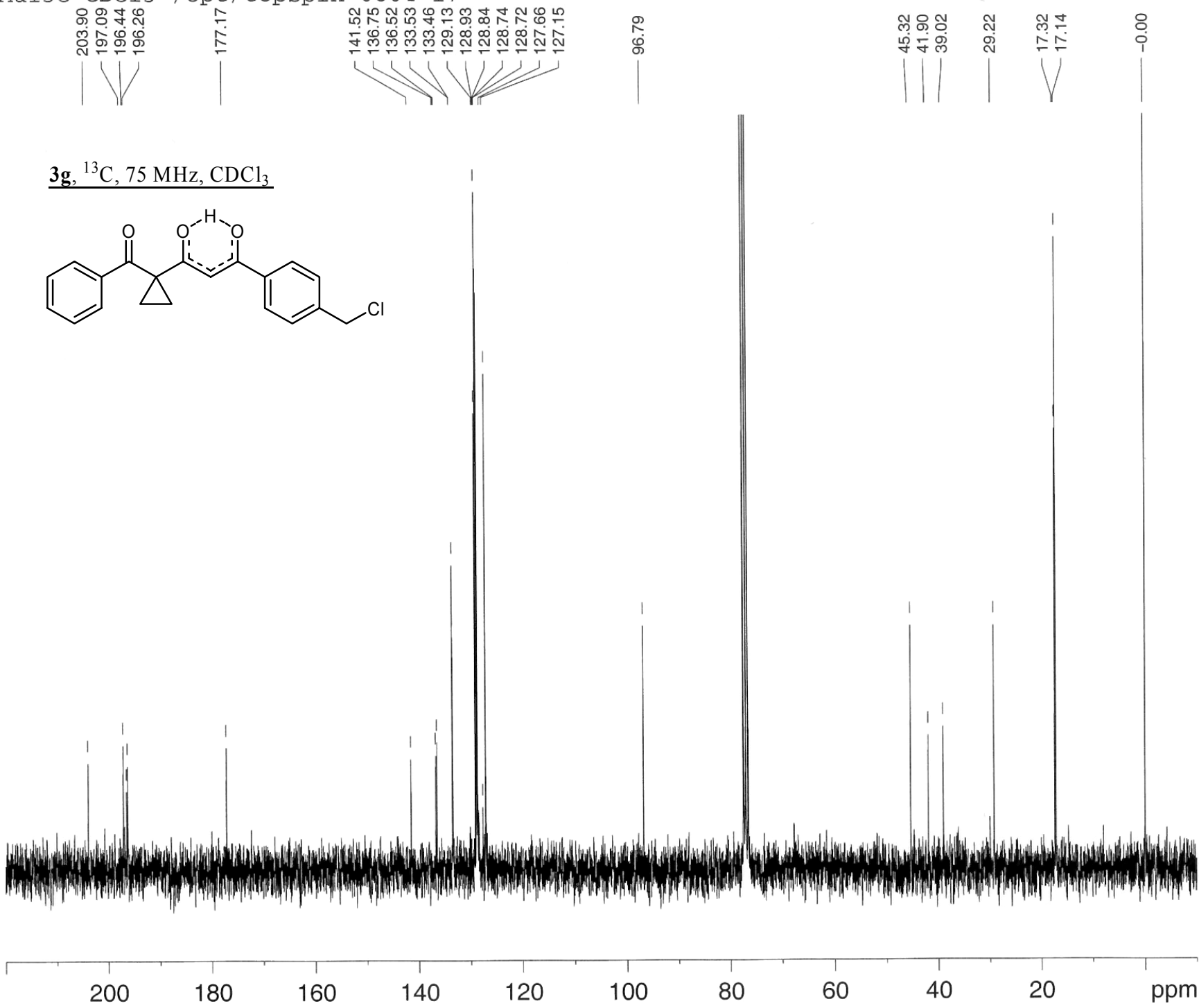
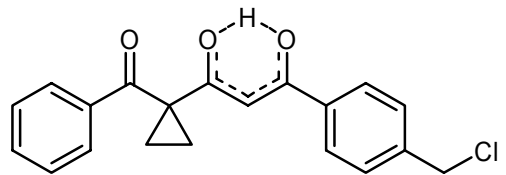
==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677536 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



AUI3C CDC13 /opt/topspin 0804 17

**3g**, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>



Current Data Parameters  
NAME 080428.317  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080428  
Time 19.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.1 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677518 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Current Data Parameters  
NAME 080521.321  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20080521  
Time 21.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.7 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====

NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

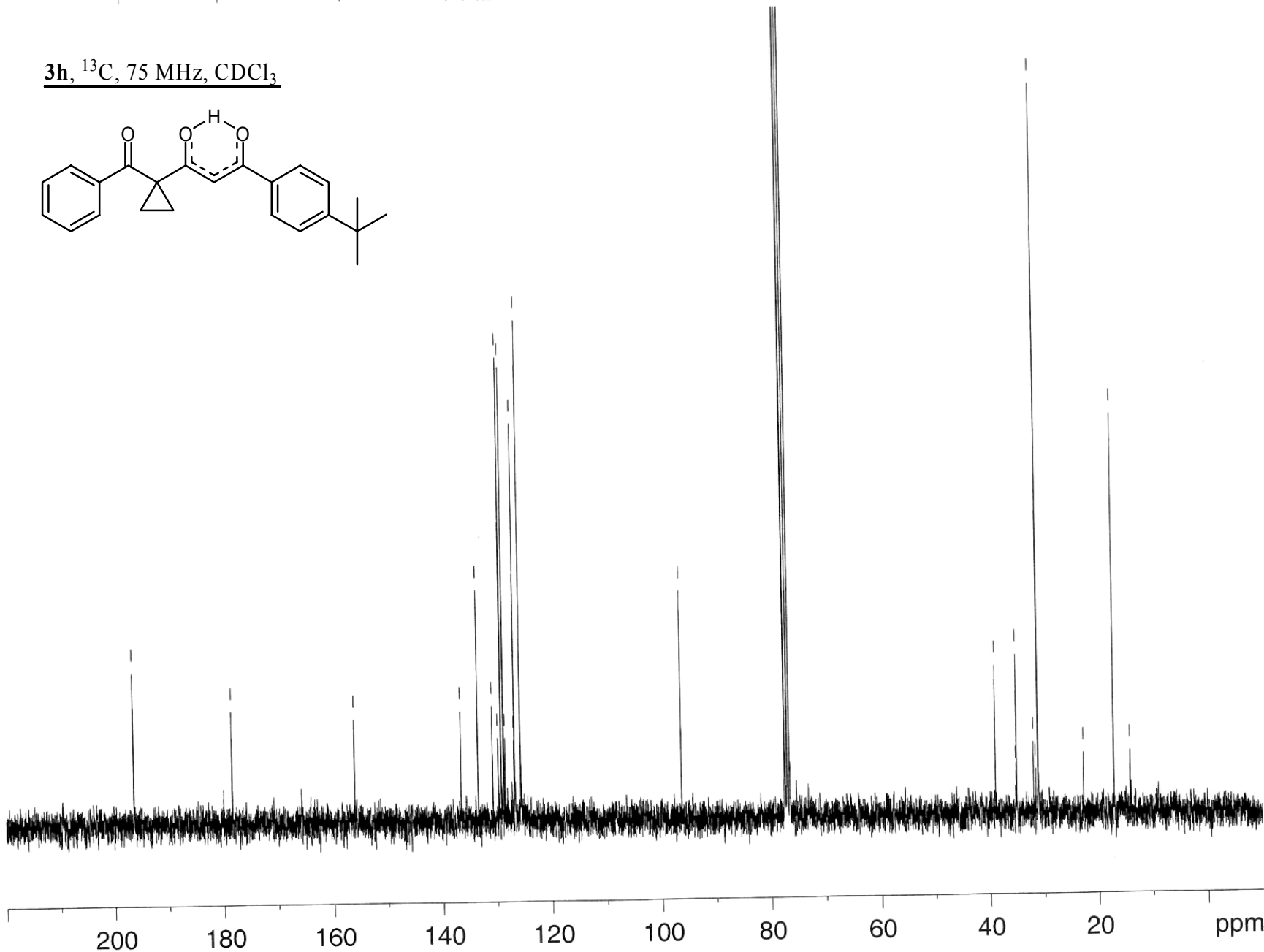
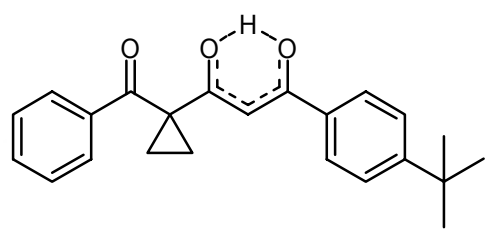
F2 - Processing parameters

SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Au13C CDCl3 /opt/topspin 0805 21

196.48 178.37 156.11 136.58 133.42 130.76 129.76 129.19 128.73 128.47 126.80 126.69 125.61 96.37 77.48 77.06 76.64 38.90 35.17 35.05 31.92 31.56 31.14 31.09 22.74 17.11 14.16

3h, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>







Current Data Parameters  
NAME 081016.318  
EXPNO 11  
PROCNO 1

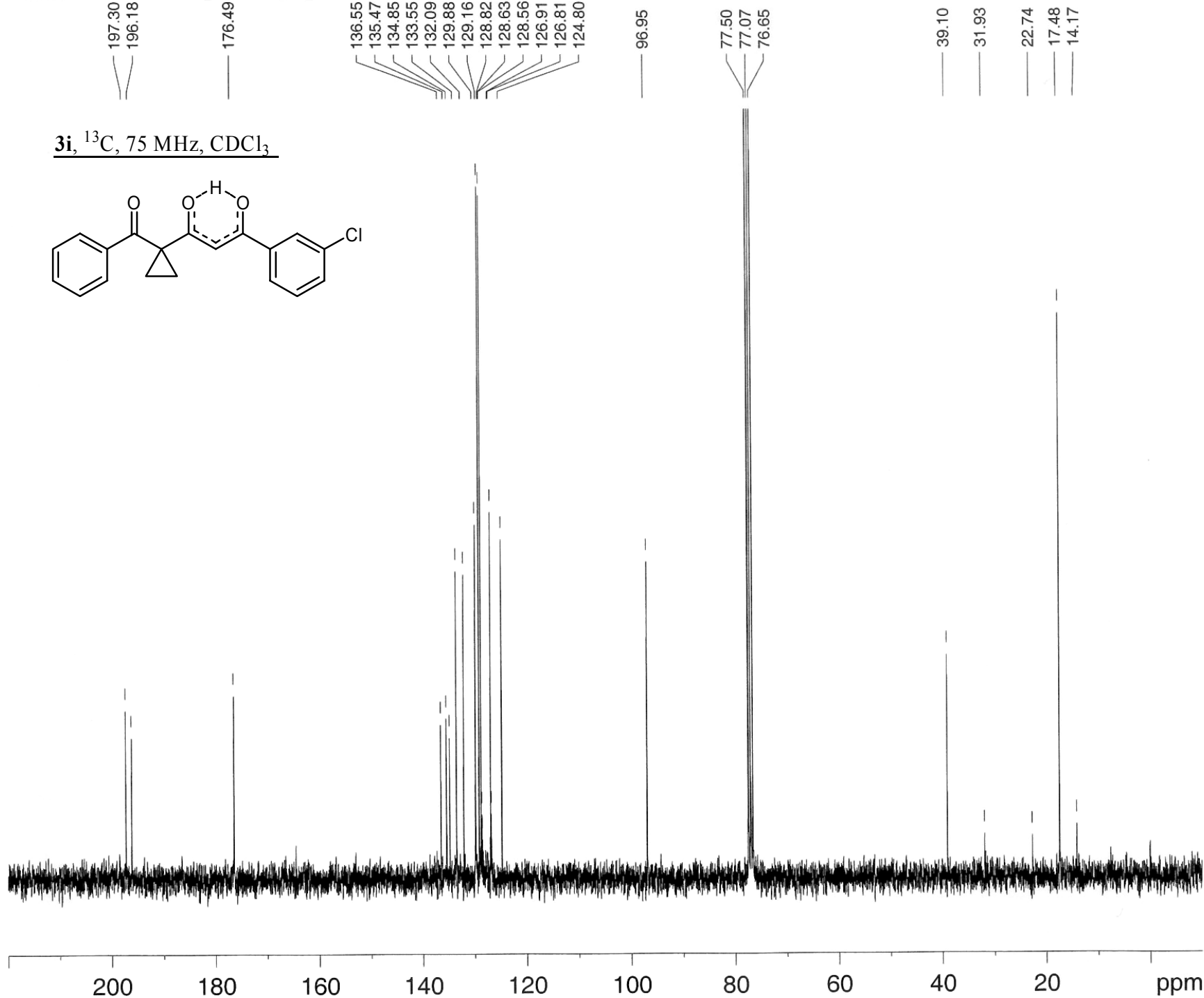
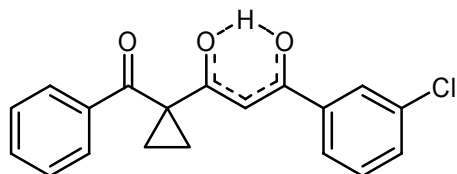
F2 - Acquisition Parameters  
Date\_ 20081016  
Time 20.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 295.2 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

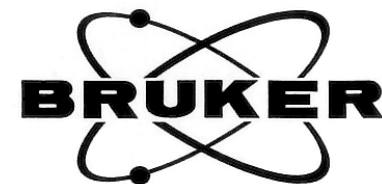
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

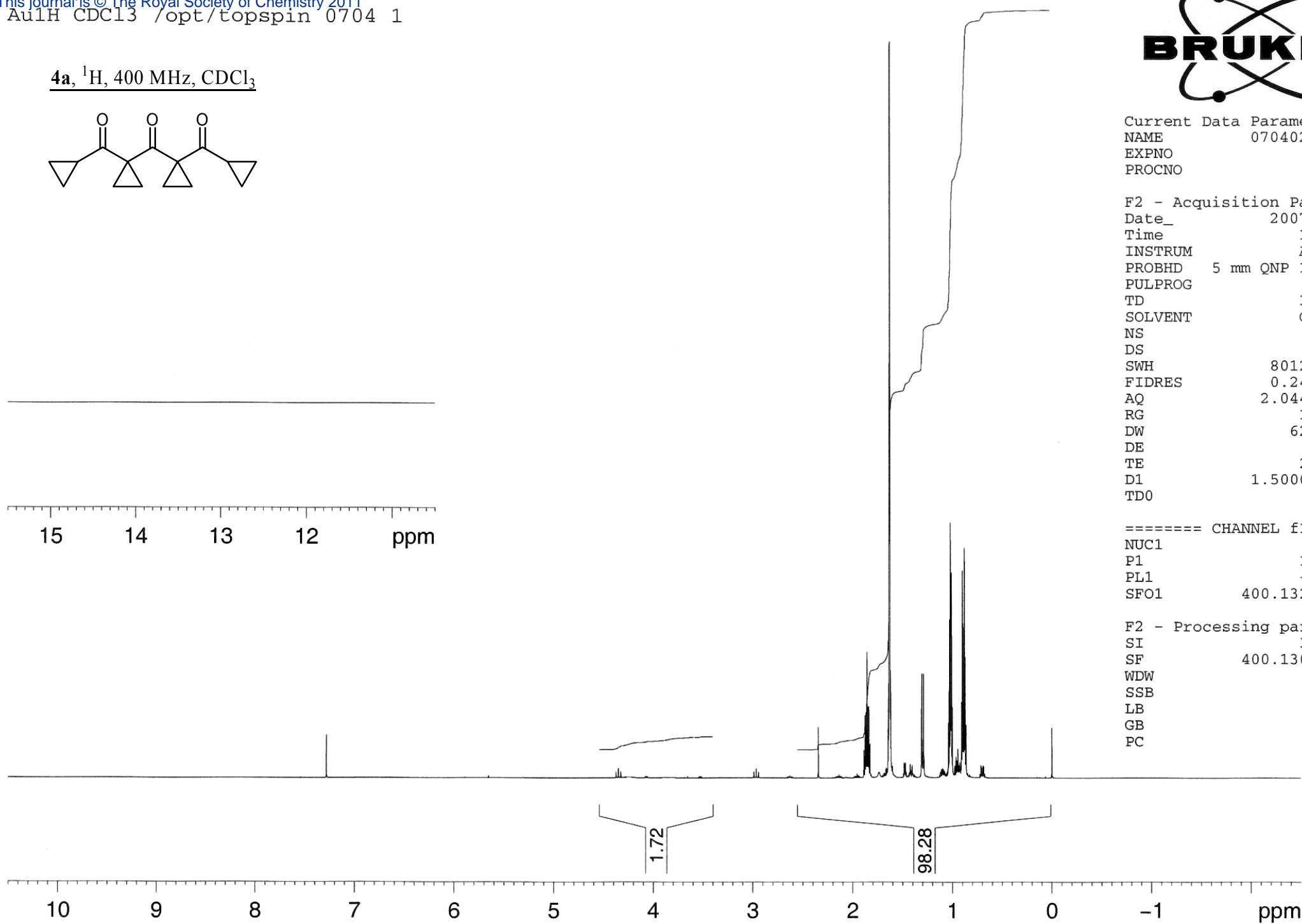
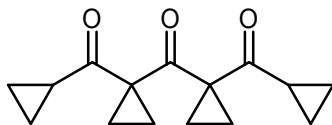
F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3i, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>





**4a**, <sup>1</sup>H, 400 MHz, CDCl<sub>3</sub>

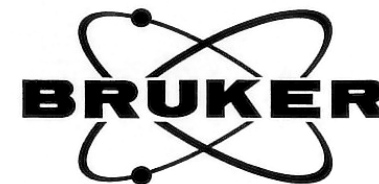


Current Data Parameters  
NAME 070402.401  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070402  
Time 15.17  
INSTRUM AV400  
PROBHD 5 mm QNP 1H/29  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 4  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 2.0447731 sec  
RG 101.6  
DW 62.400 usec  
DE 6.00 usec  
TE 297.0 K  
D1 1.50000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 10.50 usec  
PL1 -1.00 dB  
SFO1 400.1324000 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300118 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME 070402.401  
EXPNO 11  
PROCNO 1

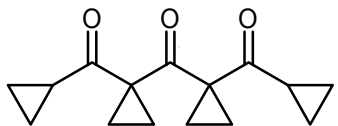
F2 - Acquisition Parameters  
Date\_ 20070402  
Time 15.30  
INSTRUM AV400  
PROBHD 5 mm QNP 1H/29  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 29940.119 Hz  
FIDRES 0.456850 Hz  
AQ 1.0945013 sec  
RG 32768  
DW 16.700 usec  
DE 6.00 usec  
TE 297.0 K  
D1 1.70000005 sec  
d11 0.03000000 sec  
DELTA 1.60000002 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PL1 -1.00 dB  
SFO1 100.6260690 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 -1.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 400.1318000 MHz

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

**4a**, <sup>13</sup>C, 100 MHz, CDCl<sub>3</sub>

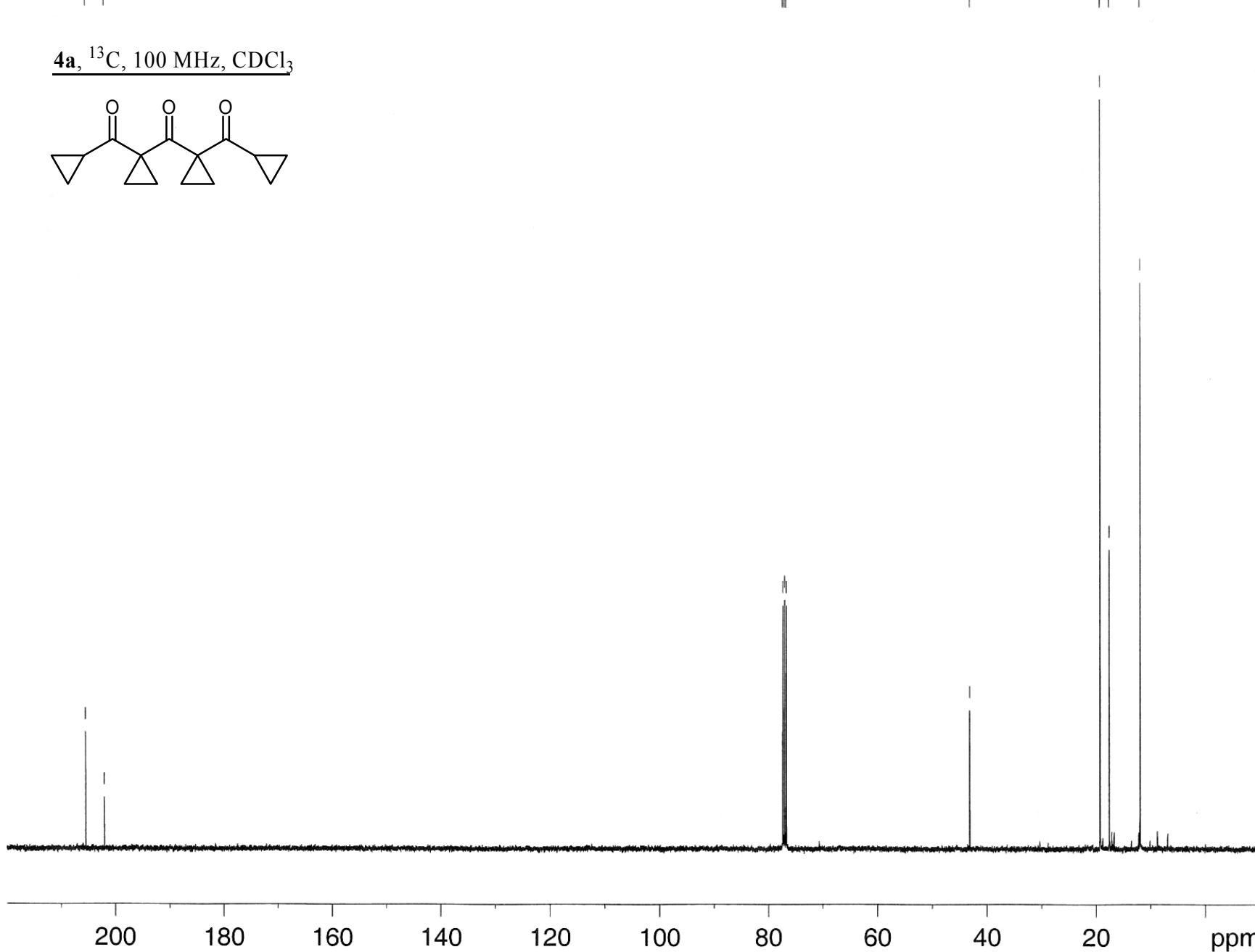


205.56  
202.09

77.39  
77.07  
76.76

43.18

19.30  
17.61  
11.98





Current Data Parameters  
NAME 070821.414  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters

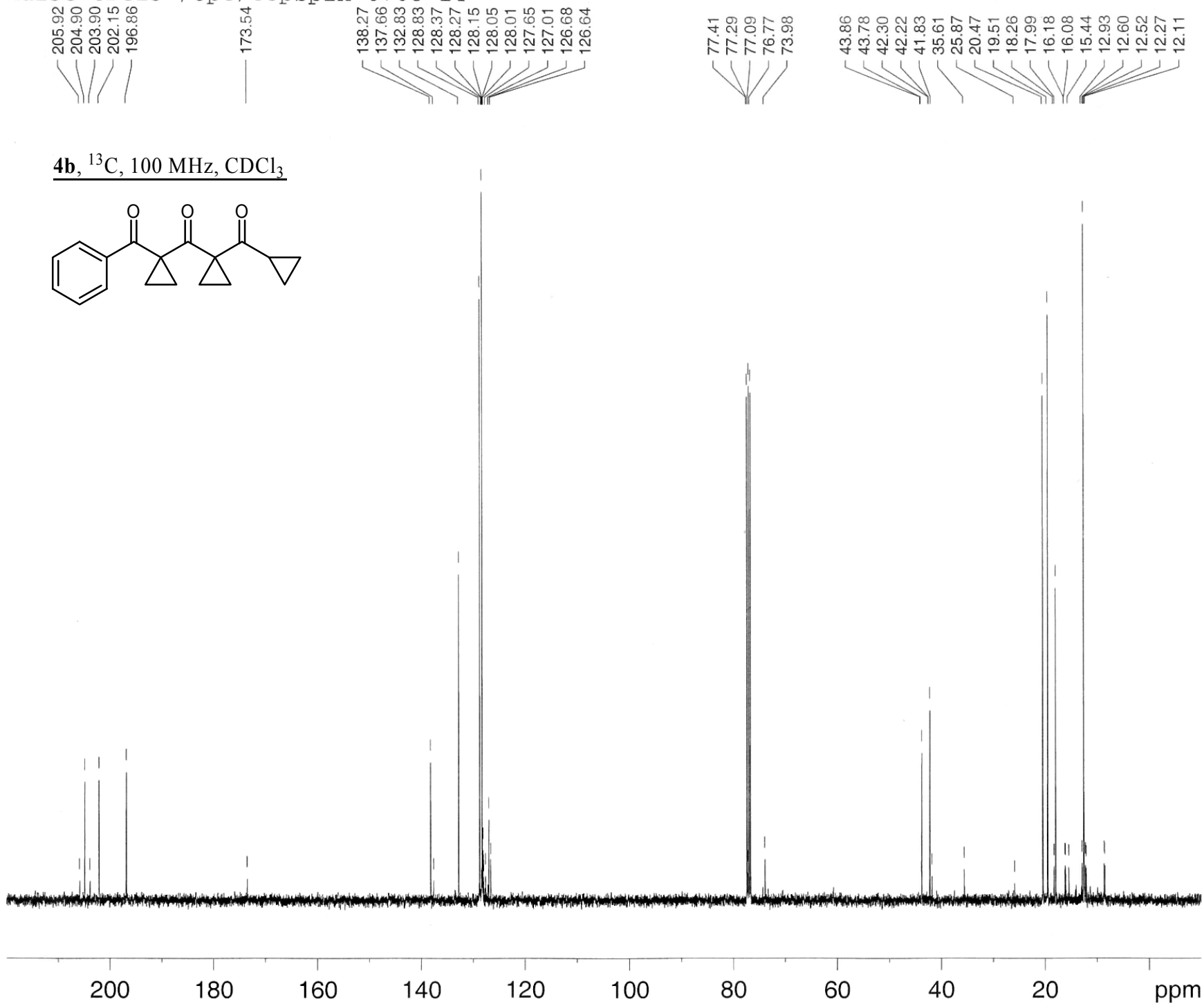
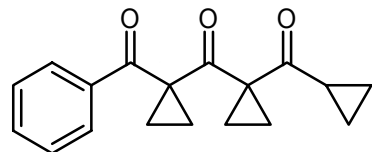
Date\_ 20070821  
Time 22.19  
INSTRUM AV400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 29940.119 Hz  
FIDRES 0.456850 Hz  
AQ 1.0945013 sec  
RG 2298.8  
DW 16.700 usec  
DE 6.00 usec  
TE 297.0 K  
D1 1.7000005 sec  
d11 0.03000000 sec  
DELTA 1.60000002 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PL1 -0.50 dB  
SFO1 100.6260690 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 -2.00 dB  
PL12 17.00 dB  
PL13 19.00 dB  
SFO2 400.1318000 MHz

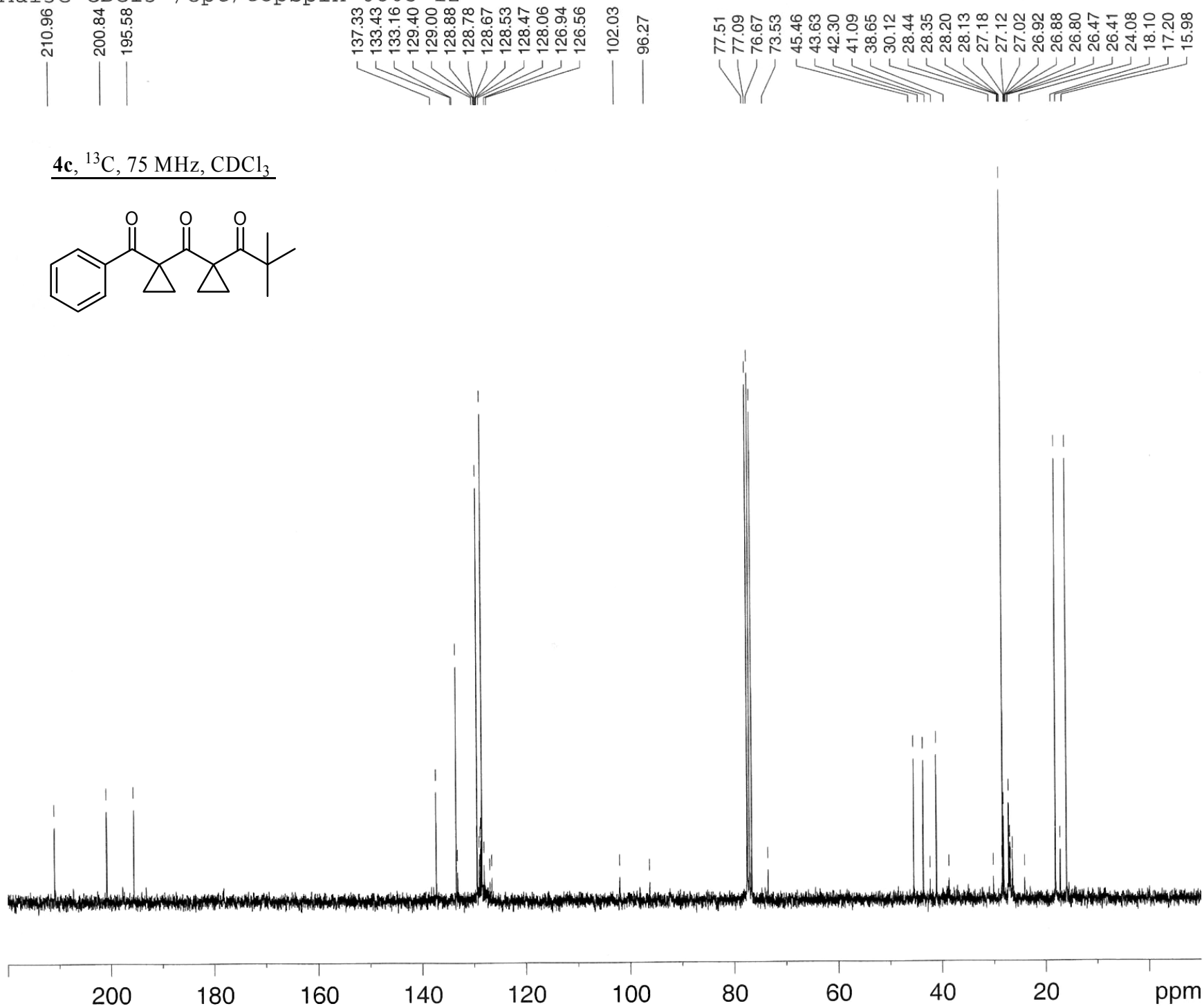
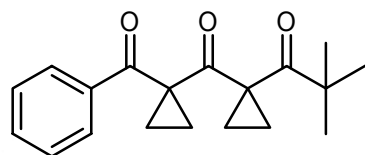
F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.00

4b, <sup>13</sup>C, 100 MHz, CDCl<sub>3</sub>





**4c**,  $^{13}\text{C}$ , 75 MHz,  $\text{CDCl}_3$



Current Data Parameters  
NAME 080519.312  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080519  
Time 14.28  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT  $\text{CDCl}_3$   
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.7 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

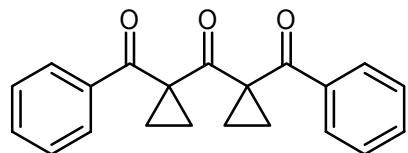
==== CHANNEL f1 =====  
NUC1  $^{13}\text{C}$   
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2  $^1\text{H}$   
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

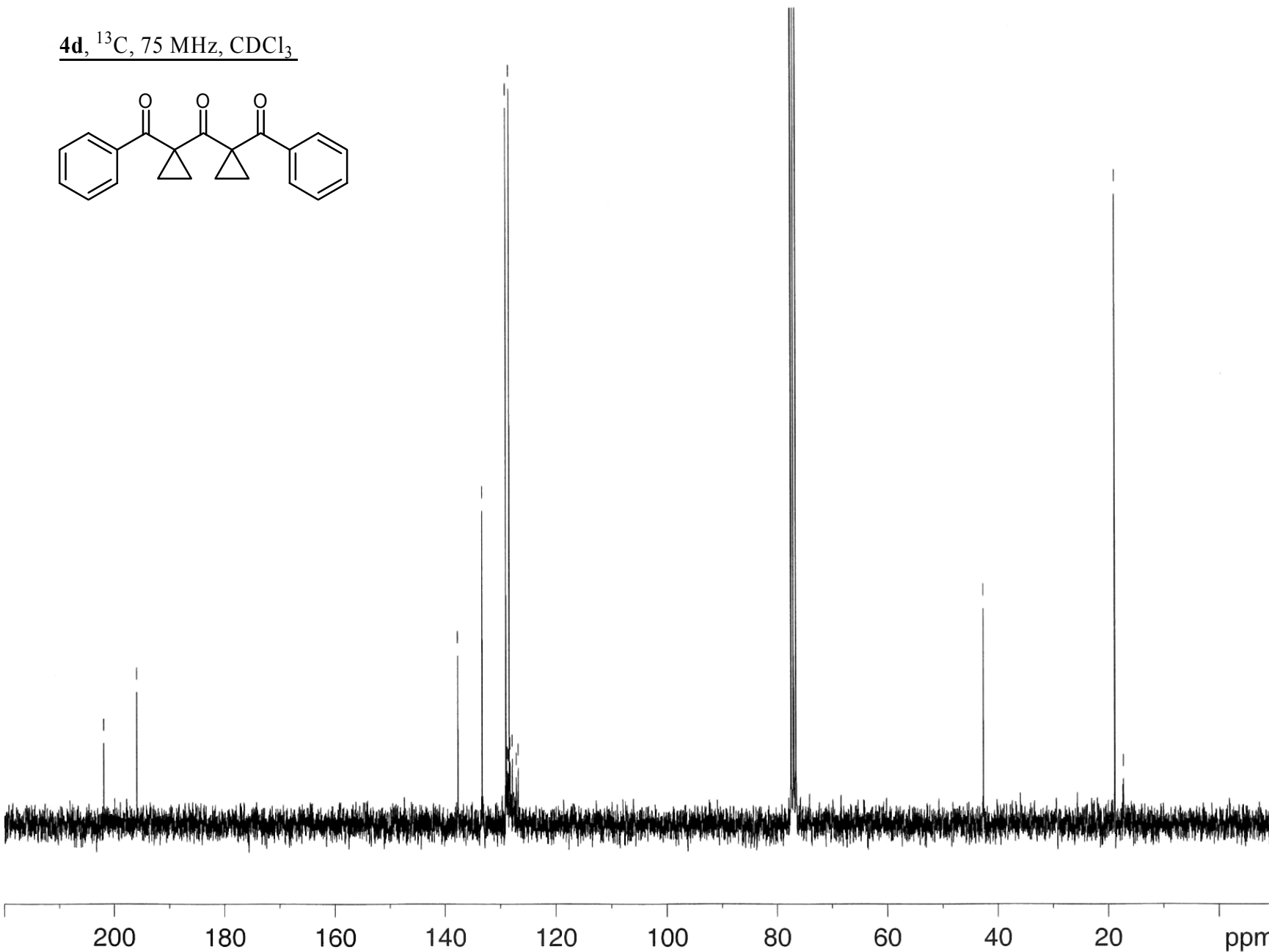
F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



4d,  $^{13}\text{C}$ , 75 MHz,  $\text{CDCl}_3$



201.92  
195.91  
137.75  
133.31  
129.08  
128.97  
128.75  
128.62  
128.47  
128.26  
127.88  
127.13  
126.78  
42.68  
18.83  
17.23



Current Data Parameters  
NAME 070820.312  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070820  
Time 23.03  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT  $\text{CDCl}_3$   
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.2 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1  
NUC1  $^{13}\text{C}$   
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2  $^1\text{H}$   
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Current Data Parameters  
 NAME 080530.315  
 EXPNO 11  
 PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20080530  
 Time 21.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDC13  
 NS 256  
 DS 4  
 SWH 21097.047 Hz  
 FIDRES 0.643831 Hz  
 AQ 0.7766516 sec  
 RG 32768  
 DW 23.700 usec  
 DE 6.00 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

## ===== CHANNEL f1 =====

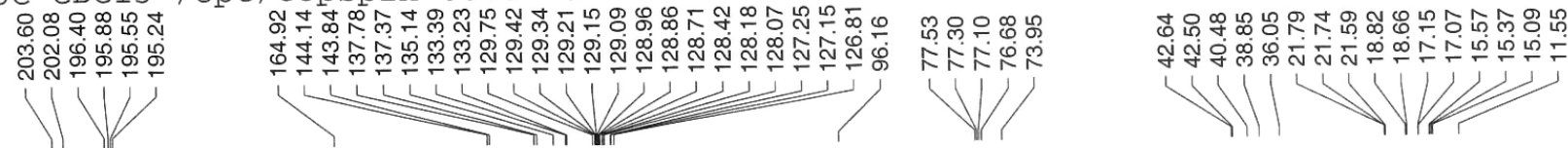
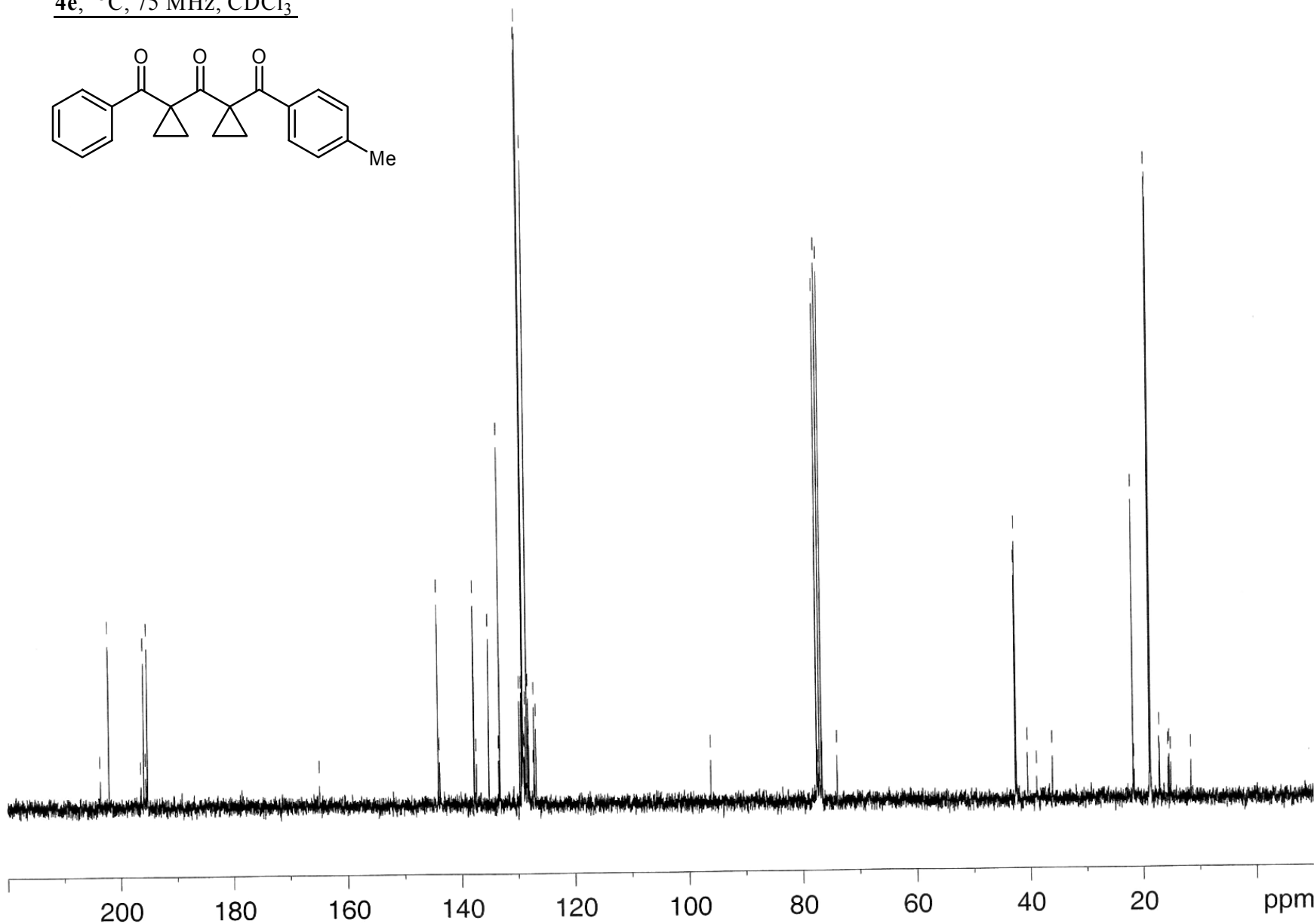
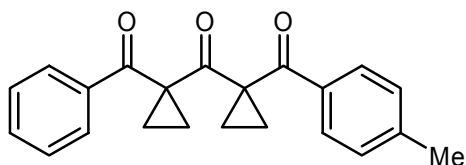
NUC1 13C  
 P1 9.60 usec  
 PL1 -1.10 dB  
 SFO1 75.4771825 MHz

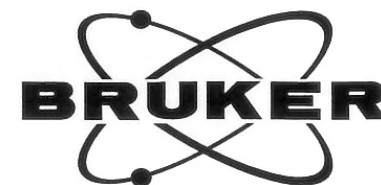
## ===== CHANNEL f2 =====

CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 0.00 dB  
 PL12 19.00 dB  
 PL13 21.00 dB  
 SFO2 300.1312005 MHz

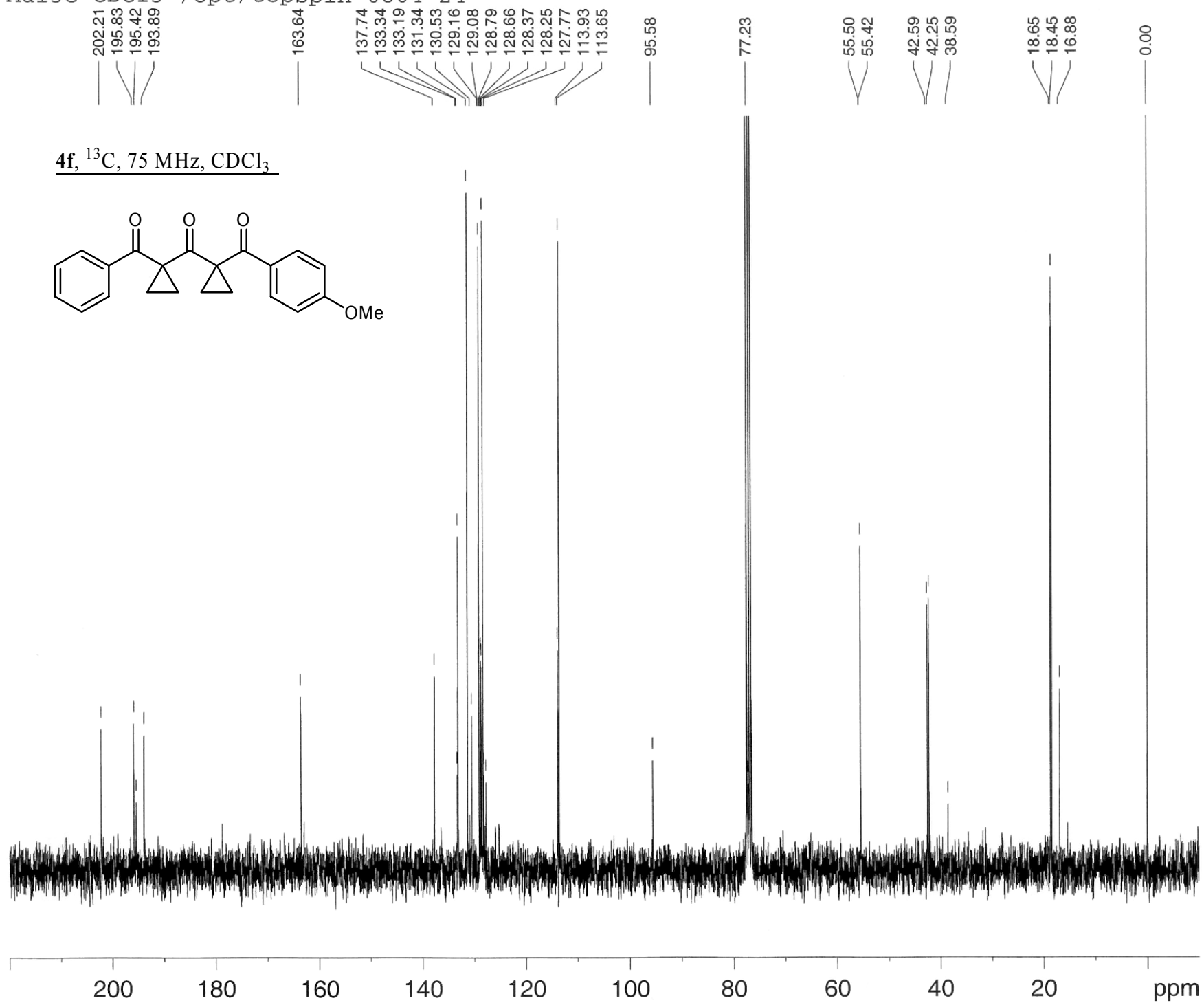
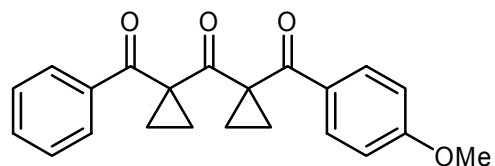
## F2 - Processing parameters

SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4e, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>



**4f**, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>



Current Data Parameters  
NAME 080422.324  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080423  
Time 7.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 295.4 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

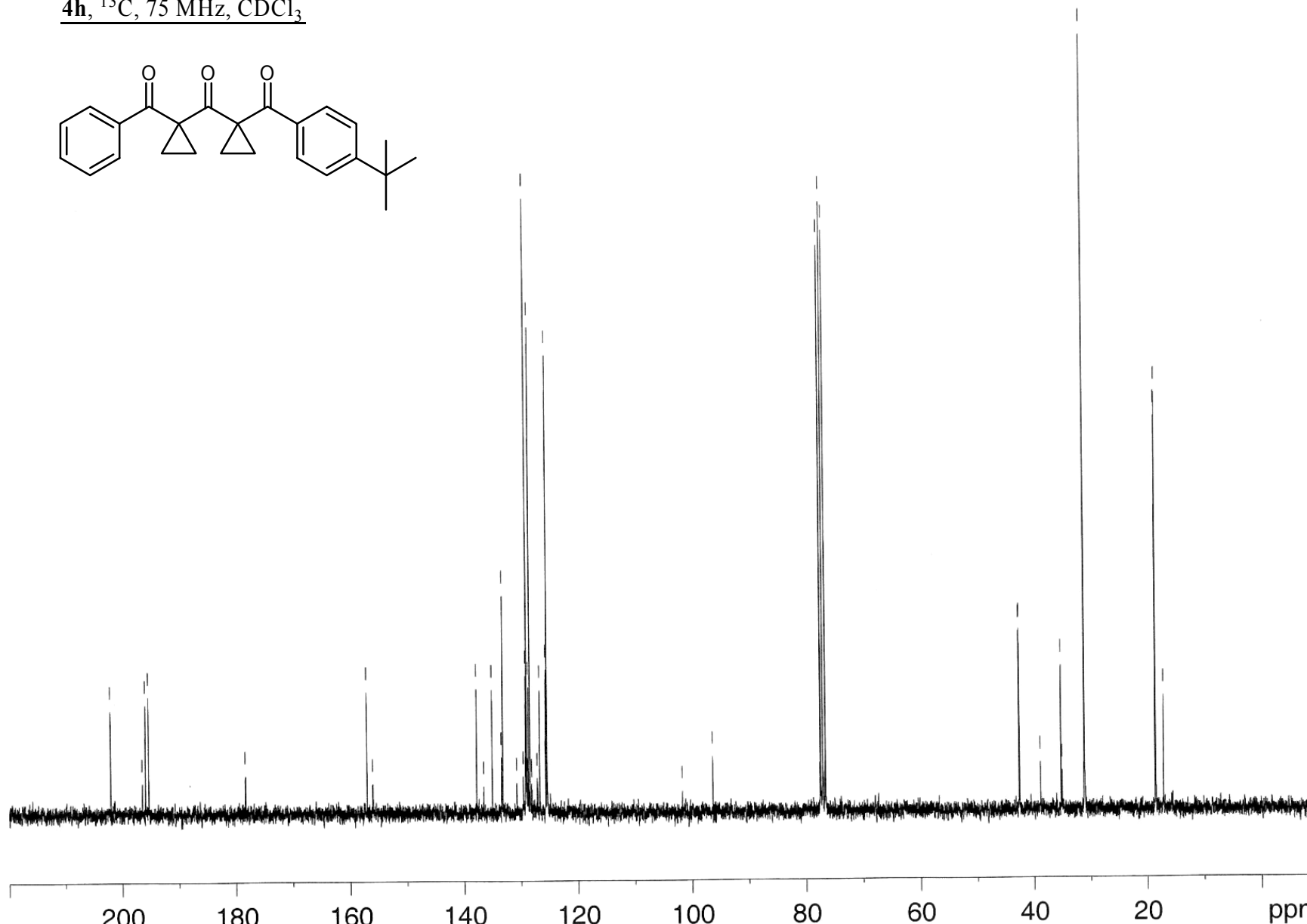
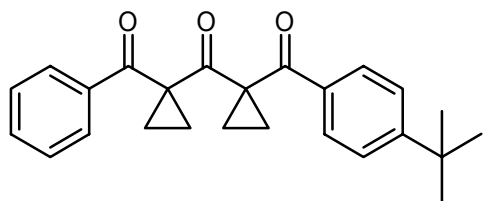
F2 - Processing parameters  
SI 32768  
SF 75.4677517 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Path: Aul3C CDC13 /opt/topspin 0806 15  
202.08  
196.49  
195.95  
195.38  
178.35  
157.12  
156.09  
137.82  
136.58  
135.10  
133.42  
133.20  
130.75  
129.60  
129.18  
129.07  
128.89  
128.72  
128.63  
128.42  
128.16  
128.08  
127.12  
126.69  
125.68  
125.61  
125.39  
101.74  
96.36  
77.51  
77.09  
76.66  
42.66  
42.56  
38.89  
35.21  
35.04  
31.14  
31.09  
18.58  
18.50  
17.11

4h, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>



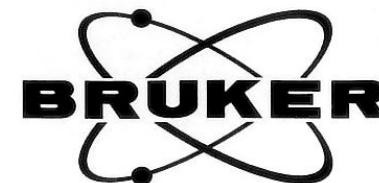
Current Data Parameters  
NAME 080616.315  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080616  
Time 21.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.2 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

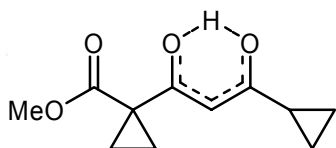
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



7a,  $^1\text{H}$ , 300 MHz,  $\text{CDCl}_3$

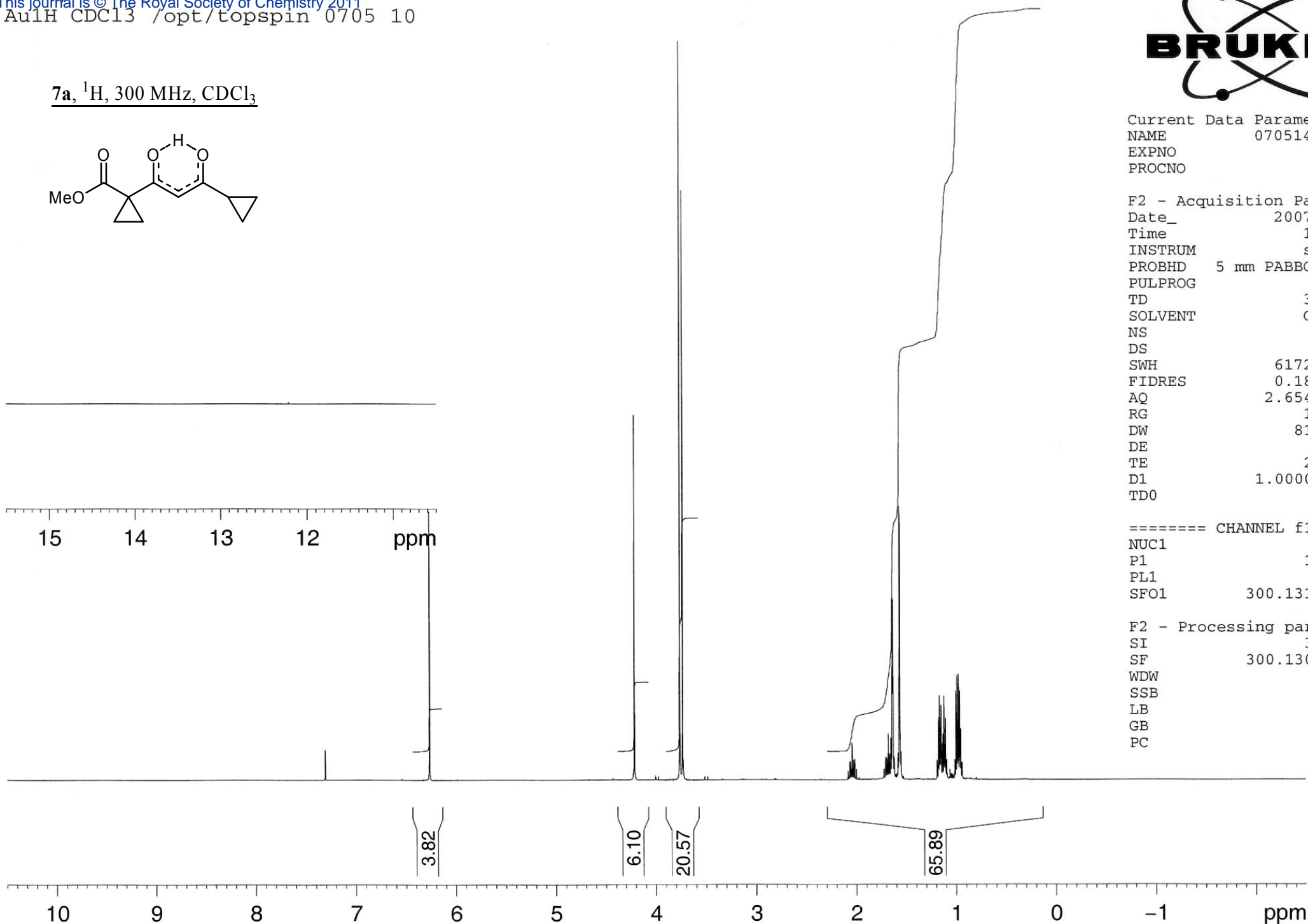


Current Data Parameters  
NAME 070514.310  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20070514  
Time 18.24  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT  $\text{CDCl}_3$   
NS 32  
DS 4  
SWH 6172.839 Hz  
FIDRES 0.188380 Hz  
AQ 2.6542580 sec  
RG 143.7  
DW 81.000 usec  
DE 6.00 usec  
TE 295.9 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1  $^1\text{H}$   
P1 11.00 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME 070514.310  
EXPNO 11  
PROCNO 1

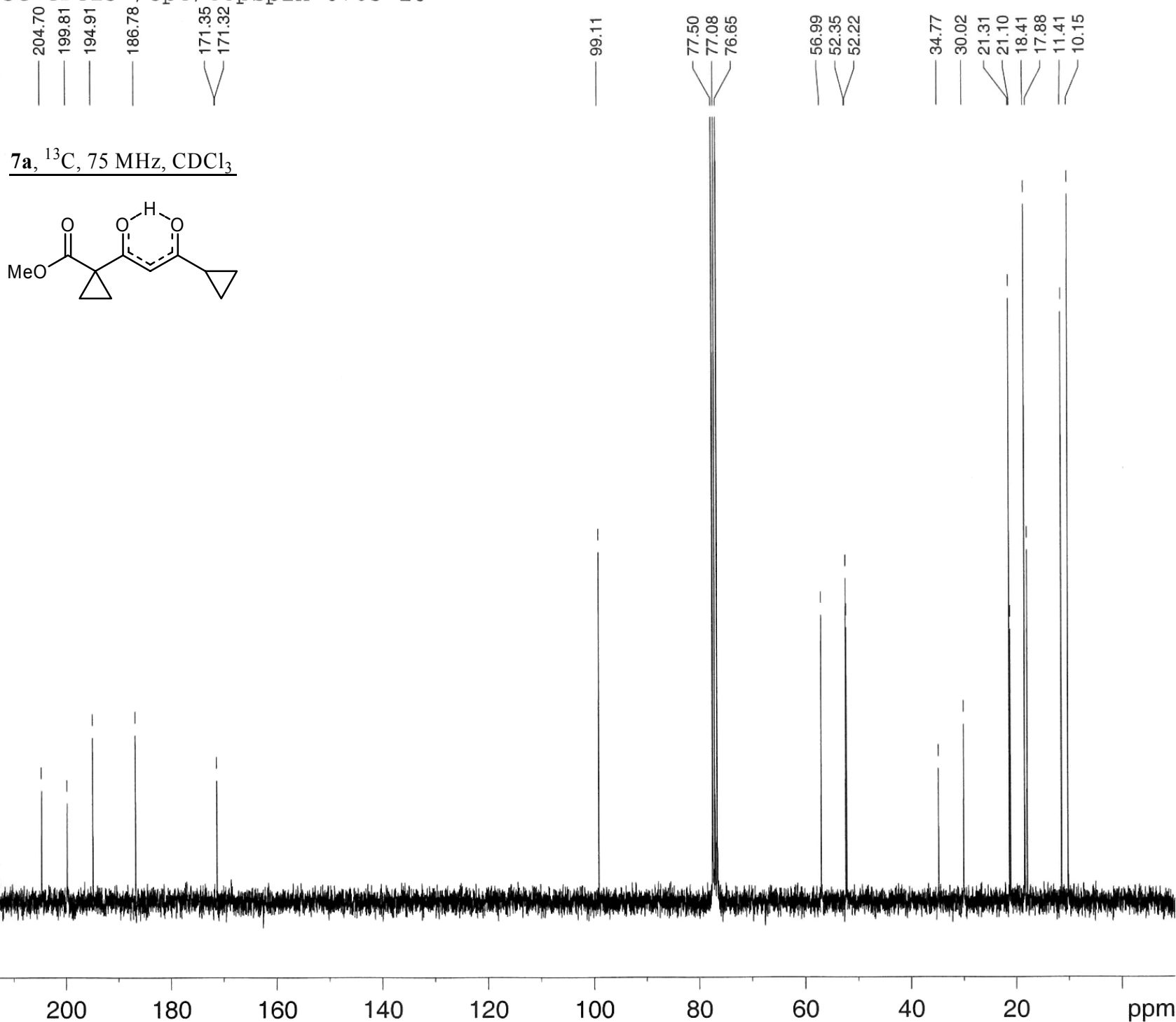
F2 - Acquisition Parameters

Date\_ 20070514  
Time 18.37  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.3 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

=====  
CHANNEL f1  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

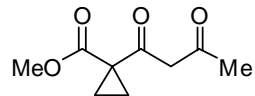
=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



15.429

**1H, 7b, 300MHz, CDCl3**



7.260

6.099

4.019

3.702

3.668

2.234

2.041

1.591

1.535

1.522

1.520

1.508

0.9

1.0

1.0

1.5

1.5

2.0

3.0

3.0

4.0

16

14

12

10

8

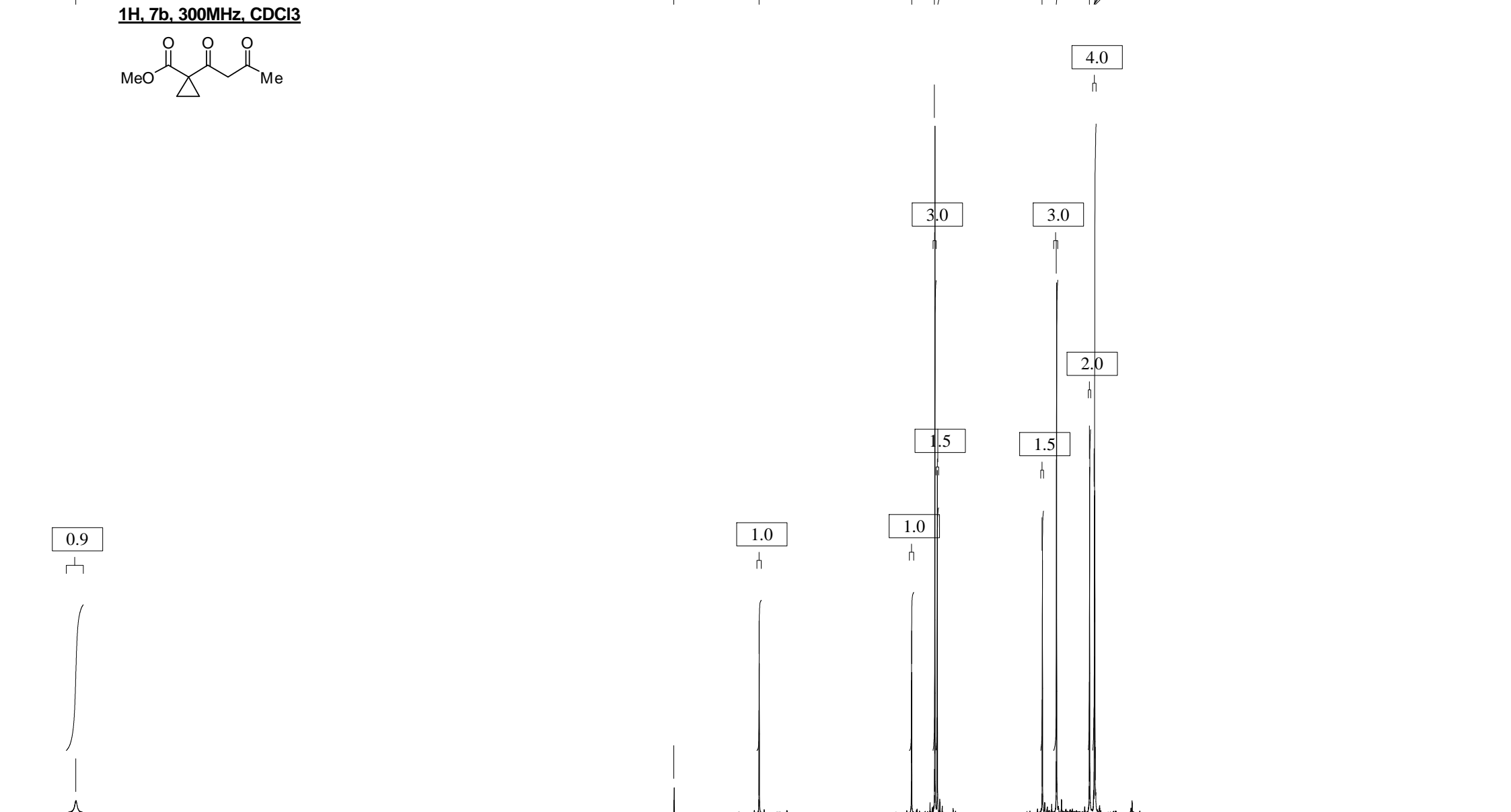
6

4

2

0

-2



202.3774  
199.6006  
192.4773  
186.2277  
171.2575  
171.1118

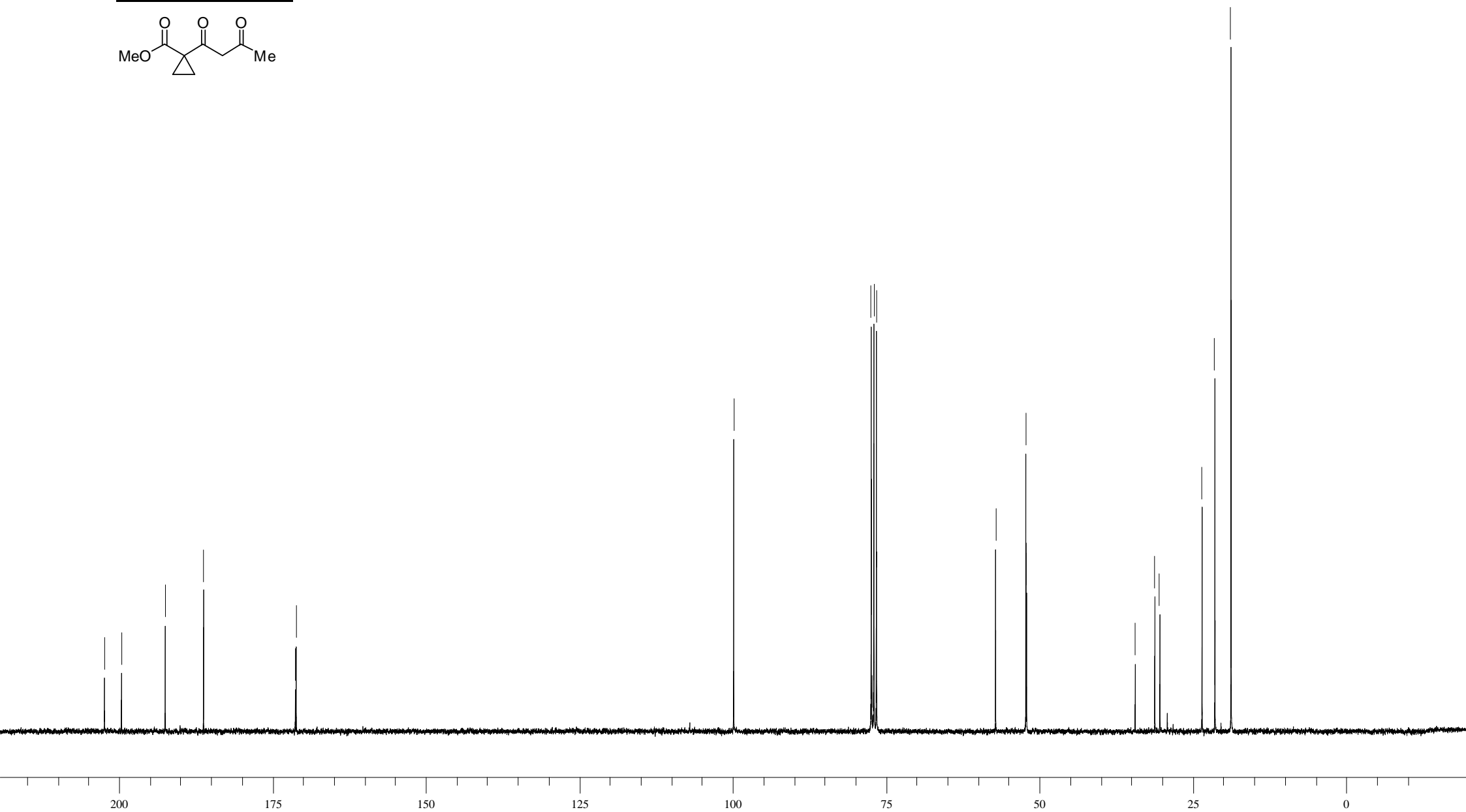
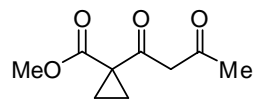
99.8334

77.416  
77.192  
76.992  
76.562

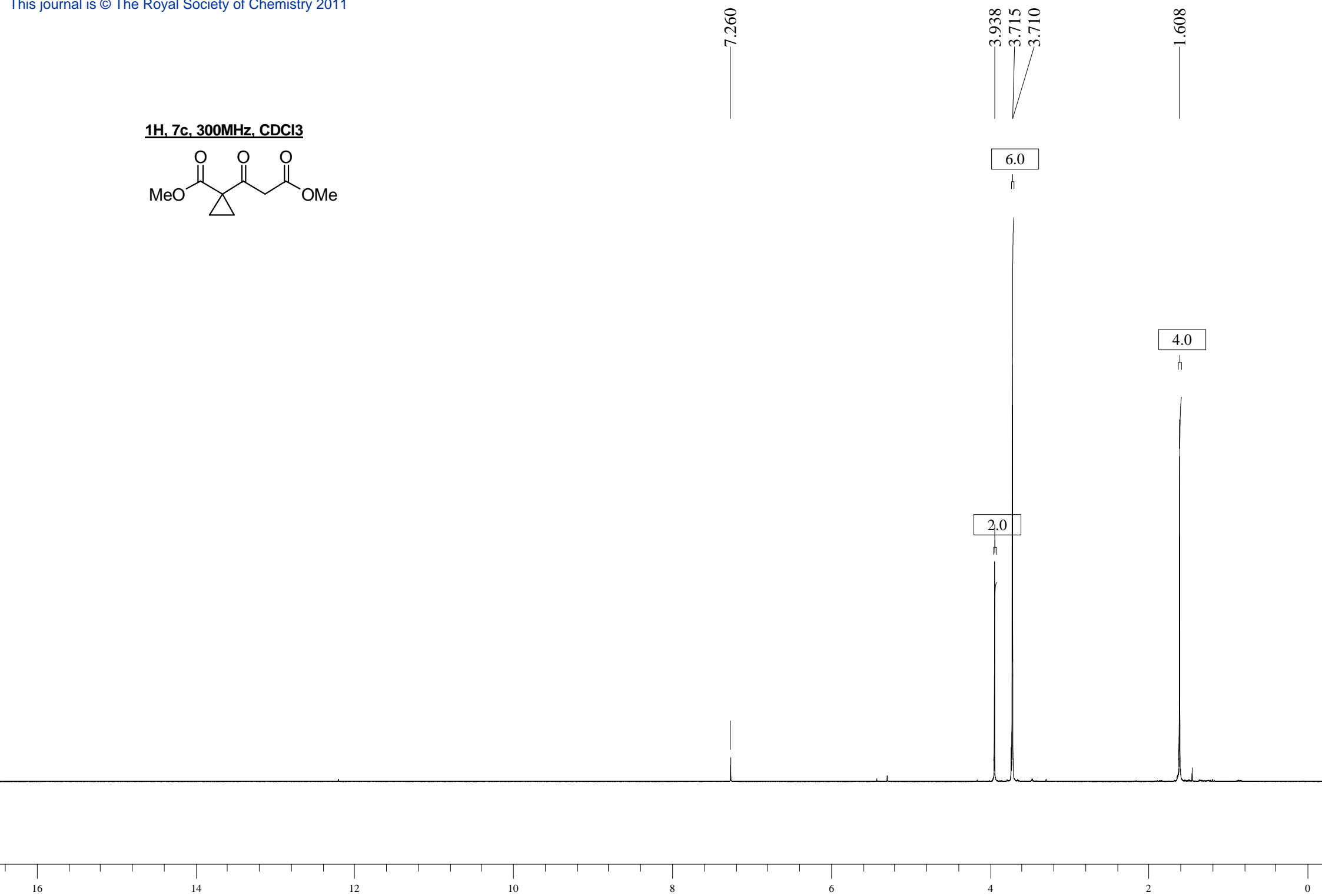
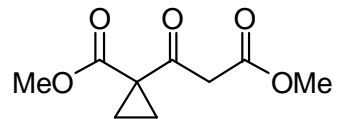
57.150  
52.214  
52.096

34.395  
31.196  
30.377  
23.495  
21.404  
18.773

**13C, 7b, 75MHz, CDCl3**



**1H, 7c, 300MHz, CDCl3**



198.119

171.074

168.074

77.496

76.993

76.485

52.241

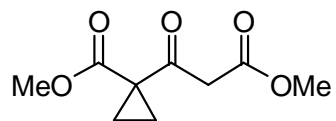
52.162

48.683

34.431

21.382

**13C, 7c, 63MHz, CDCl3**



200

175

150

125

100

75

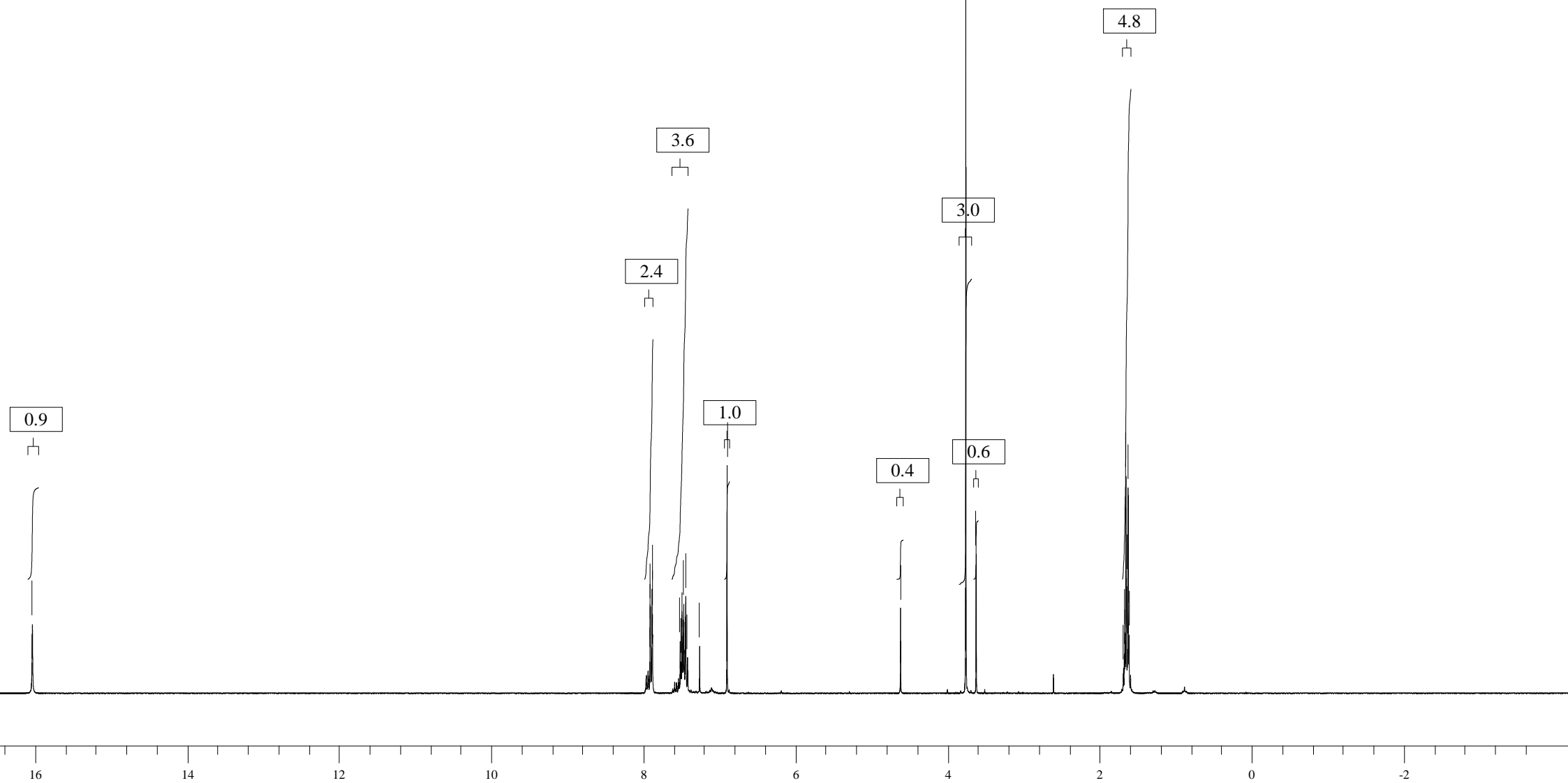
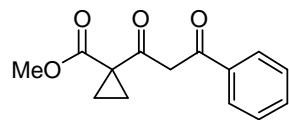
50

25

0

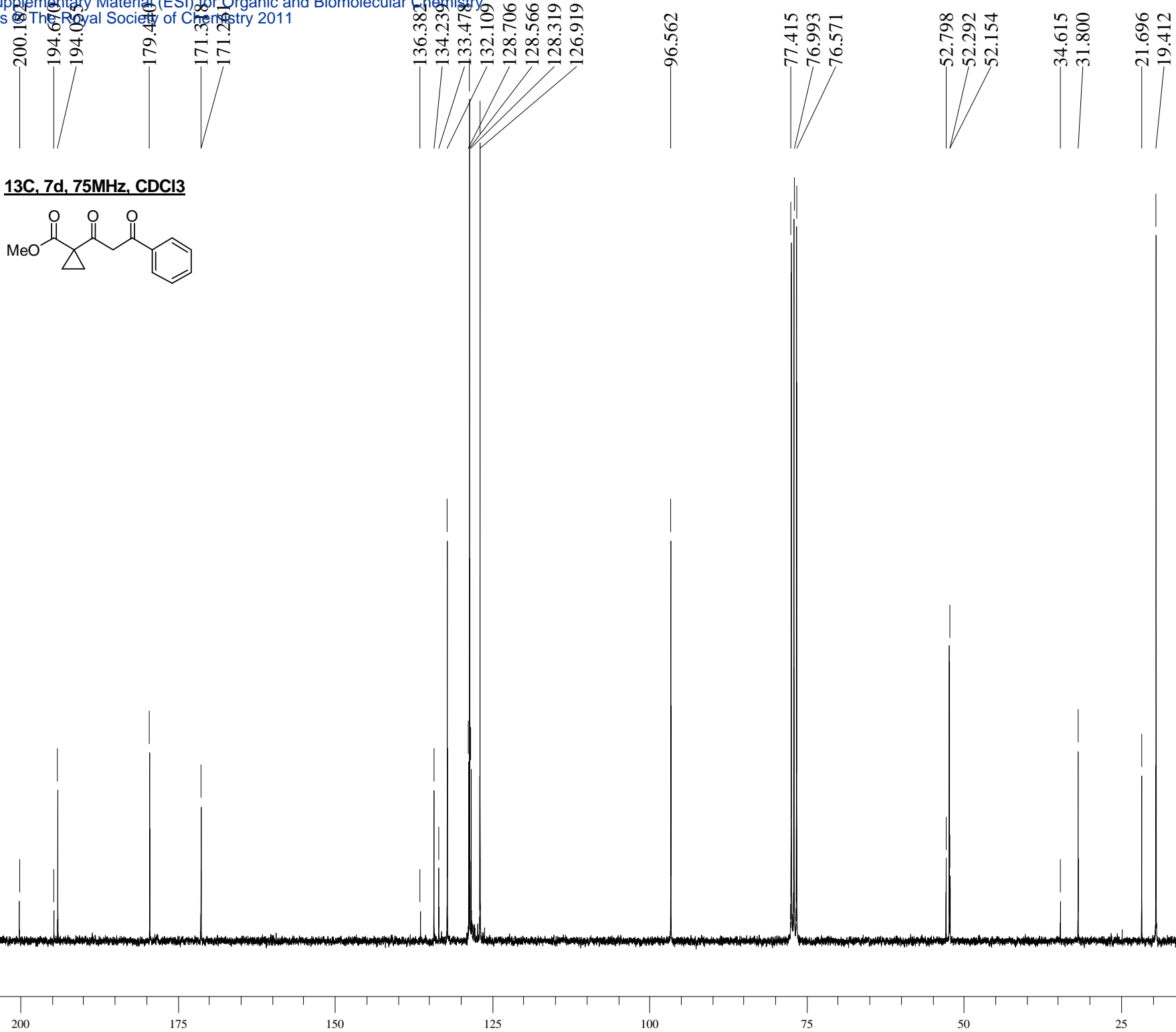
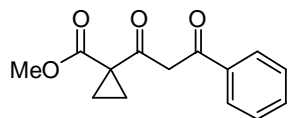
16.035

**1H, 7d, 300MHz, CDCl3**

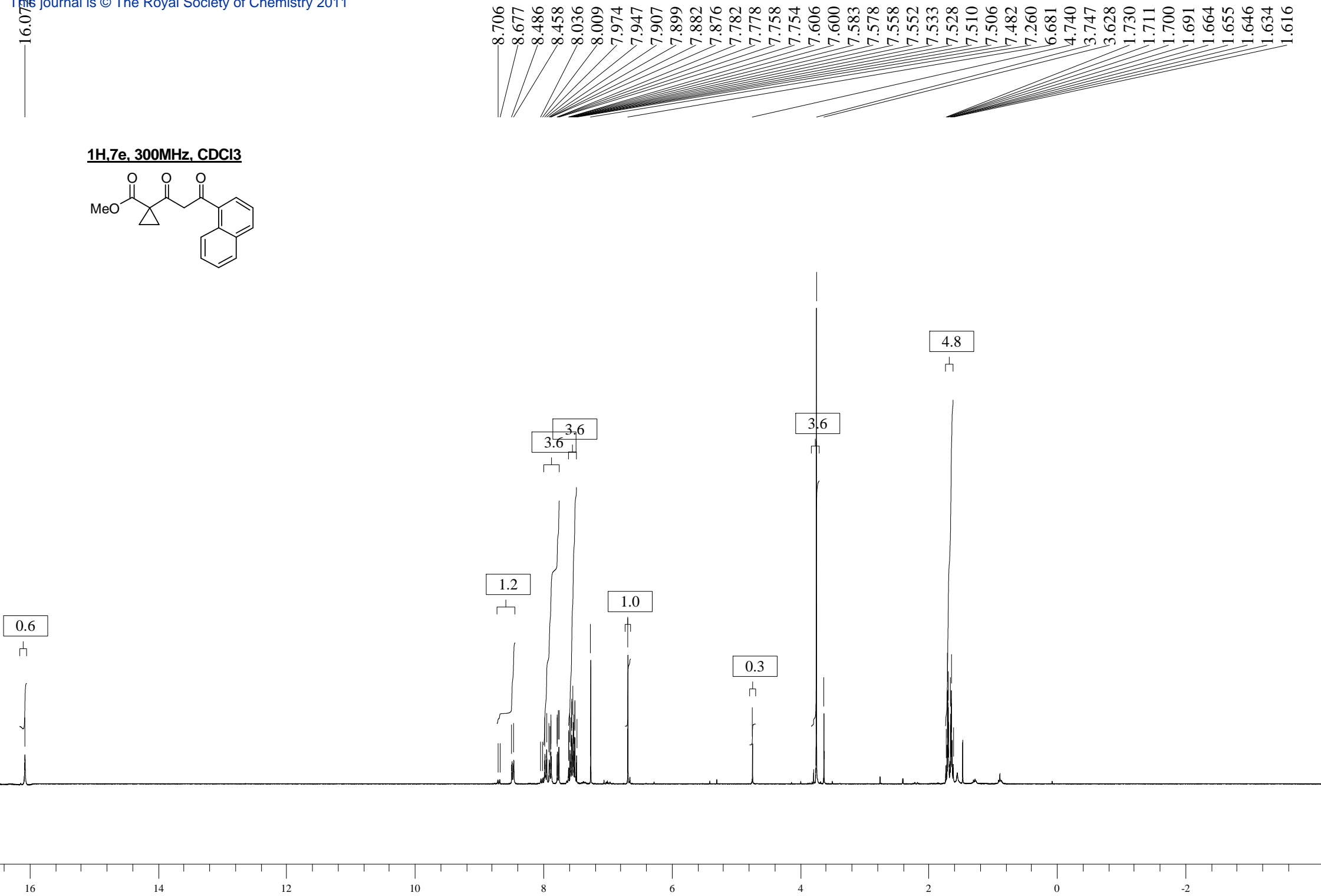
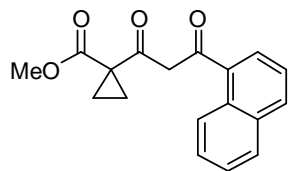




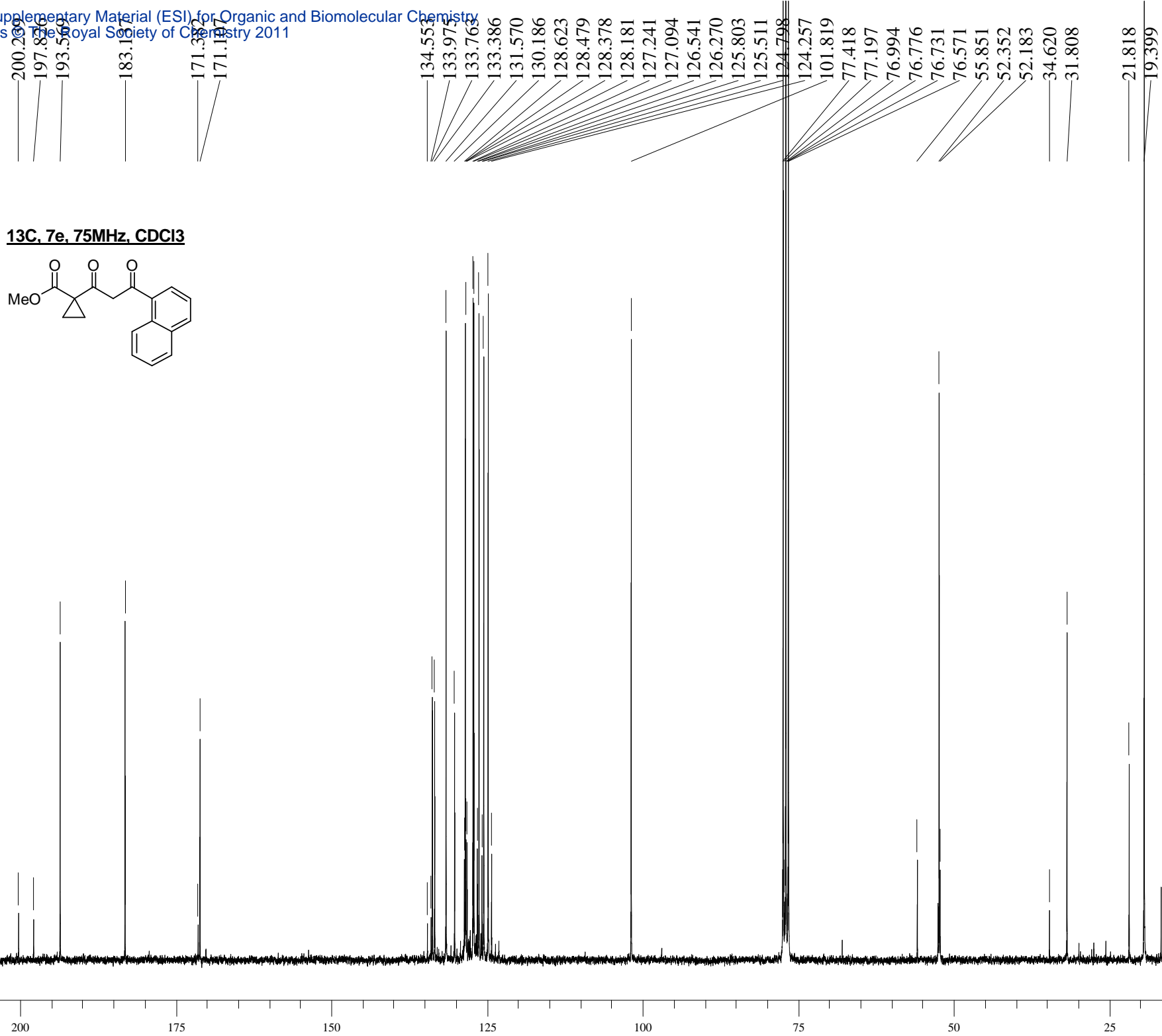
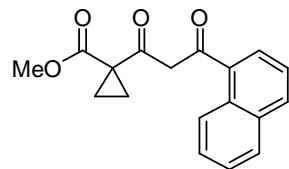
**13C, 7d, 75MHz, CDCl3**



**1H, 7e, 300MHz, CDCl3**



**13C, 7e, 75MHz, CDCl3**



15.566

7.260

6.132

4.099

3.713

3.665

2.457

2.446

2.435

2.224

2.213

2.203

2.187

2.176

2.165

2.149

2.138

2.127

1.885

1.845

1.777

1.702

1.692

1.670

1.659

1.601

1.598

1.545

1.541

1.536

1.532

1.469

1.402

1.363

1.333

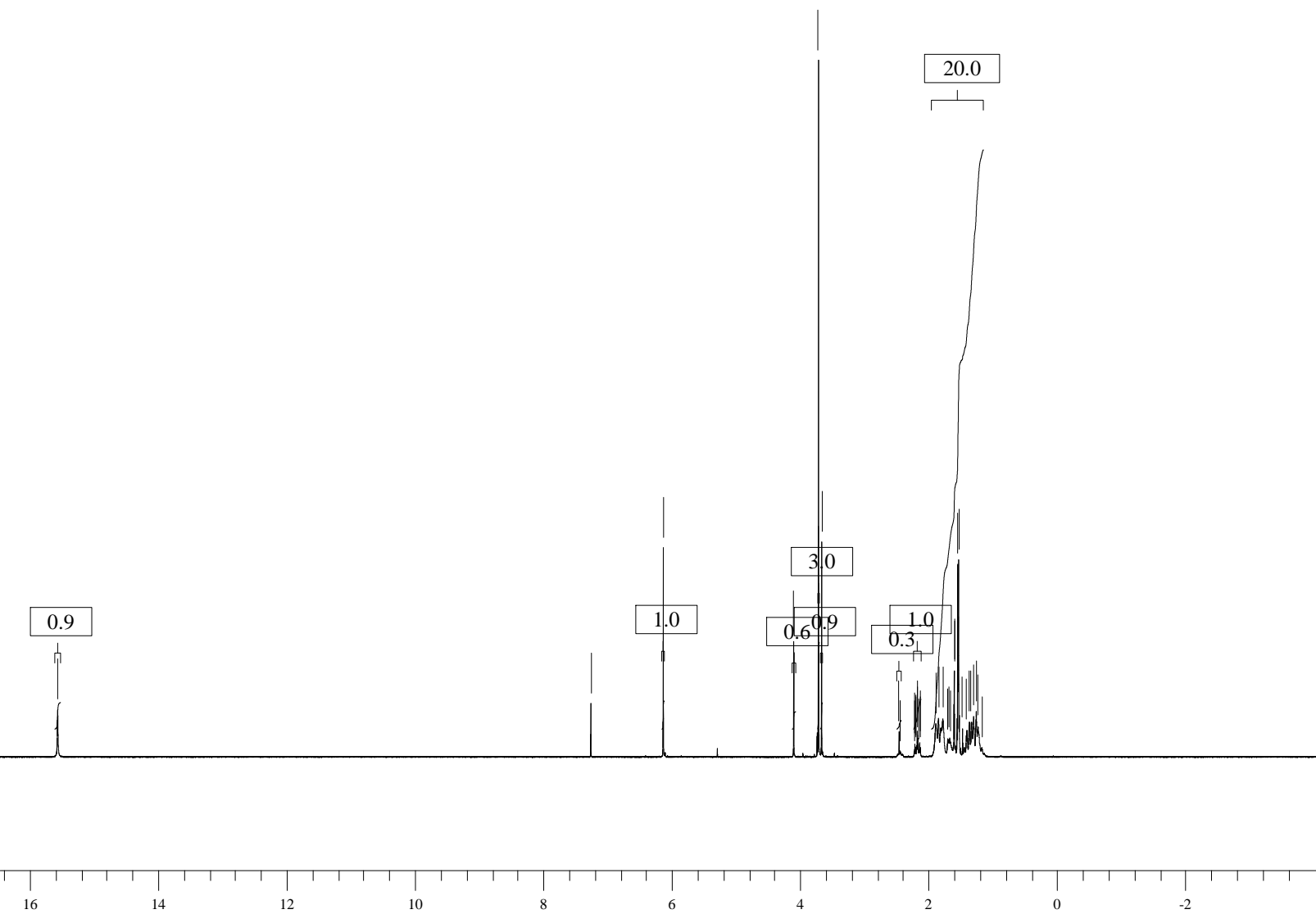
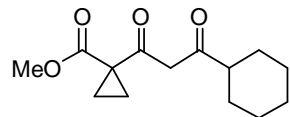
1.297

1.258

1.230

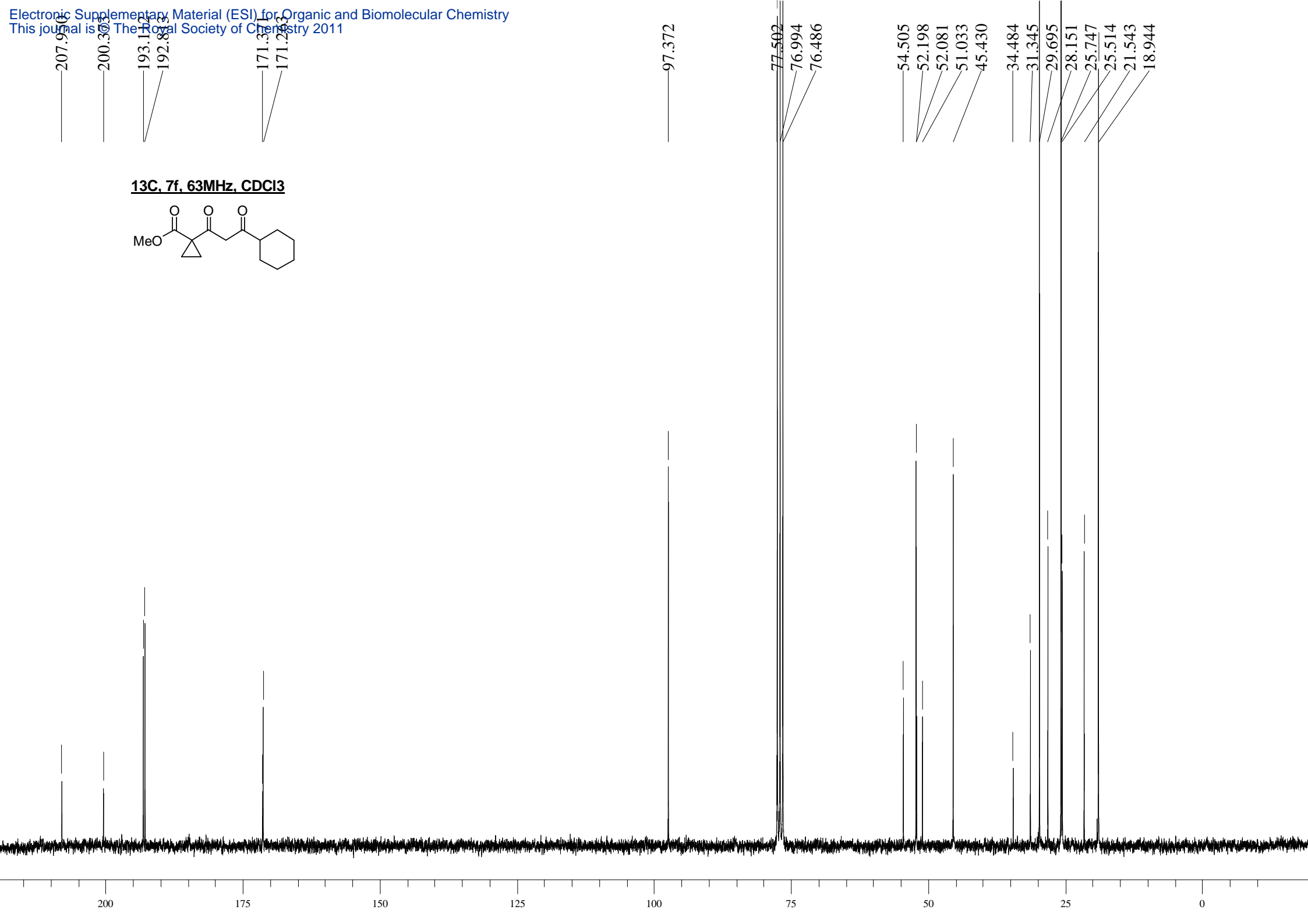
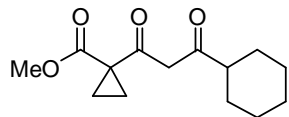
1.170

**1H, 7f, 300MHz, CDCl3**



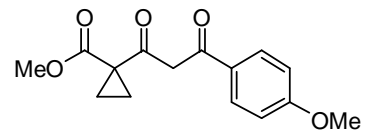


**13C, 7f, 63MHz, CDCl3**



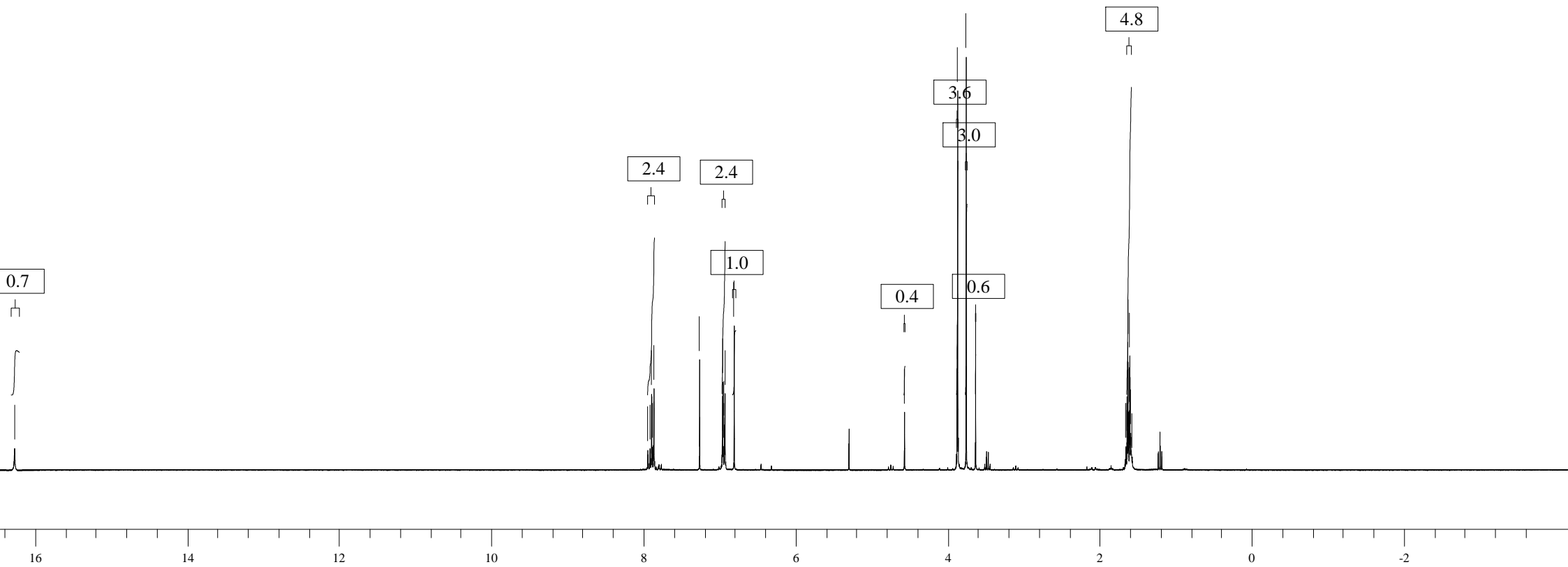
16.269

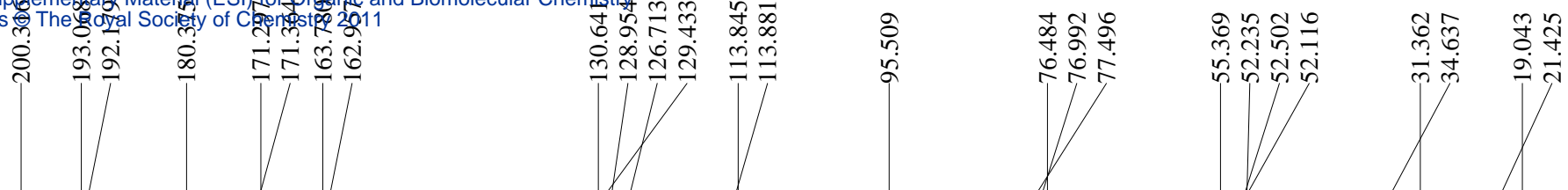
**1H,7g, 300MHz, CDCl3**



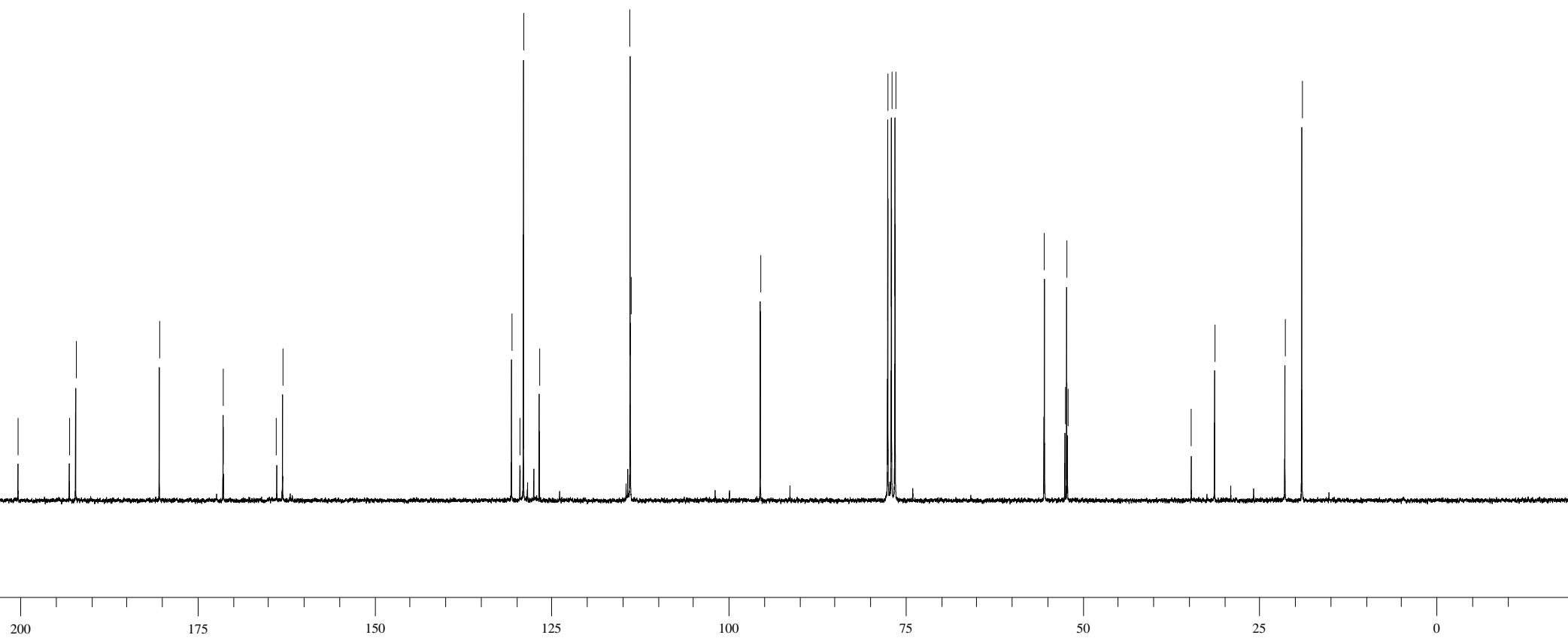
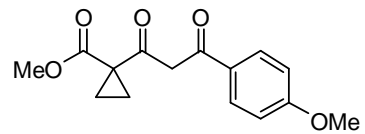
7.941  
7.912  
7.891  
7.884  
7.868  
7.861  
7.260  
6.964  
6.957  
6.950  
6.934  
6.926  
6.806  
4.565  
3.874  
3.867  
3.754  
3.632

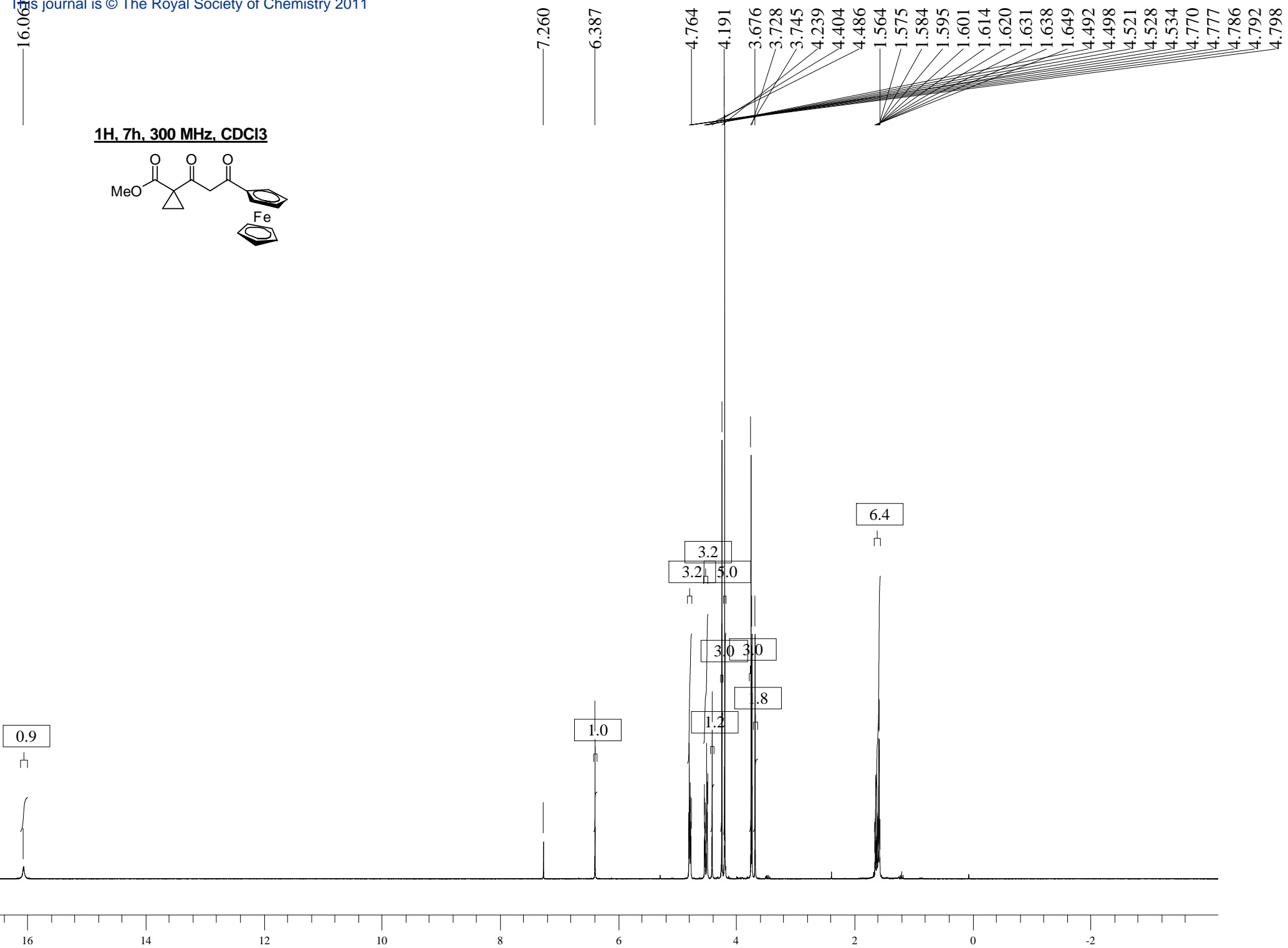
1.655  
1.648  
1.640  
1.636  
1.629  
1.622  
1.609  
1.603  
1.590  
1.571



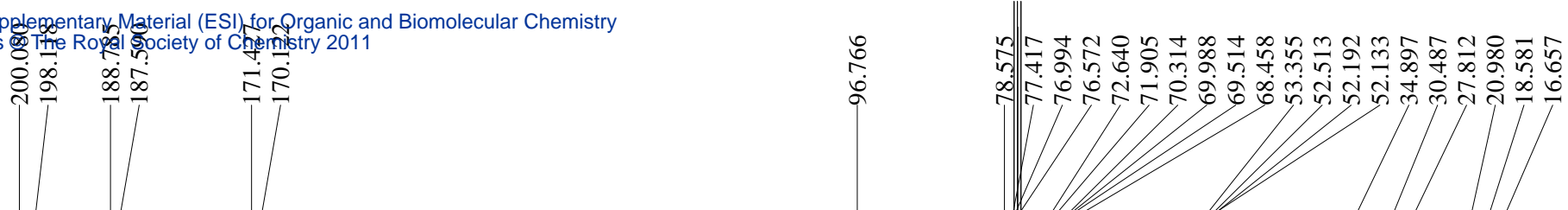


**13C, 7g, 63 MHz, CDCl<sub>3</sub>**

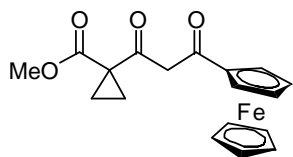








**13C, 7h, 75MHz, CDCl3**



200

175

150

125

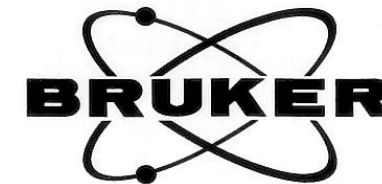
100

75

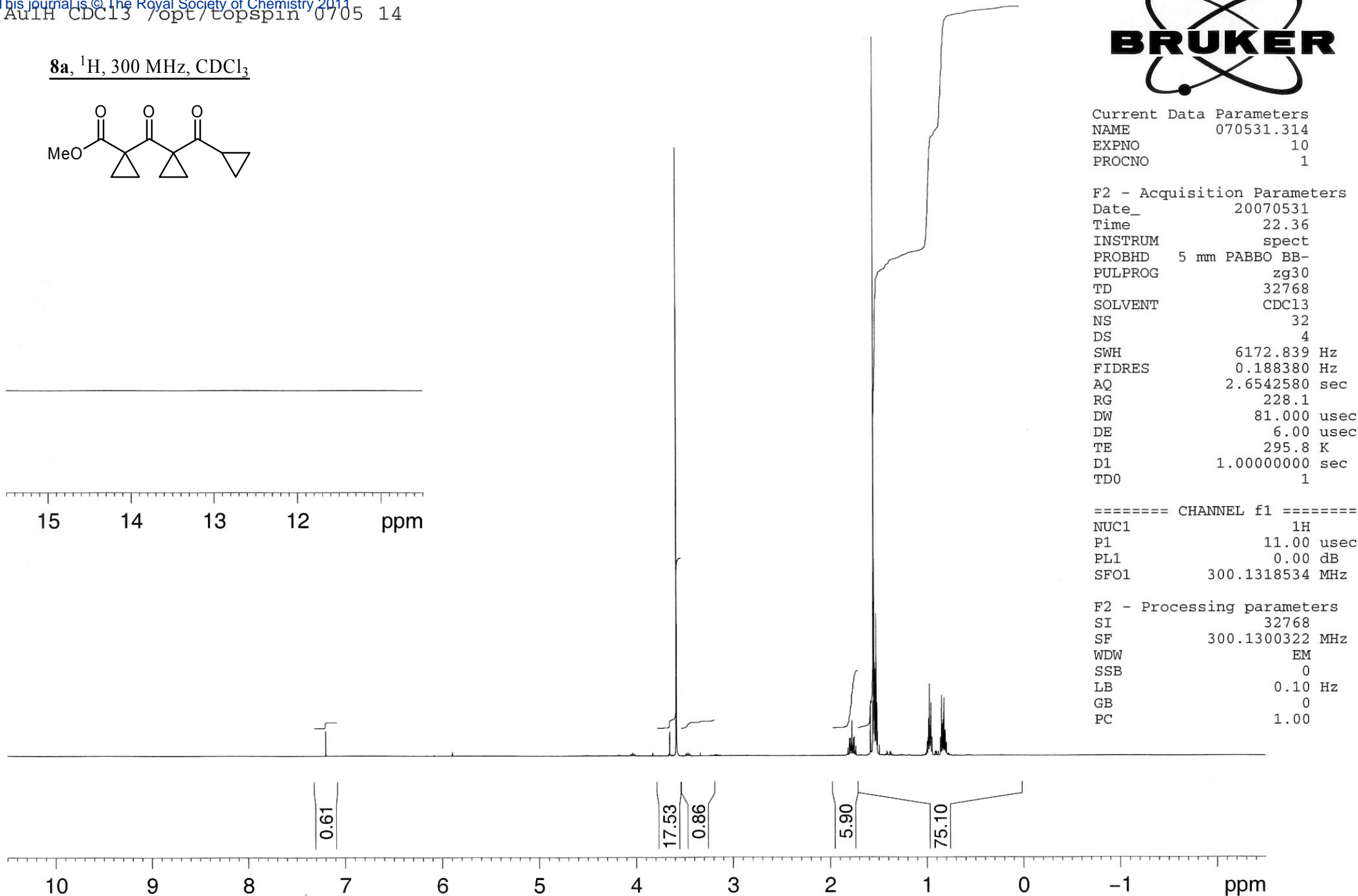
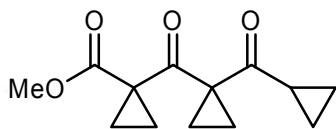
50

25

0



**8a**,  $^1\text{H}$ , 300 MHz,  $\text{CDCl}_3$





Current Data Parameters  
NAME 070531.314  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20070531  
Time 22.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.2 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

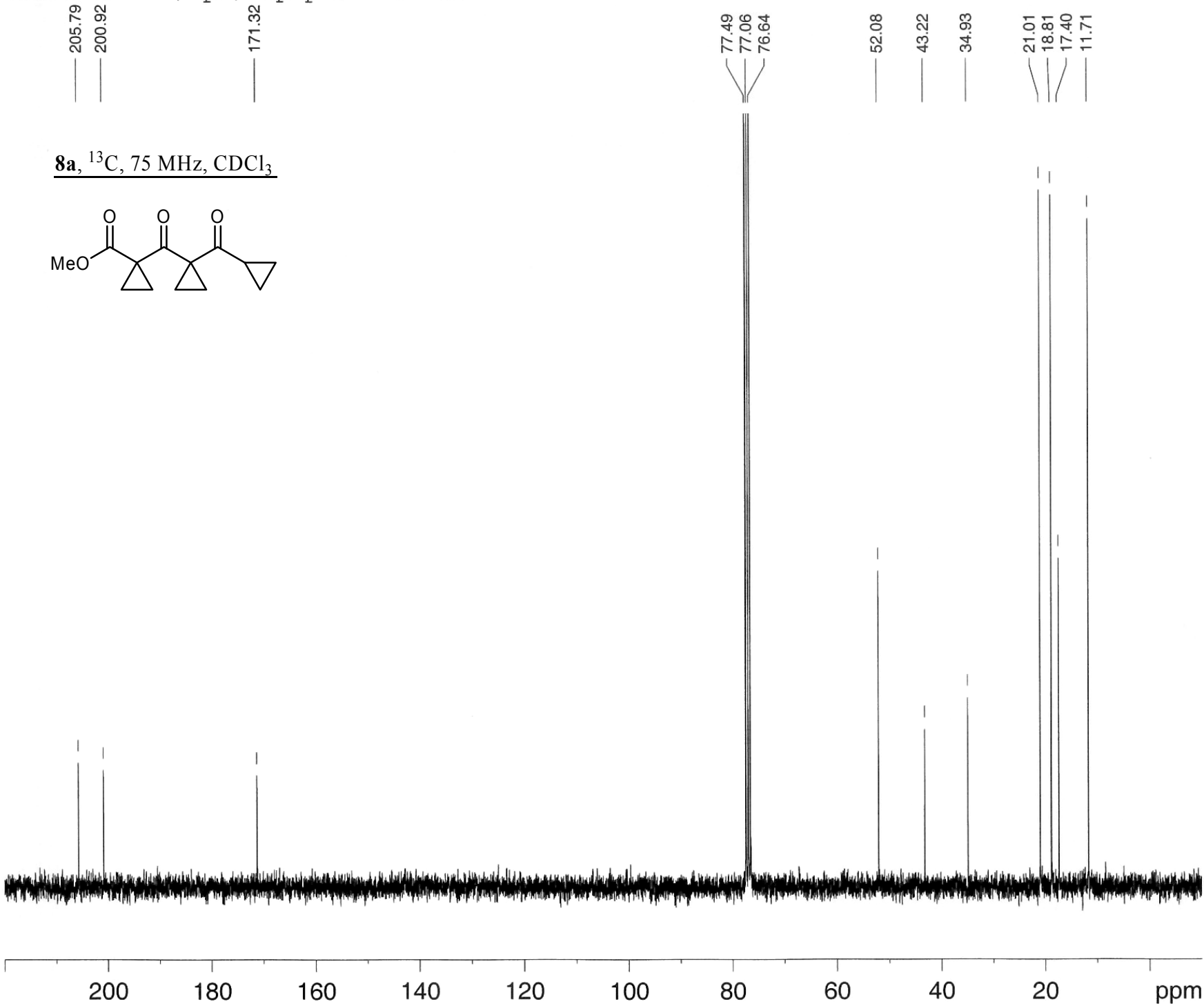
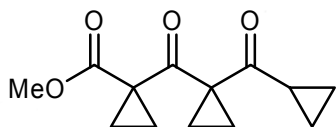
=====  
CHANNEL f1  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

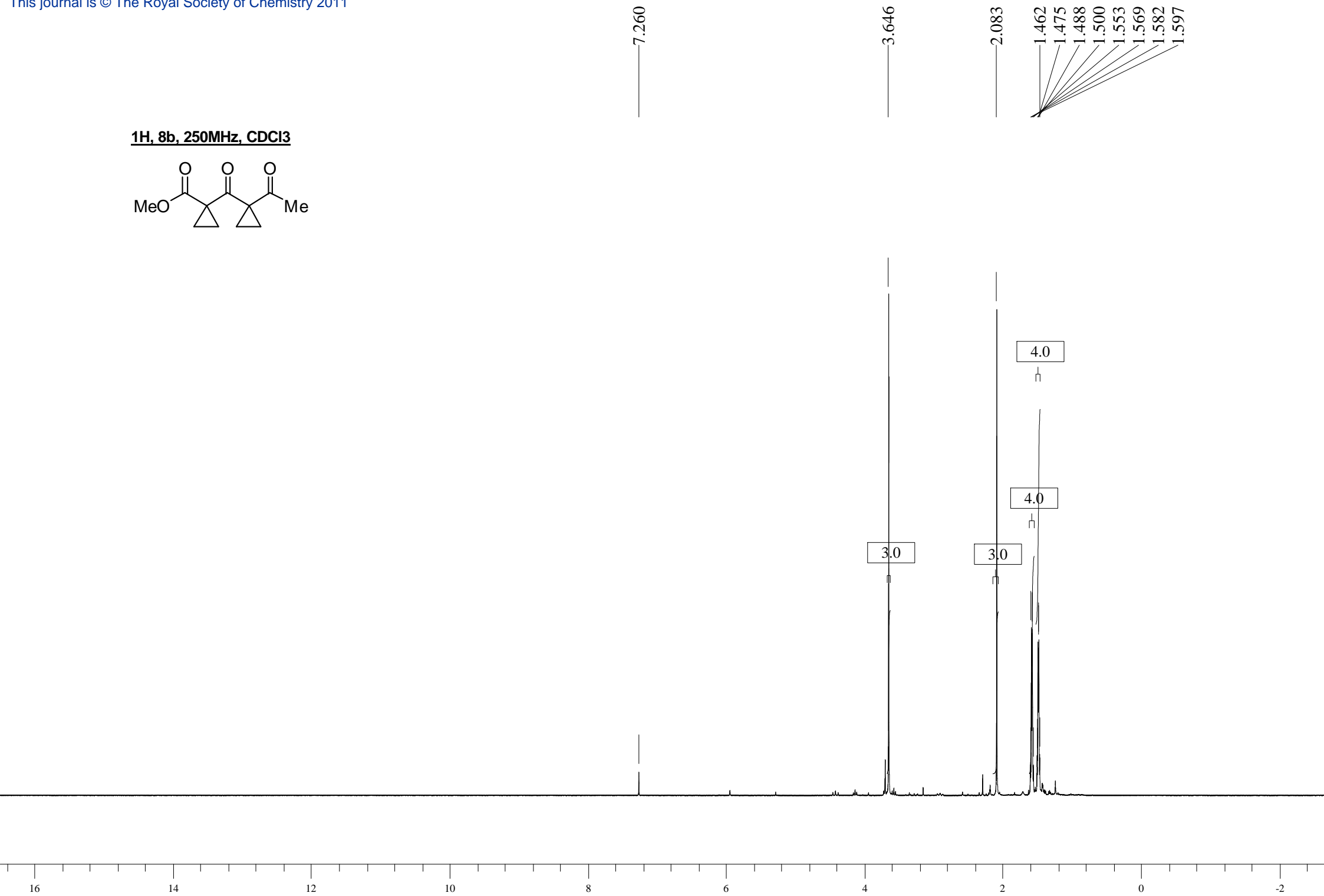
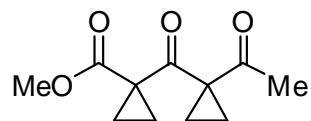
F2 - Processing parameters

SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

**8a**, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>

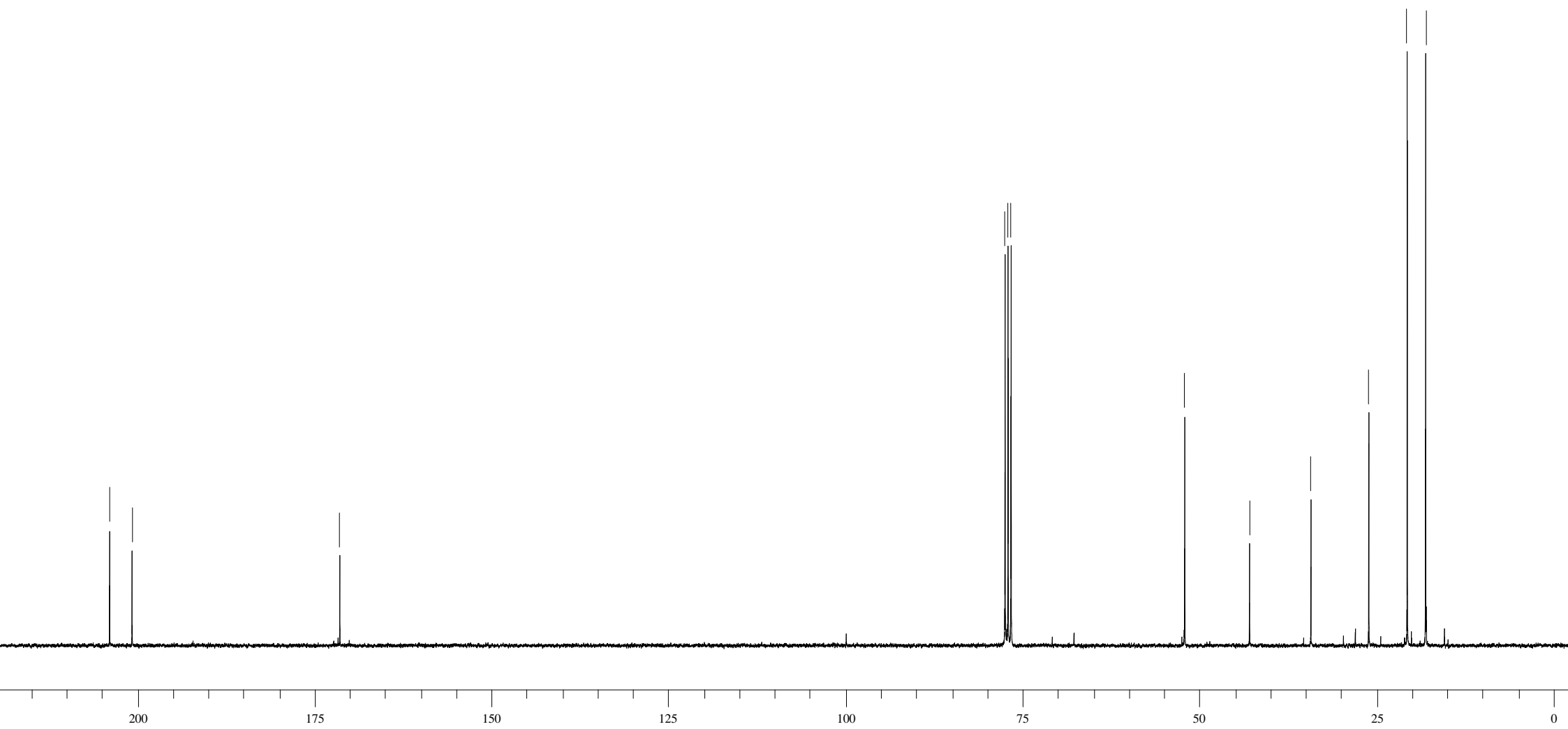
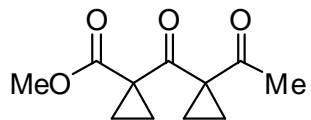


**1H, 8b, 250MHz, CDCl3**

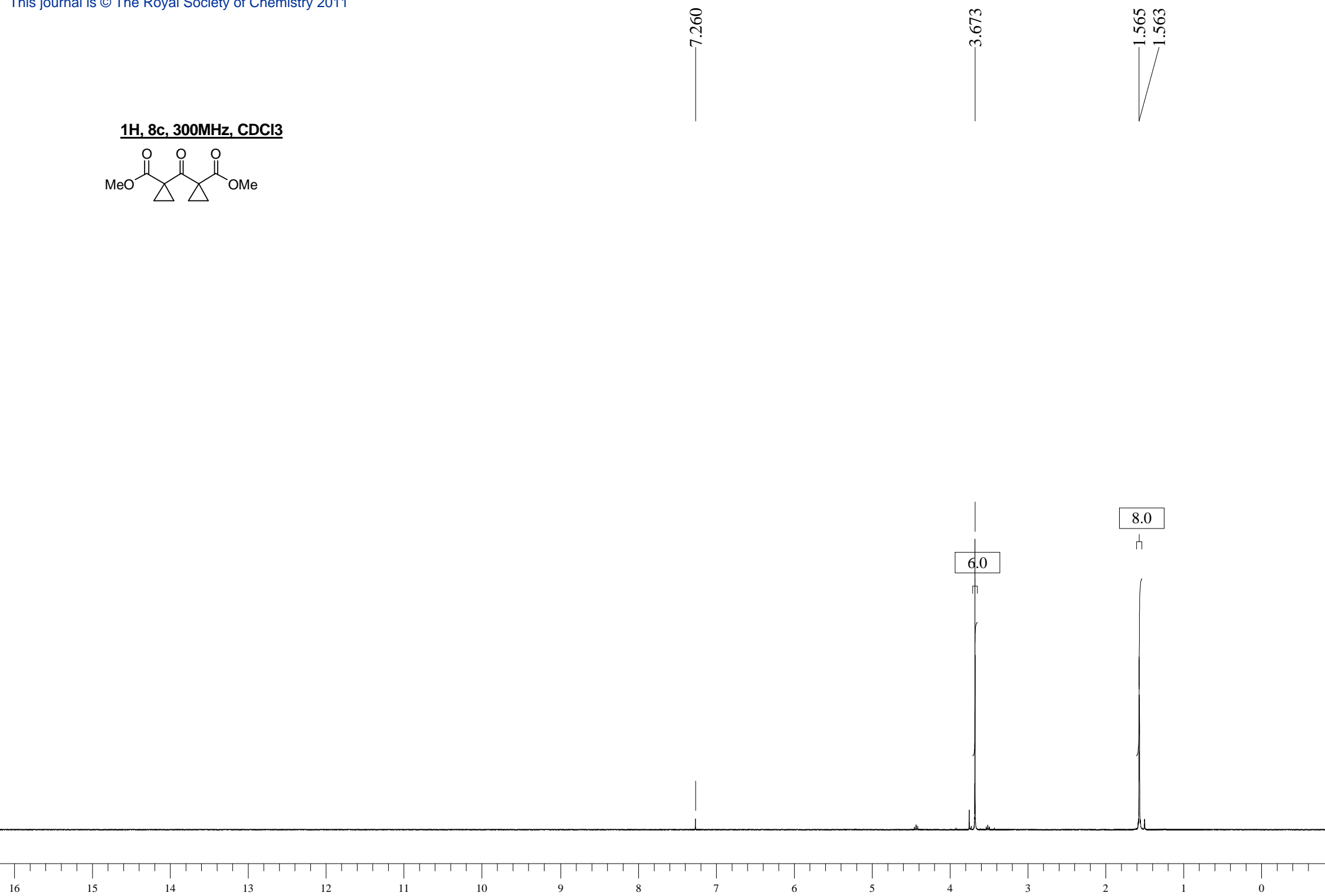
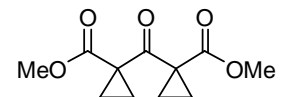




**13C, 8b, 75MHz, CDCl3**



**1H, 8c, 300MHz, CDCl3**



199.41

171.60

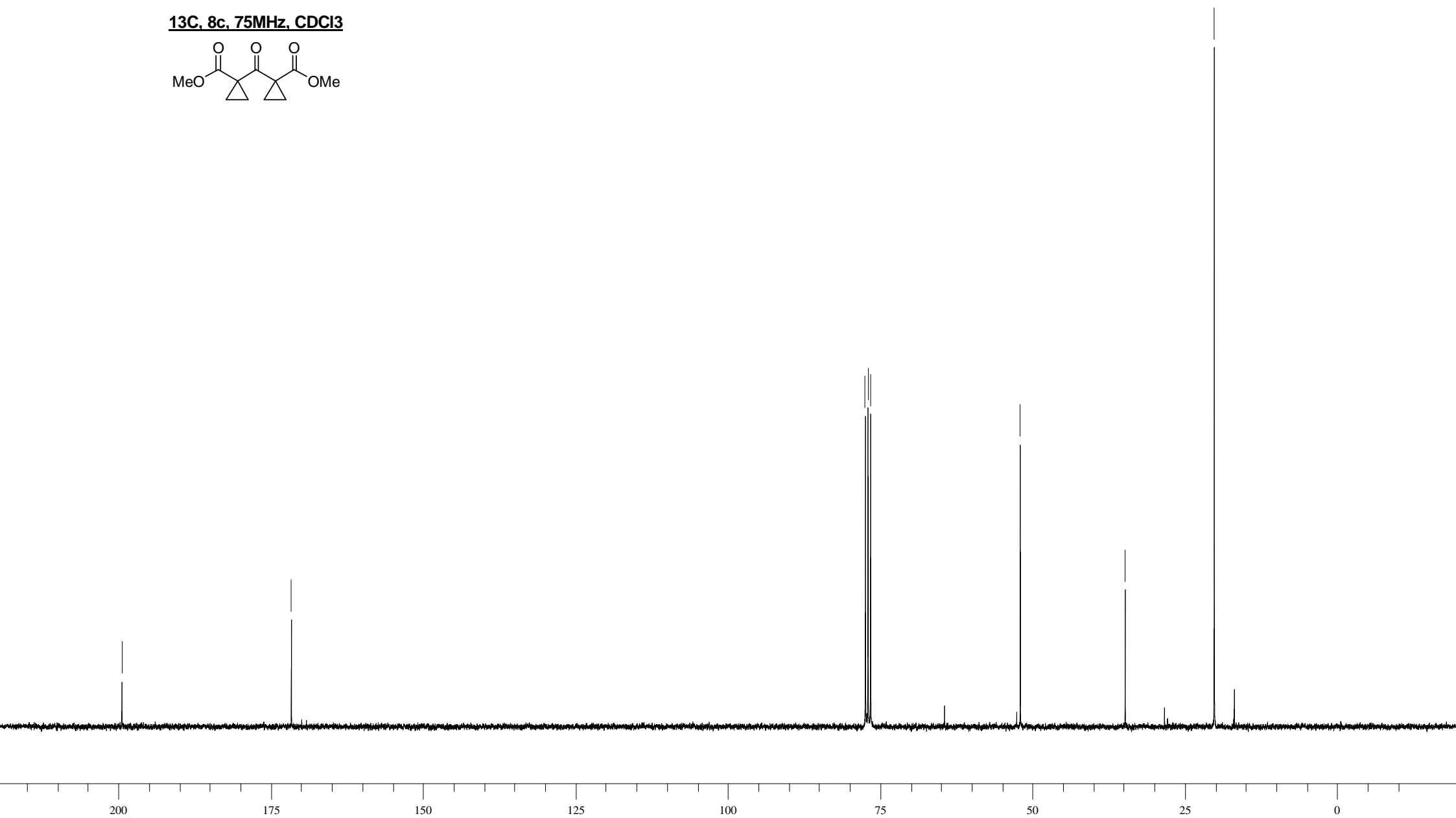
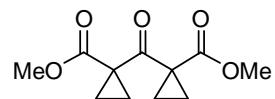
77.416  
76.994  
76.572

52.002

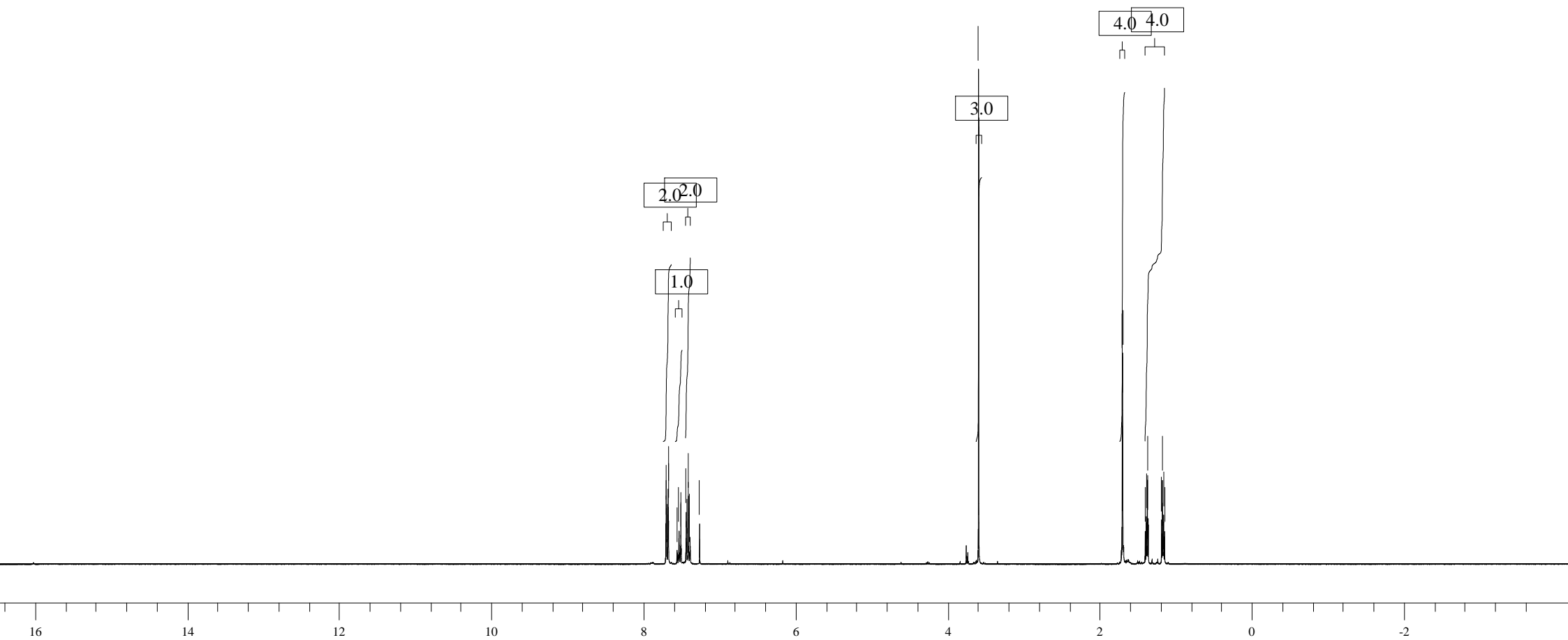
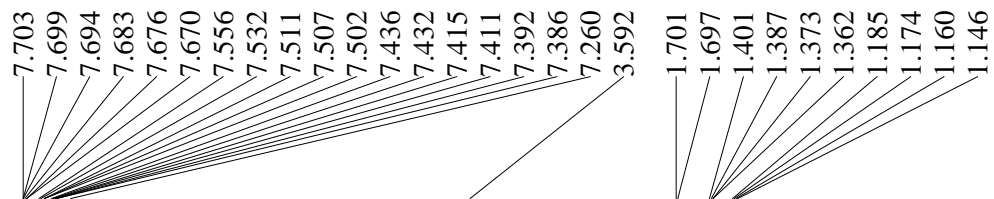
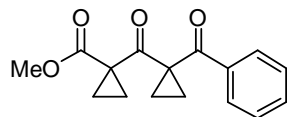
34.796

20.180

**13C, 8c, 75MHz, CDCl3**



**1H, 8d, 300MHz, CDCl3**





200.986  
196.940

170.495

138.152  
132.824  
128.449  
128.384

77.416  
76.994  
76.572

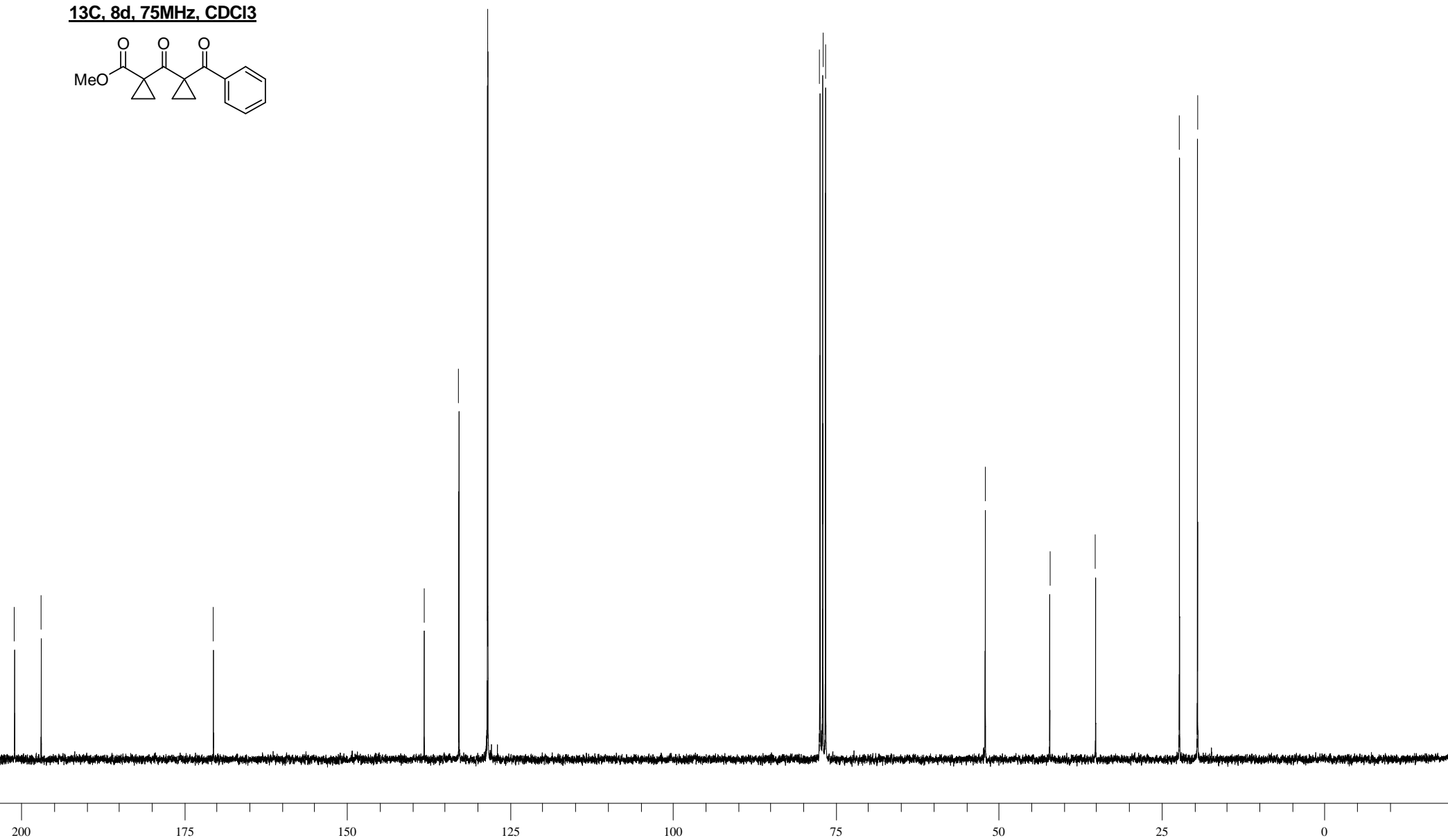
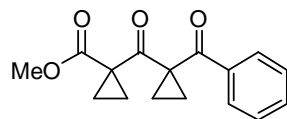
52.051

42.158

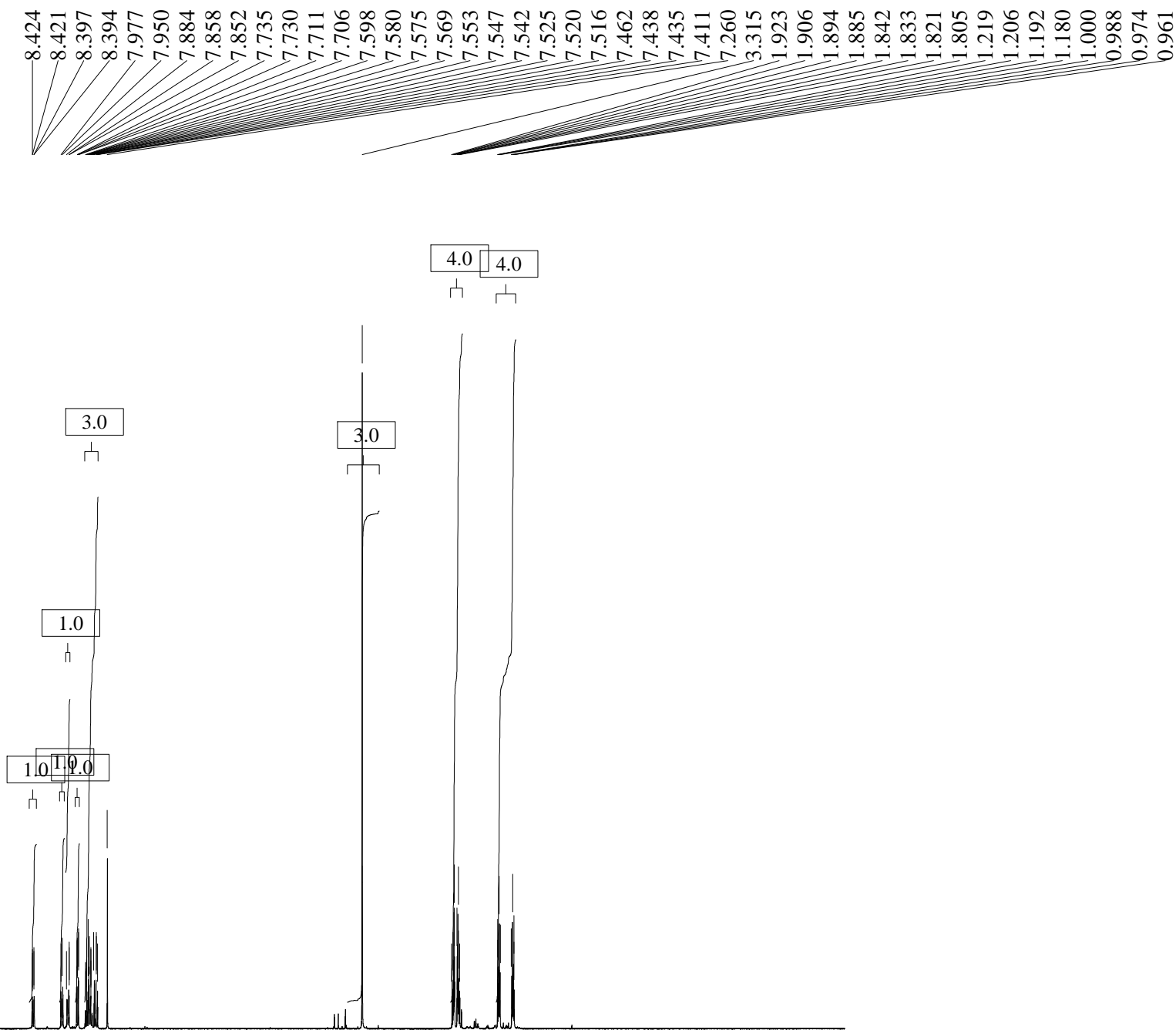
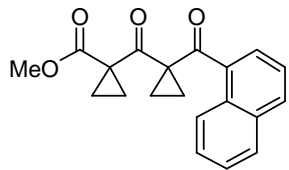
35.118

22.240  
19.486

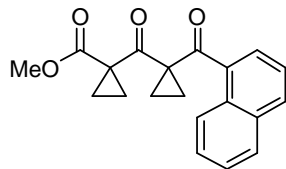
**13C, 8d, 75MHz, CDCl3**



**1H, 8e, 300MHz, CDCl3**



**13C, 8e, 75MHz, CDCl3**



201.068  
198.970  
170.677

135.822  
133.831  
132.445  
130.105  
128.346  
128.129  
127.554  
126.548  
125.732  
123.974

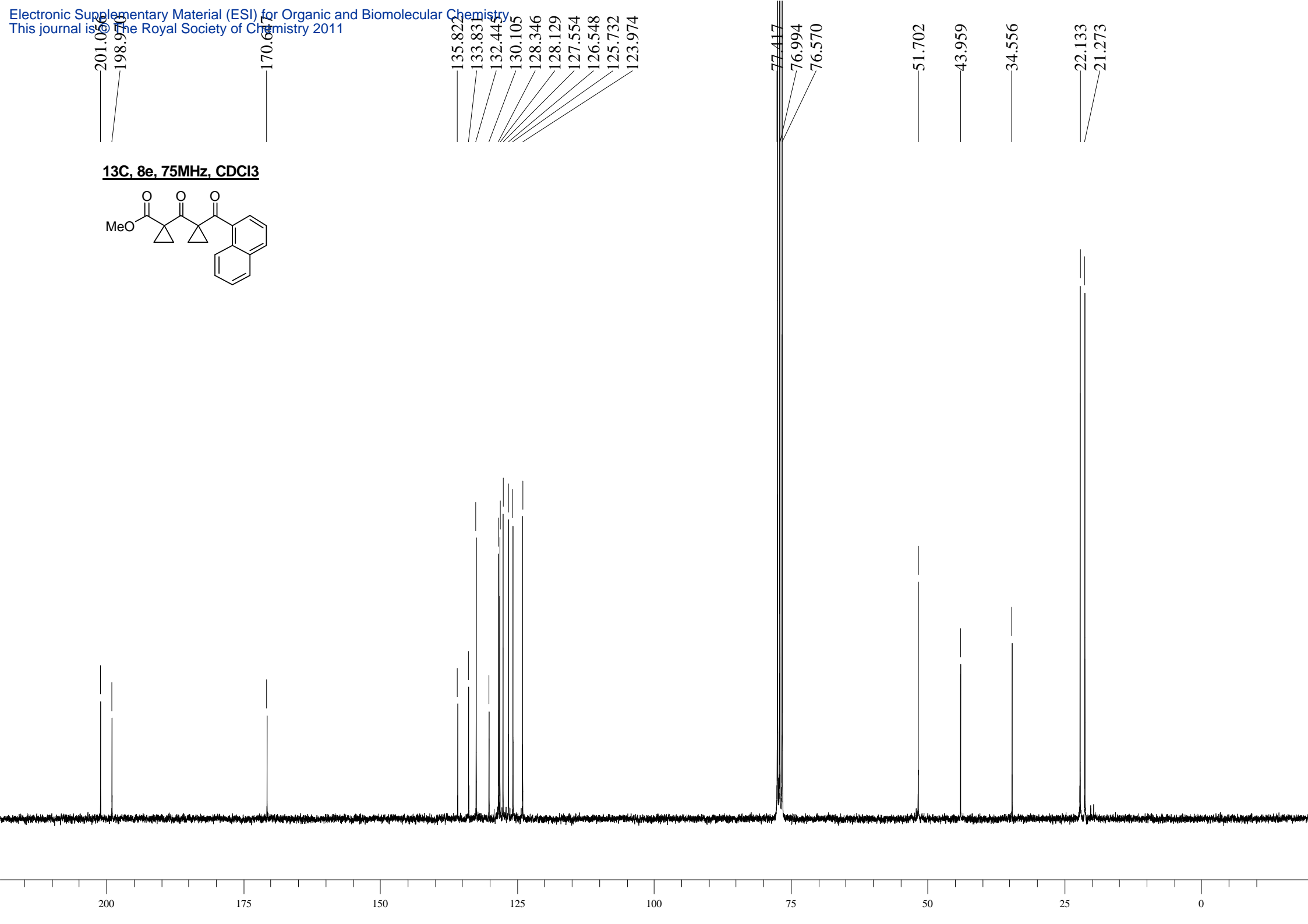
77.417  
76.994  
76.570

51.702

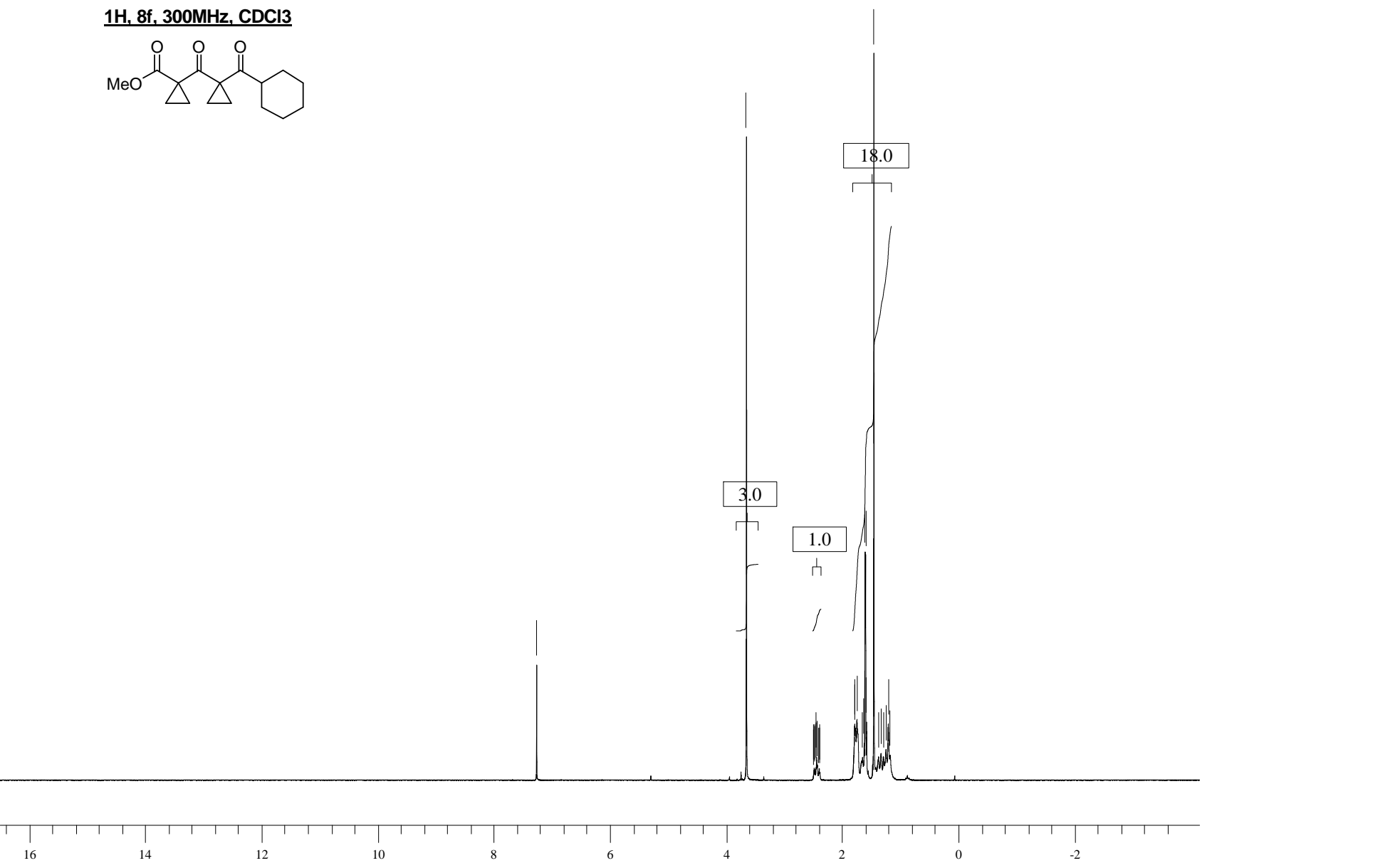
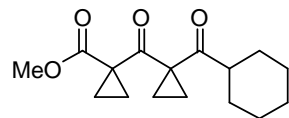
43.959

34.556

22.133  
21.273



**1H, 8f, 300MHz, CDCl3**

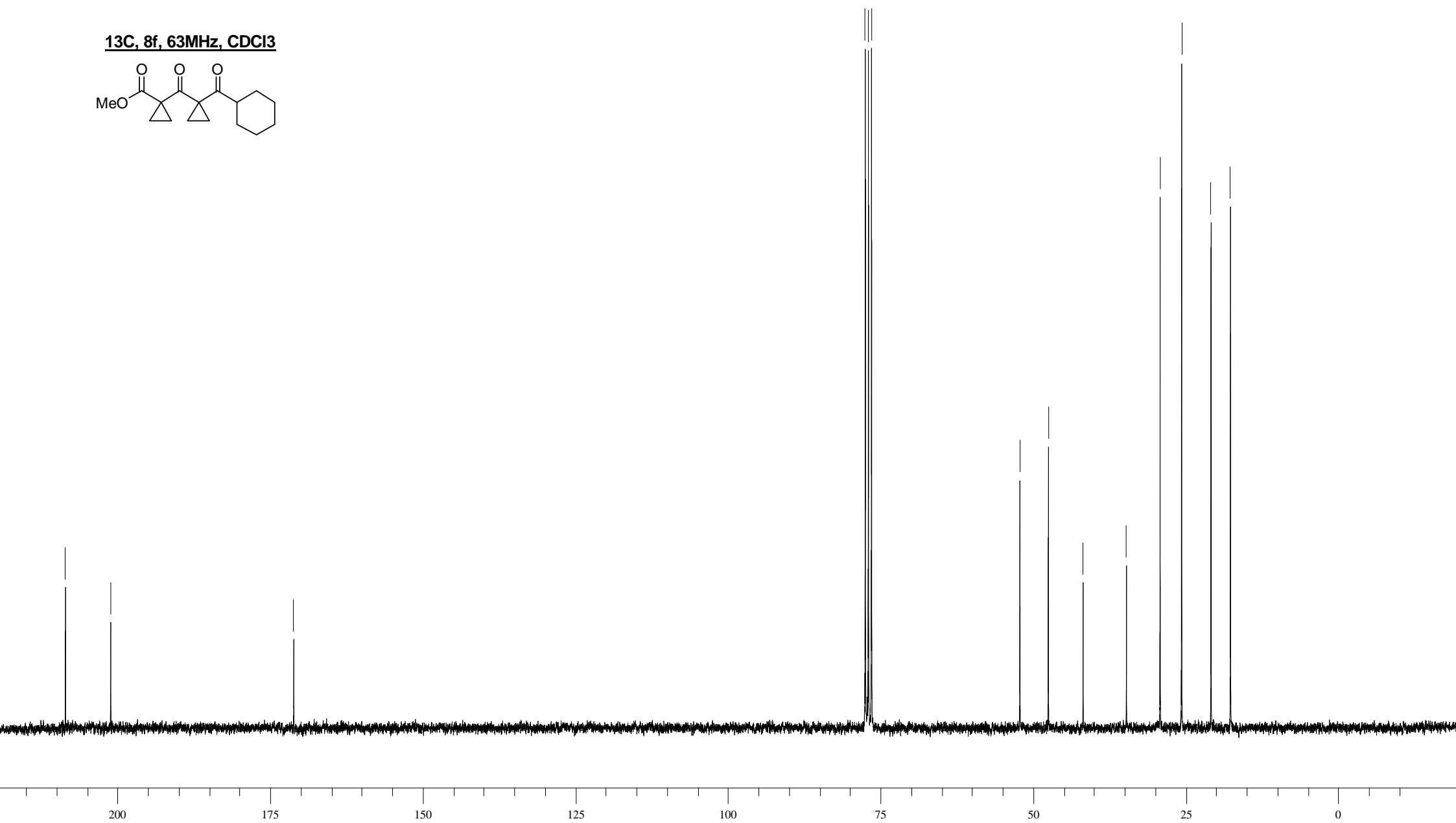
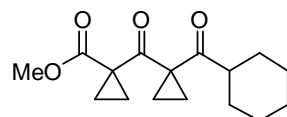


208.51  
201.17  
171.18

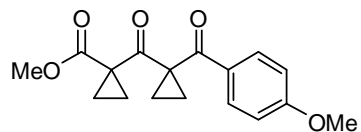
77.503  
76.992  
76.492

52.175  
47.519  
41.832  
34.730  
29.212  
25.691  
20.864  
17.678

**13C, 8f, 63MHz, CDCl3**



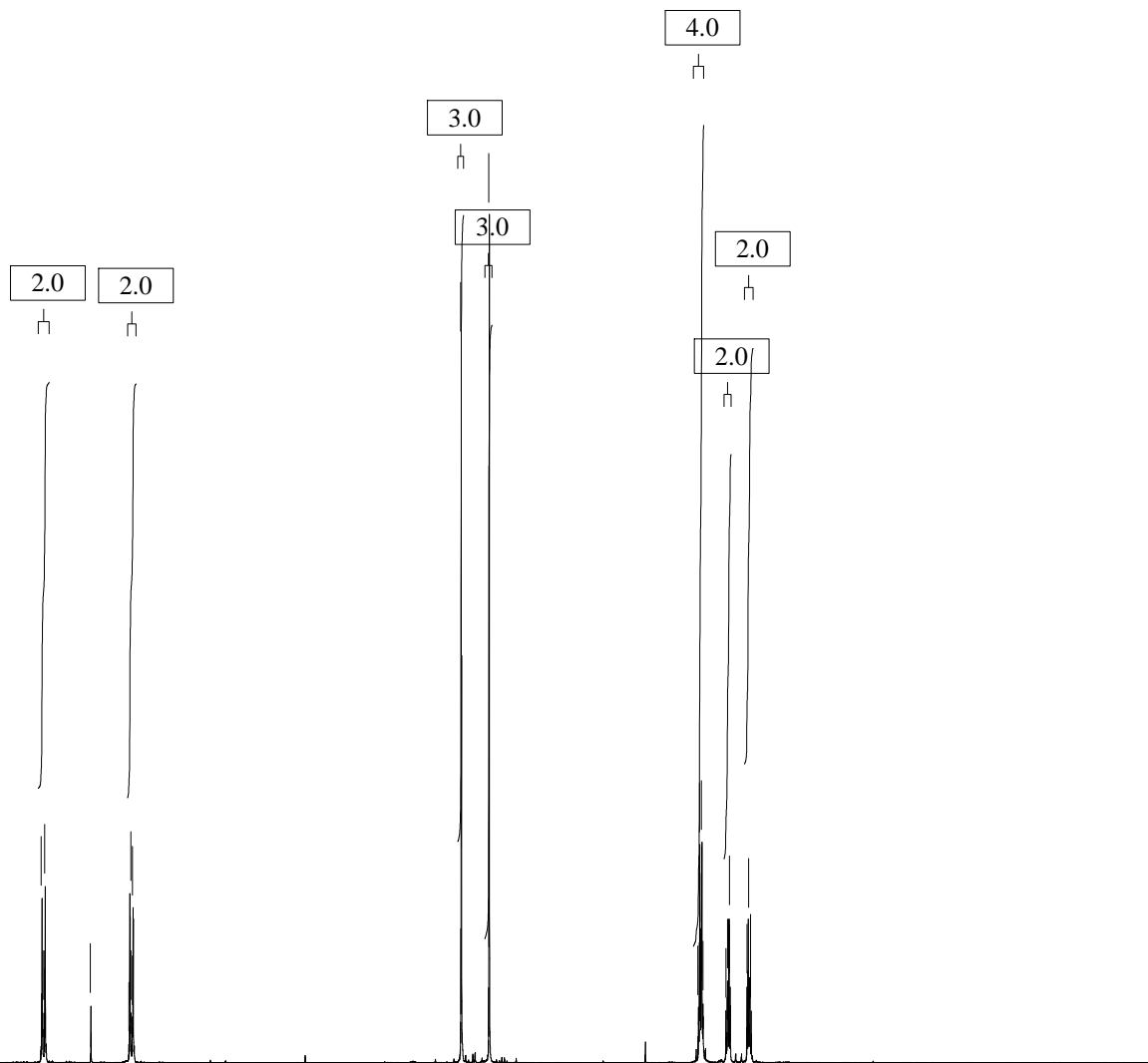
**1H, 8q, 300 MHz, CDCl3**

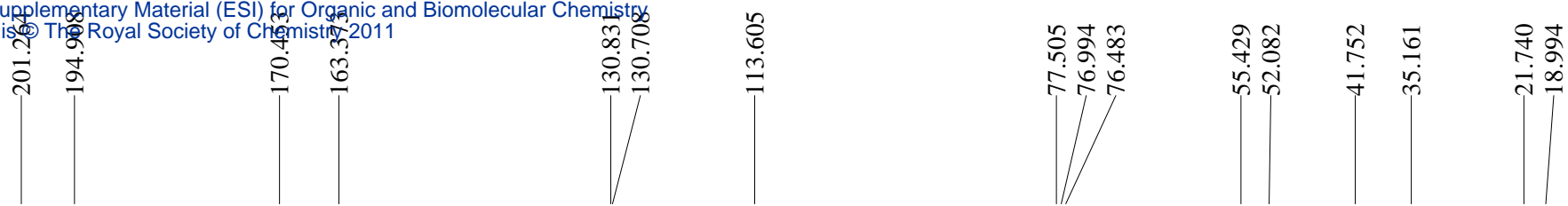


7.710  
7.703  
6.910  
6.901  
6.894  
6.878  
6.871  
7.687  
7.680  
7.260

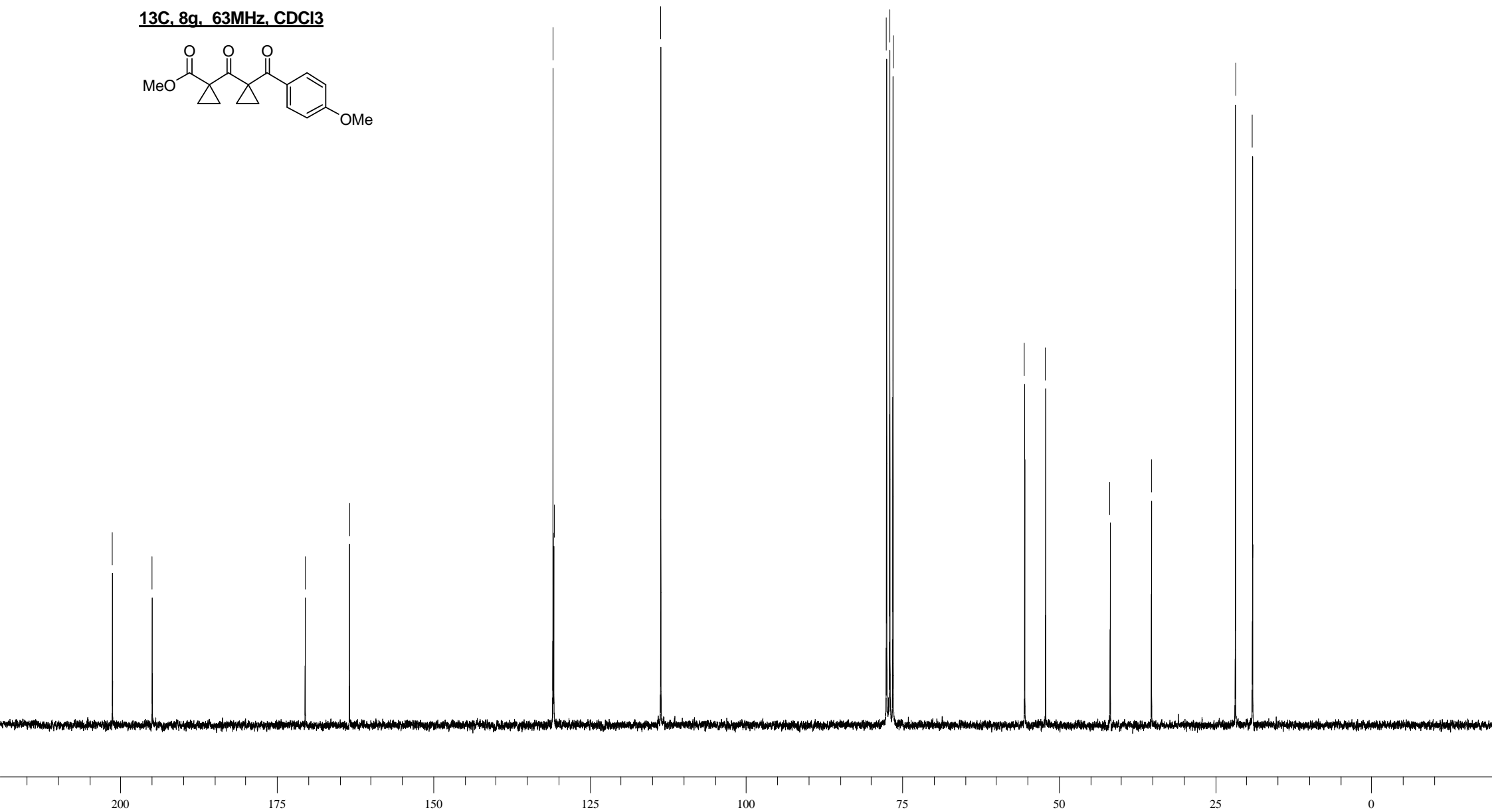
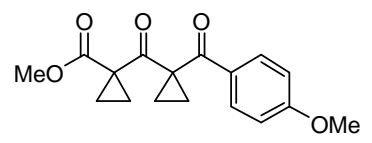
3.851  
3.594

1.667  
1.656  
1.651  
1.642  
1.636  
1.626  
1.414  
1.400  
1.386  
1.375  
1.221  
1.210  
1.196  
1.182

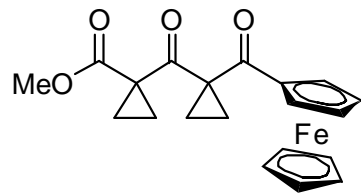




**13C, 8q, 63MHz, CDCl<sub>3</sub>**

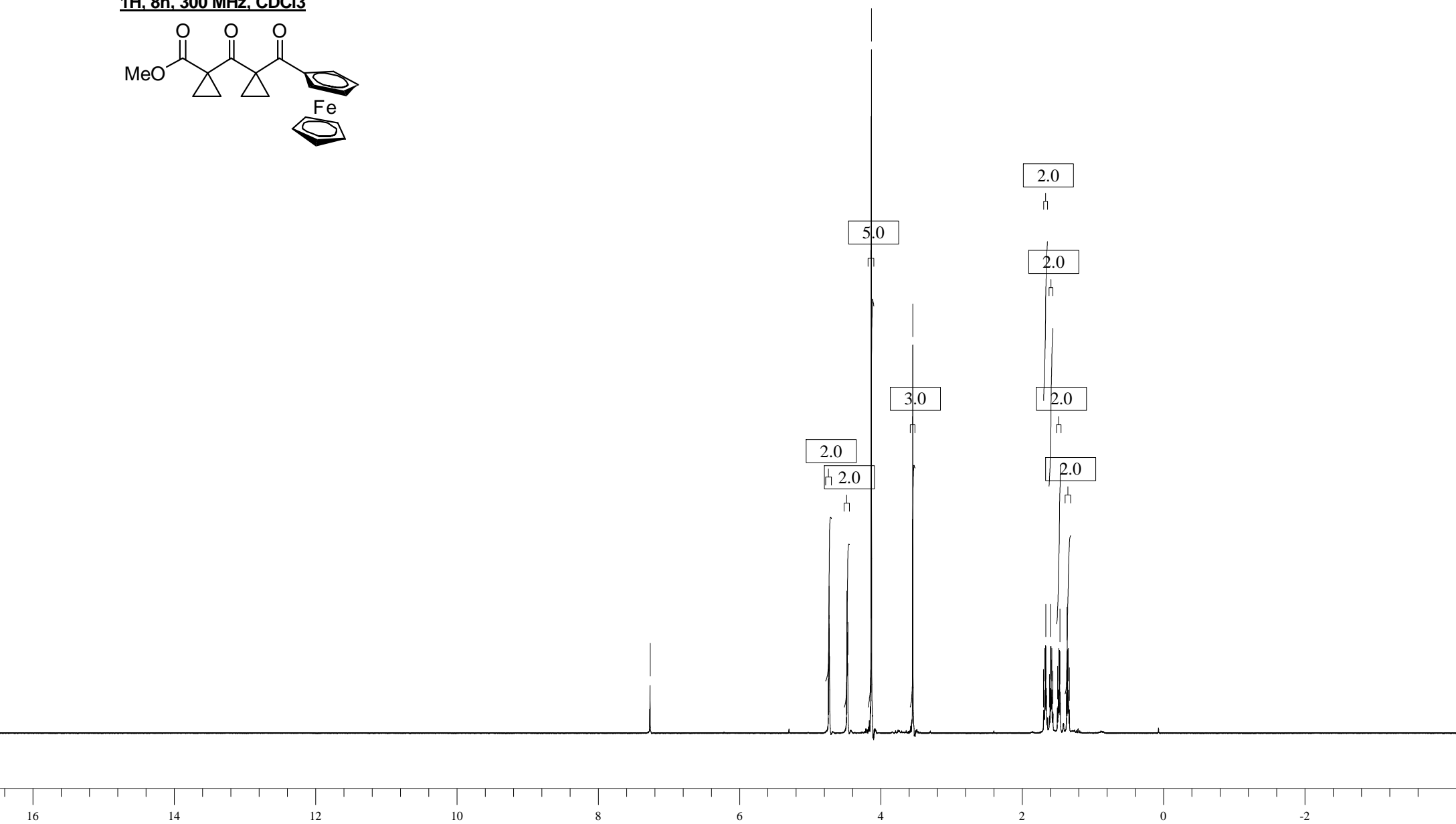


**1H, 8h, 300 MHz, CDCl3**



7.260

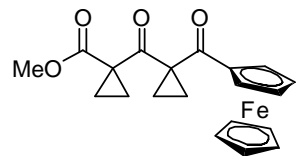
4.732  
4.126  
3.540  
4.725  
4.720  
4.473  
4.468  
1.688  
1.683  
1.671  
1.660  
1.650  
1.606  
1.594  
1.584  
1.573  
1.556  
1.492  
1.477  
1.464  
1.453  
1.362  
1.351  
1.339  
1.324  
4.462



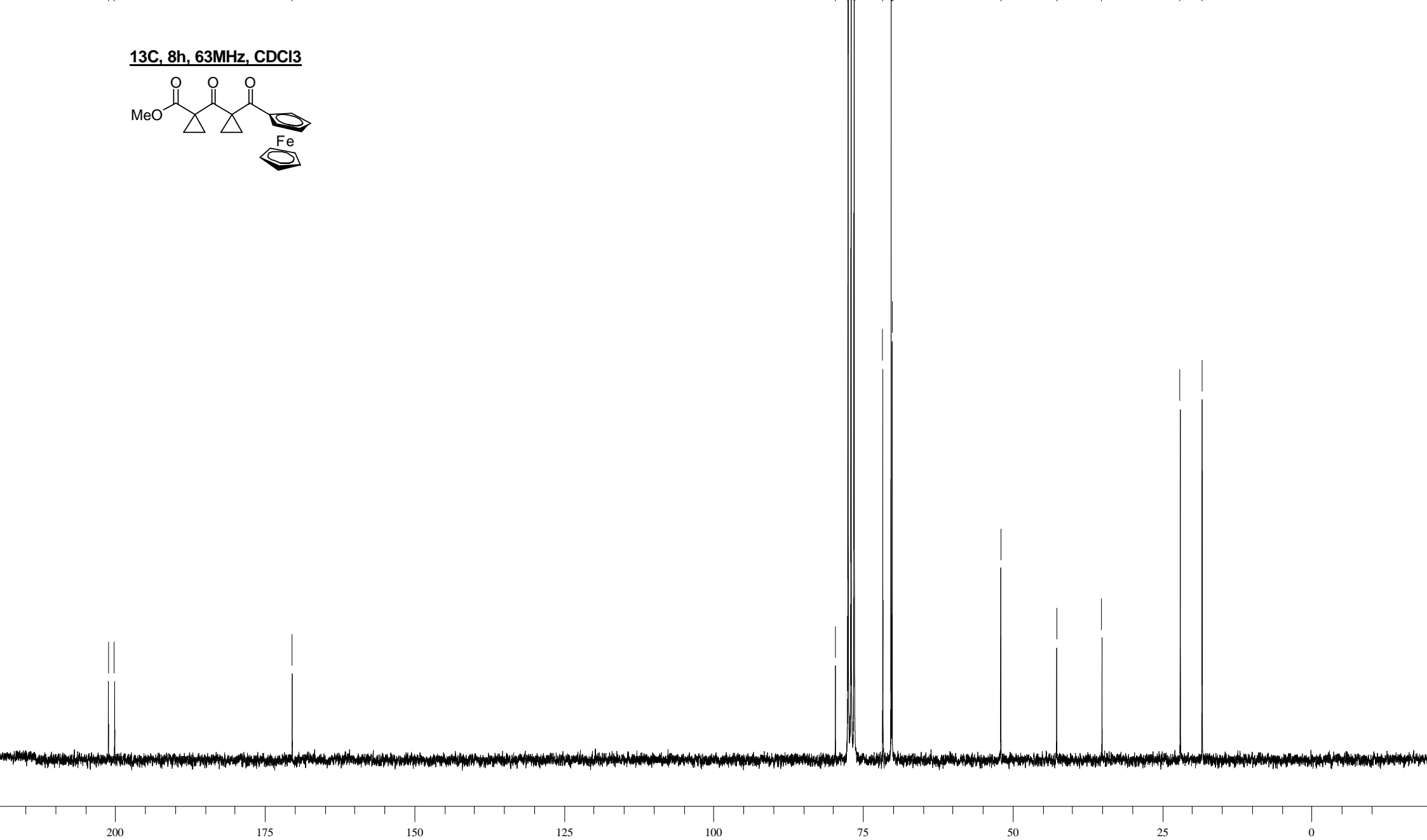


201.177  
200.090  
170.410

**13C, 8h, 63MHz, CDCl3**



79.630  
77.512  
77.001  
76.498  
71.696  
70.322  
70.147  
51.973  
42.640  
35.059  
21.977  
18.326





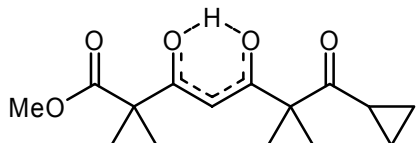
205.97  
193.10  
188.02  
170.23

100.22  
99.99

76.65

56.77  
52.61  
52.36  
39.99  
30.70  
27.89  
24.06  
21.56  
20.74  
19.78  
19.71  
19.41  
18.74  
18.58  
18.51  
17.90  
17.64  
16.76  
16.42  
12.40  
12.34

9, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>



Current Data Parameters  
NAME 070524.305  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters

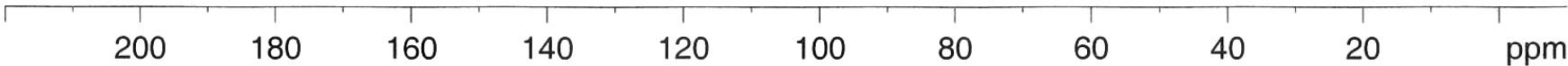
Date\_ 20070524  
Time 20.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.4 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

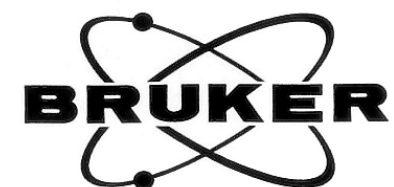
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
NAME 080627.323  
EXPNO 11  
PROCNO 1

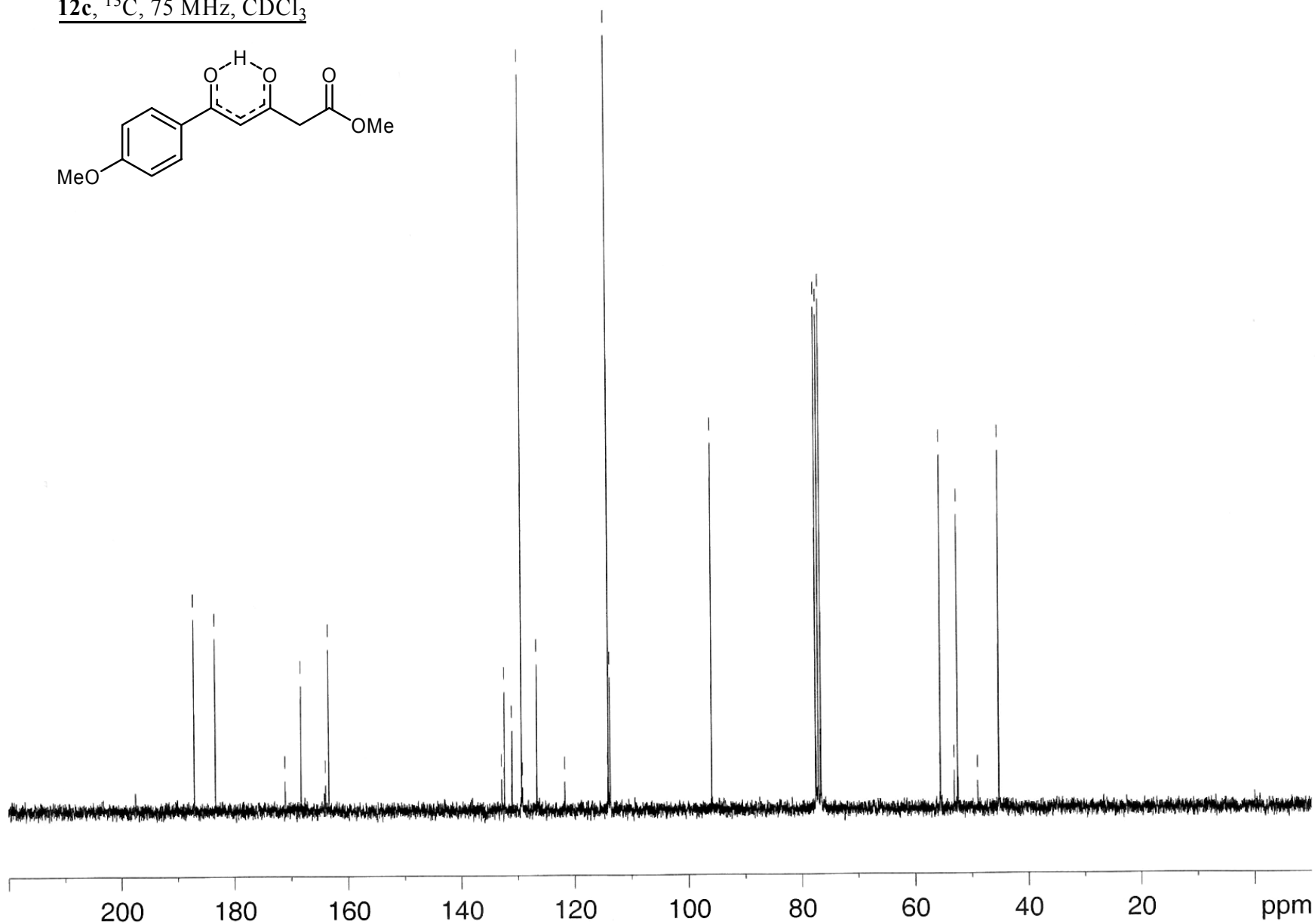
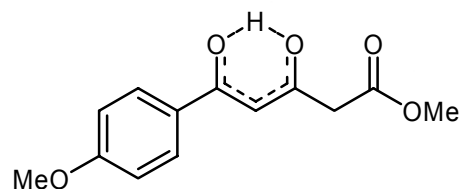
F2 - Acquisition Parameters  
Date\_ 20080627  
Time 23.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.2 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

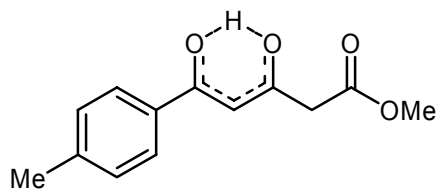
F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

12c, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>





**12d**,  $^1\text{H}$ , 300 MHz,  $\text{CDCl}_3$

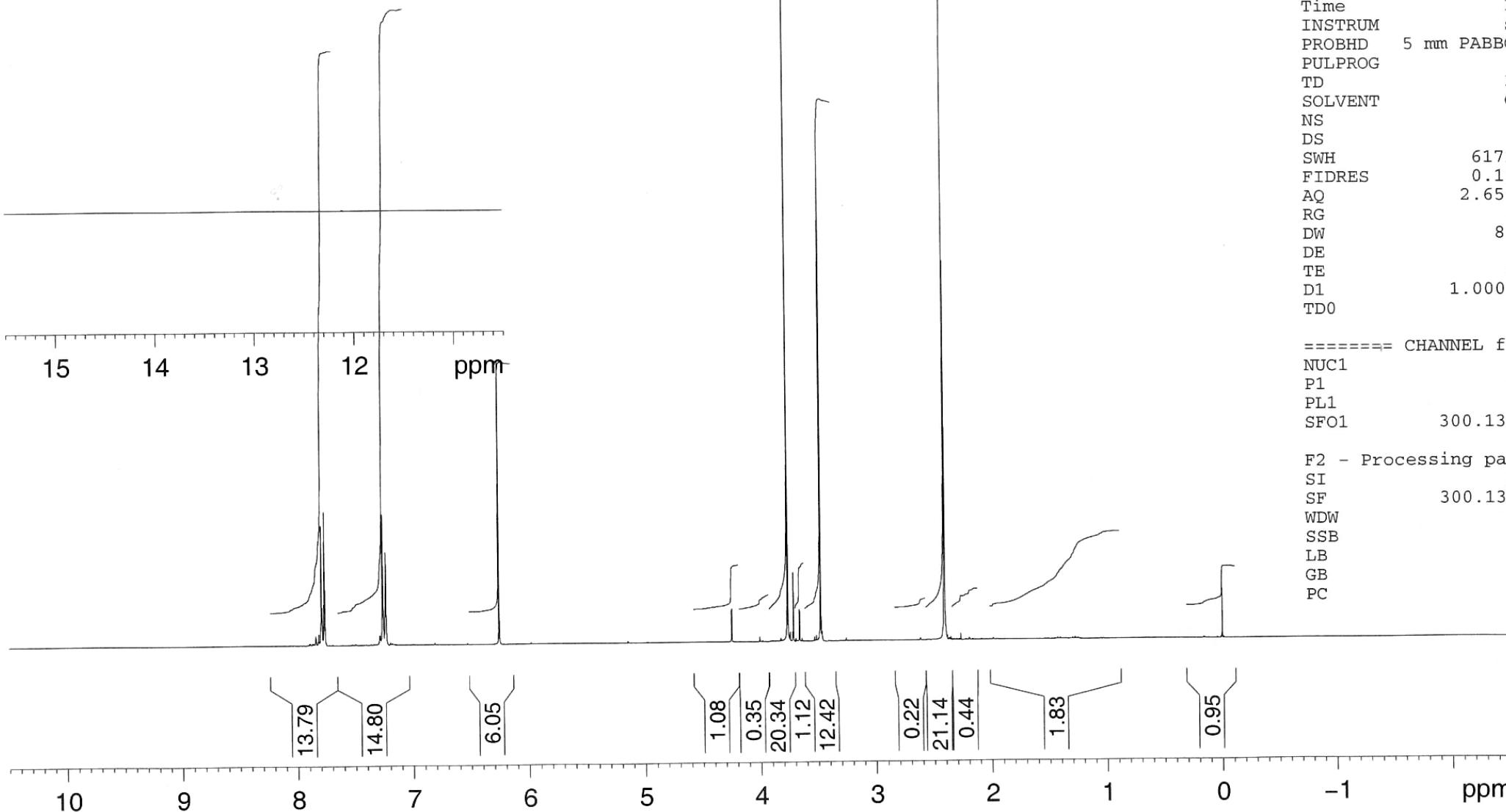


Current Data Parameters  
NAME 080725.306  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080725  
Time 19.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT  $\text{CDCl}_3$   
NS 32  
DS 4  
SWH 6172.839 Hz  
FIDRES 0.188380 Hz  
AQ 2.6542580 sec  
RG 143.7  
DW 81.000 usec  
DE 6.00 usec  
TE 295.6 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1  $^1\text{H}$   
P1 11.00 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300135 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME 080725.306  
EXPNO 11  
PROCNO 1

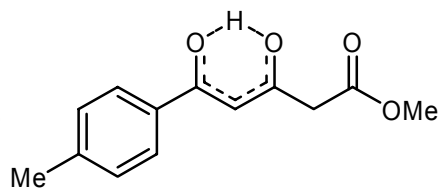
F2 - Acquisition Parameters  
Date\_ 20080725  
Time 19.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

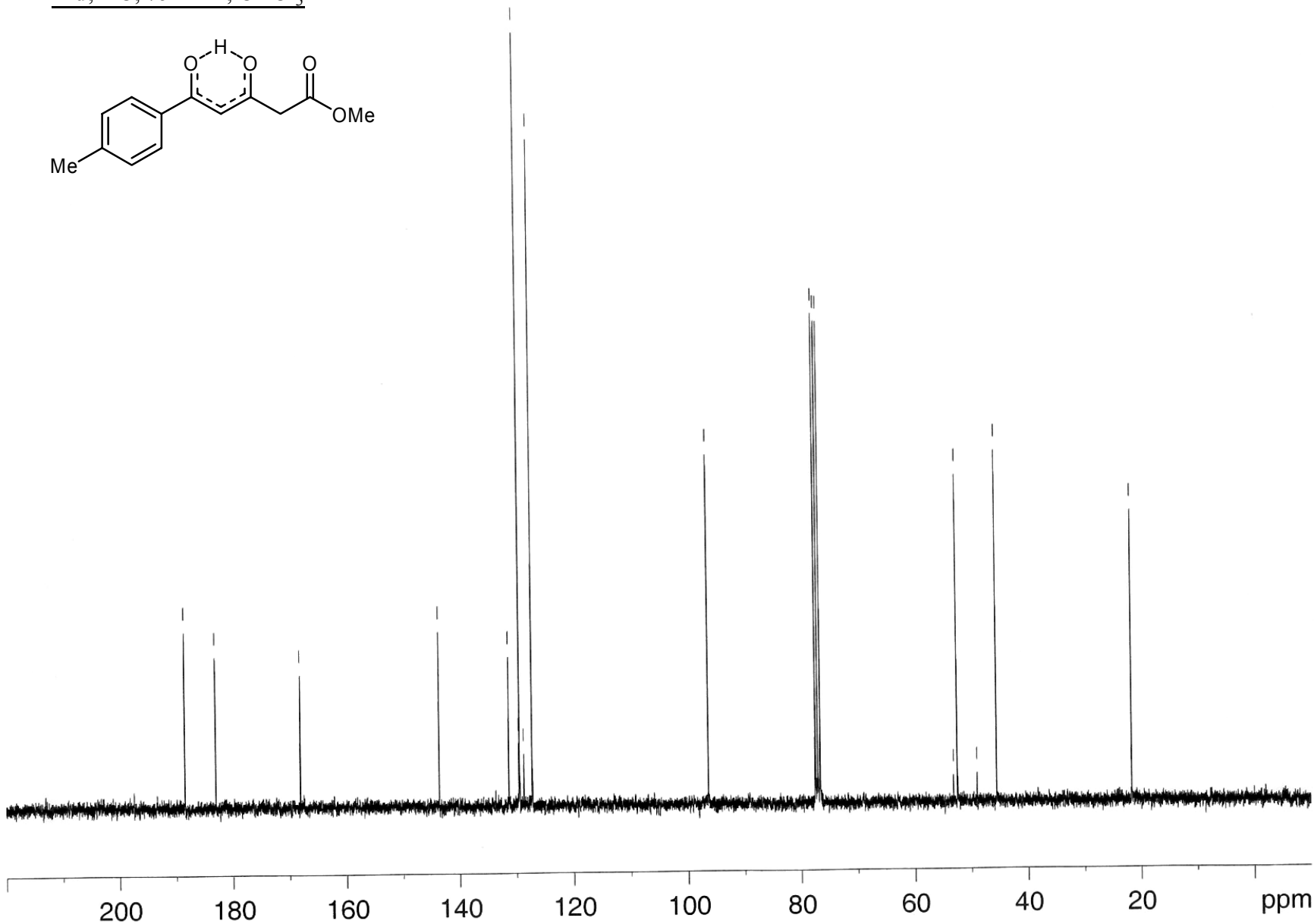
==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

12d, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>

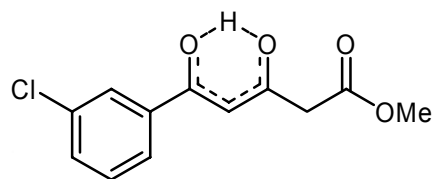


188.47  
183.07  
168.14  
143.63  
131.35  
129.58  
129.47  
128.73  
127.23  
96.43  
77.52  
77.10  
76.68  
53.16  
52.54  
52.45  
49.03  
45.58  
21.75  
21.68

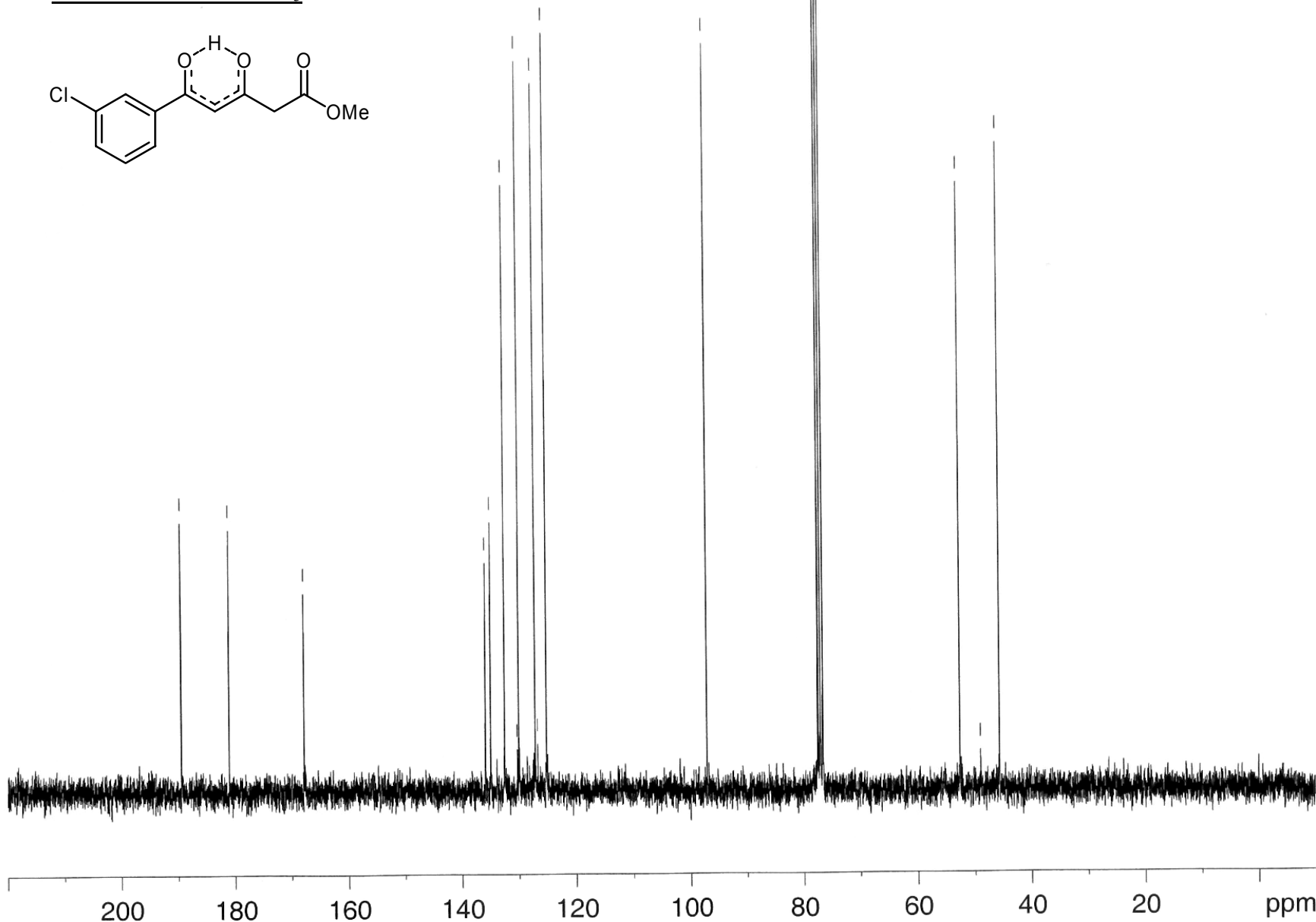




**12e**,  $^{13}\text{C}$ , 75 MHz,  $\text{CDCl}_3$



189.49  
181.05  
167.84  
135.90  
134.98  
132.55  
130.31  
130.02  
127.22  
126.73  
125.21  
97.11  
77.51  
77.09  
76.67  
52.61  
48.98  
45.66



Current Data Parameters  
NAME 080730.309  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080730  
Time 20.37  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT  $\text{CDCl}_3$   
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.9 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

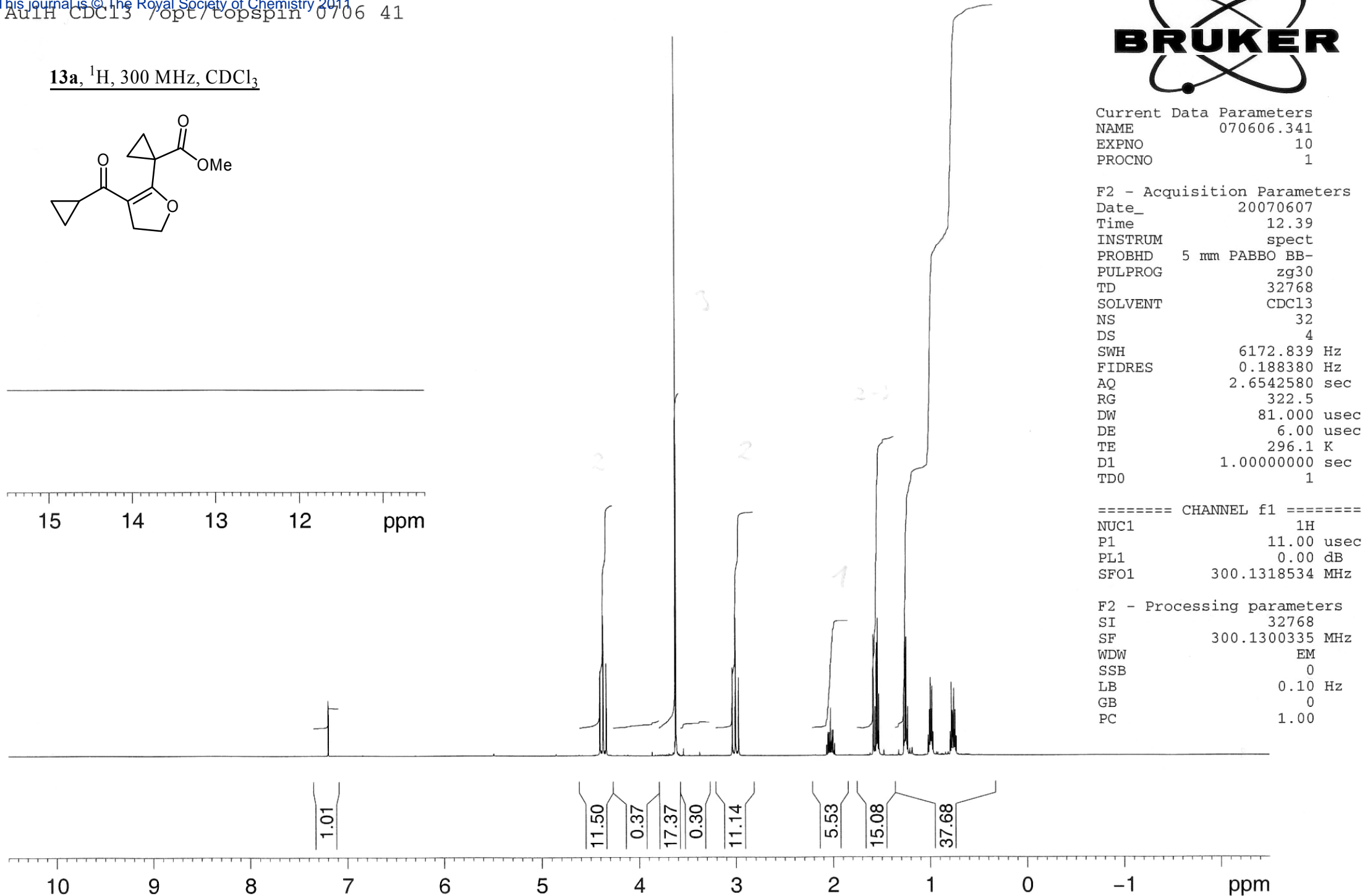
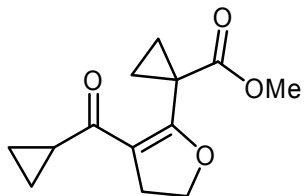
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

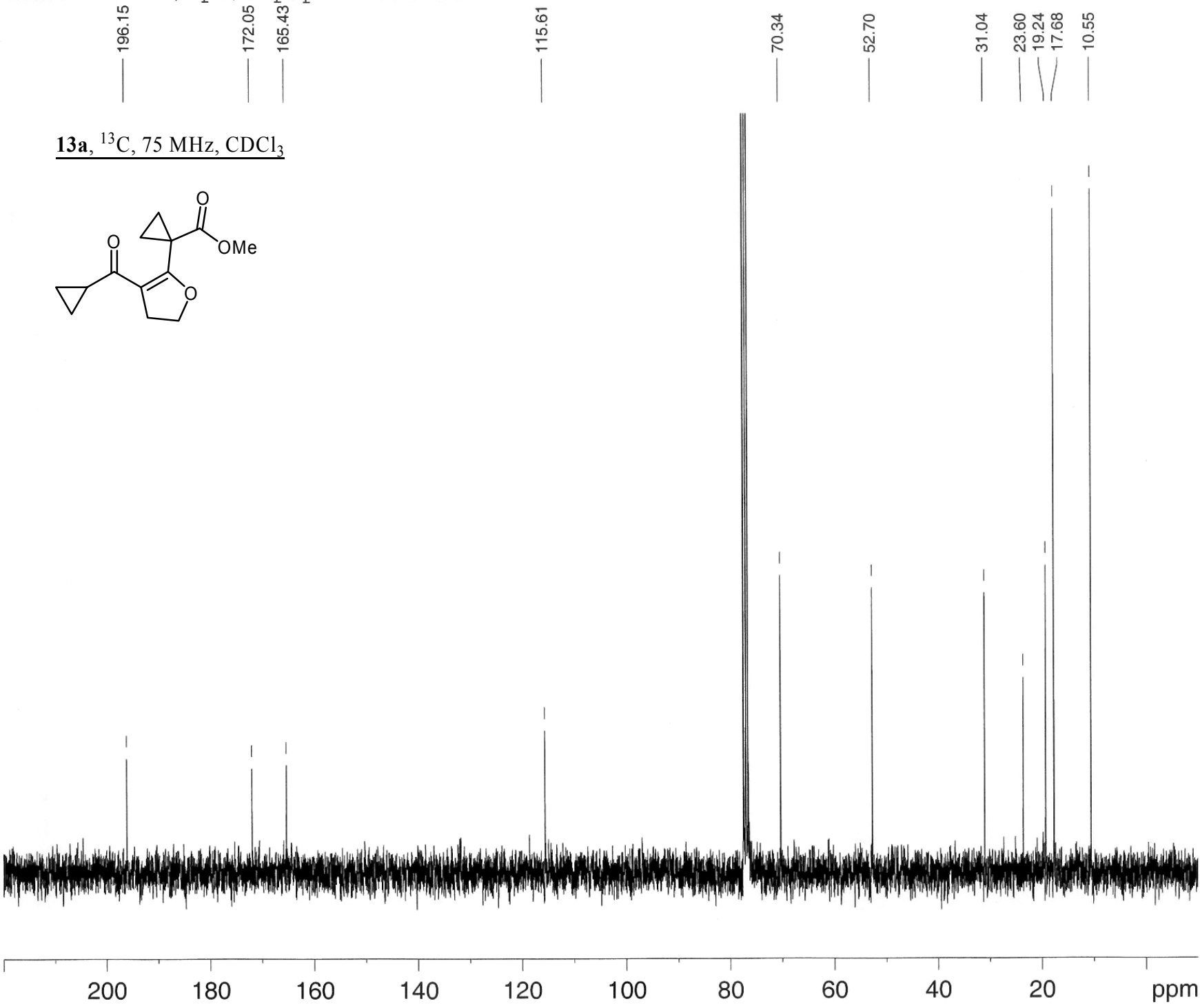
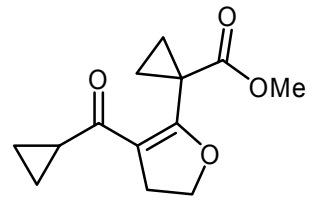
AuH CDCl3 /opt/topspin 0706 41

**13a**, <sup>1</sup>H, 300 MHz, CDCl<sub>3</sub>





**13a**, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>



Current Data Parameters  
NAME 070606.341  
EXPNO 11  
PROCNO 1

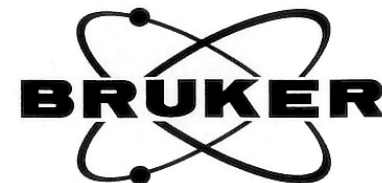
F2 - Acquisition Parameters  
Date\_ 20070607  
Time 12.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.6 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

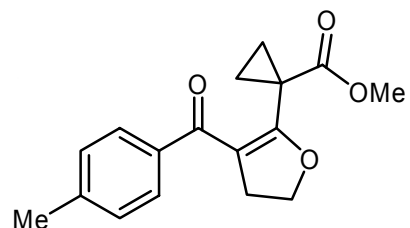
==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





**13d**, <sup>1</sup>H, 300 MHz, CDCl<sub>3</sub>

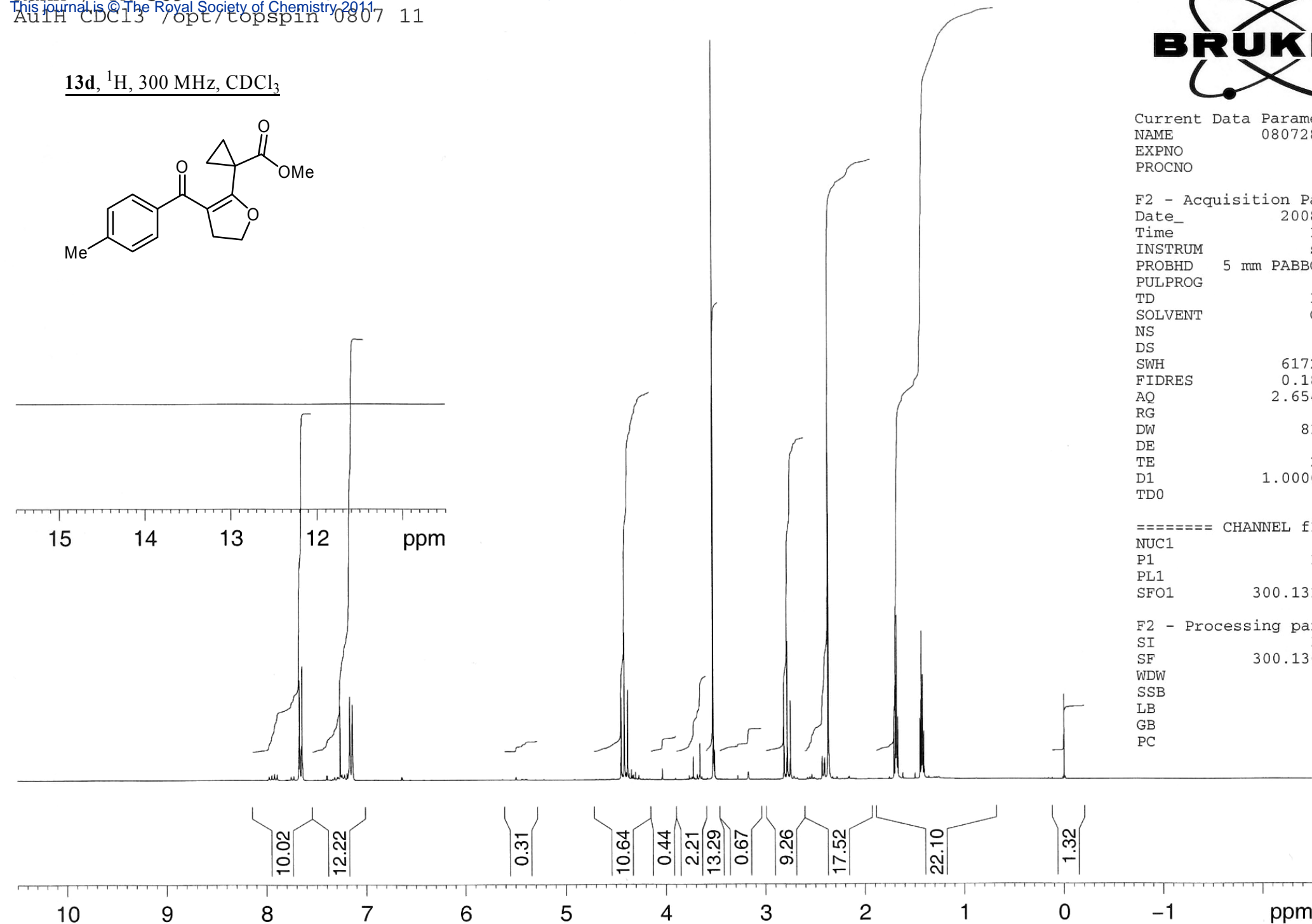


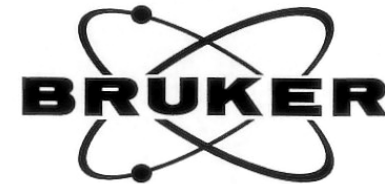
Current Data Parameters  
NAME 080728.311  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080728  
Time 19.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 4  
SWH 6172.839 Hz  
FIDRES 0.188380 Hz  
AQ 2.6542580 sec  
RG 256  
DW 81.000 usec  
DE 6.00 usec  
TE 297.0 K  
D1 1.0000000 sec  
TDO 1

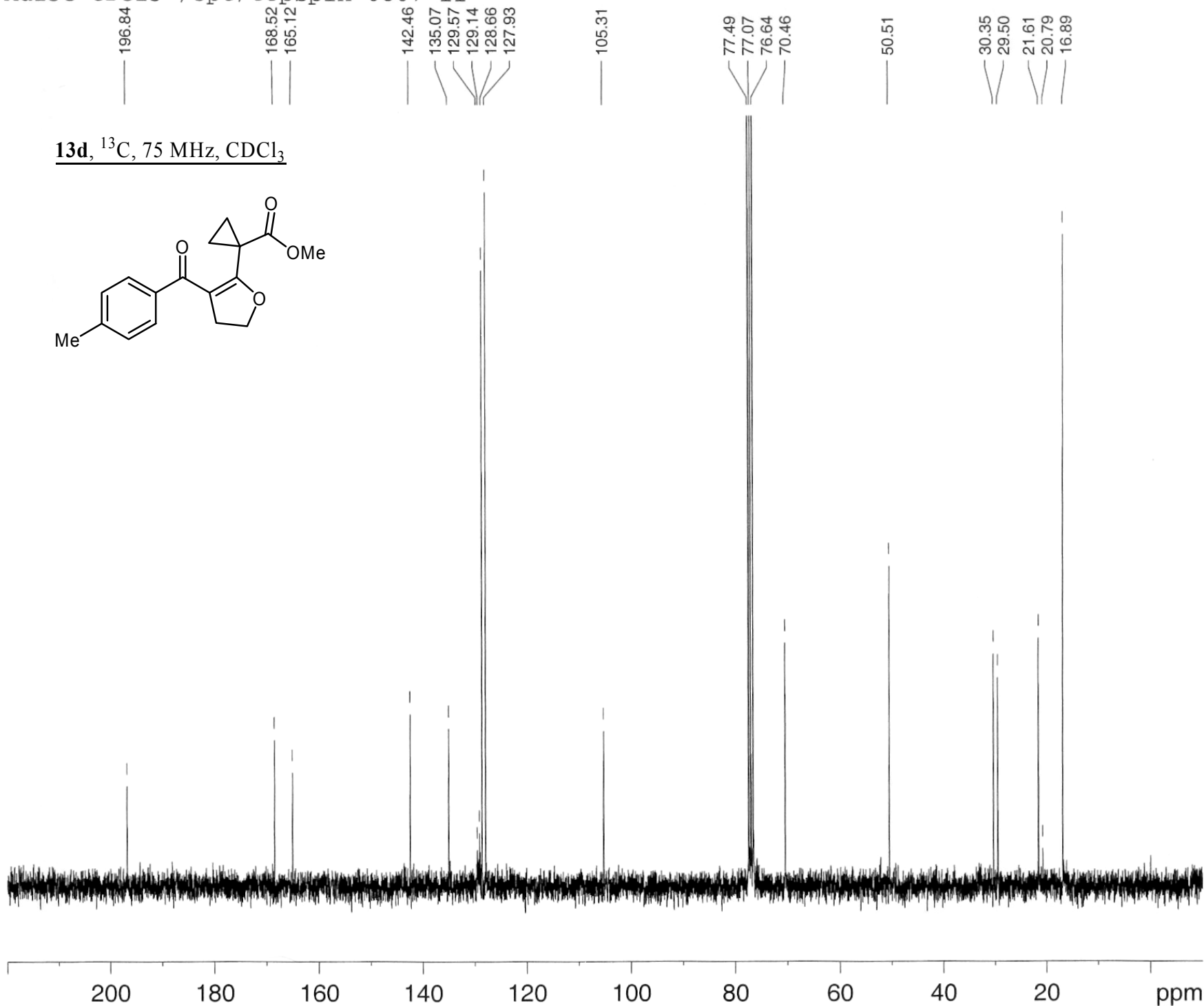
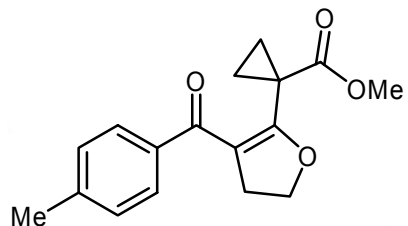
==== CHANNEL f1 =====  
NUC1 1H  
P1 11.00 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300134 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





**13d**,  $^{13}\text{C}$ , 75 MHz,  $\text{CDCl}_3$



Current Data Parameters  
NAME 080728.311  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080728  
Time 20.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT  $\text{CDCl}_3$   
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 297.4 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TDO 1

=====  
CHANNEL f1  
NUC1  $^{13}\text{C}$   
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

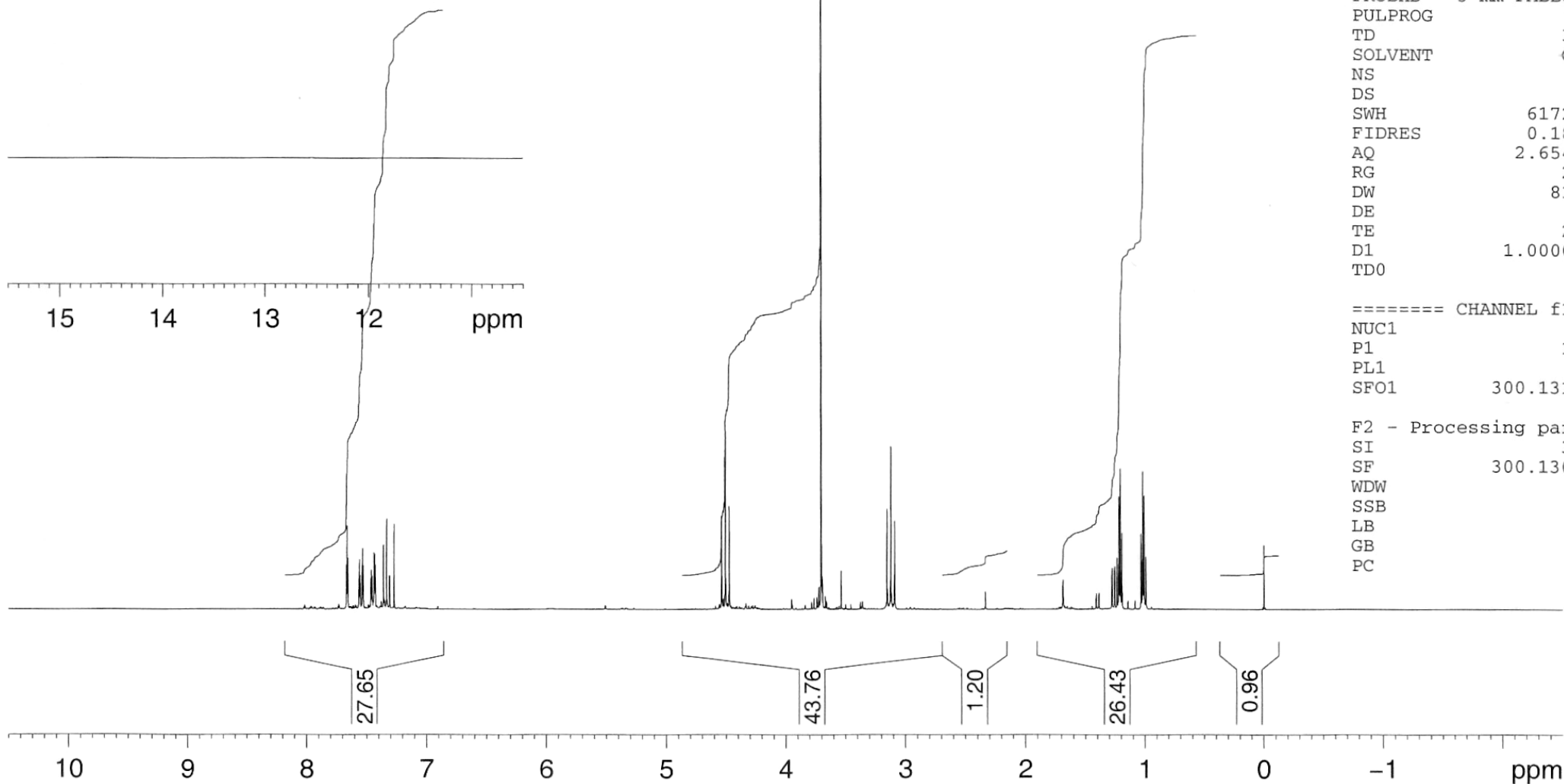
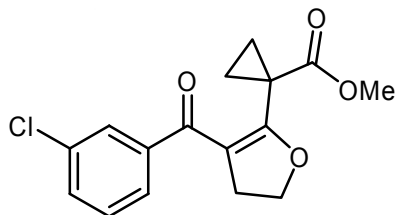
=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2  $^1\text{H}$   
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

AUIH CDC13 /opt/topspin 0808 6



13e, <sup>1</sup>H, 300 MHz, CDCl<sub>3</sub>



Current Data Parameters  
NAME 080801.306  
EXPNO 10  
PROCNO 1

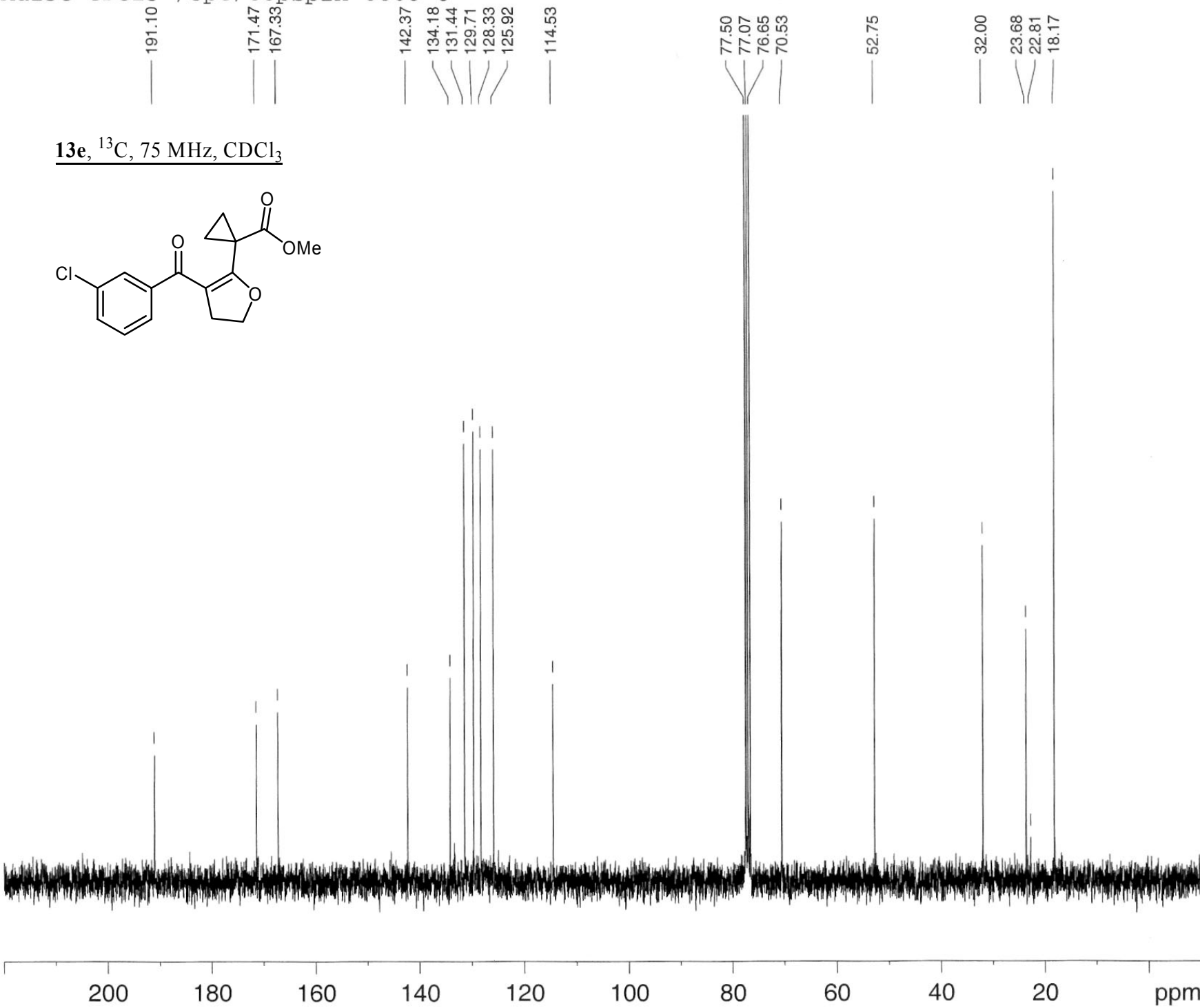
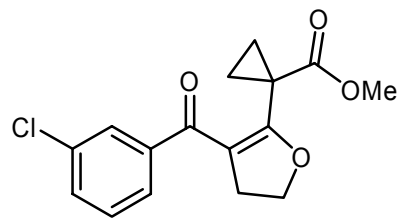
F2 - Acquisition Parameters  
Date\_ 20080801  
Time 17.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 4  
SWH 6172.839 Hz  
FIDRES 0.188380 Hz  
AQ 2.6542580 sec  
RG 228.1  
DW 81.000 usec  
DE 6.00 usec  
TE 296.5 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 11.00 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300116 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00



**13e**, <sup>13</sup>C, 75 MHz, CDCl<sub>3</sub>



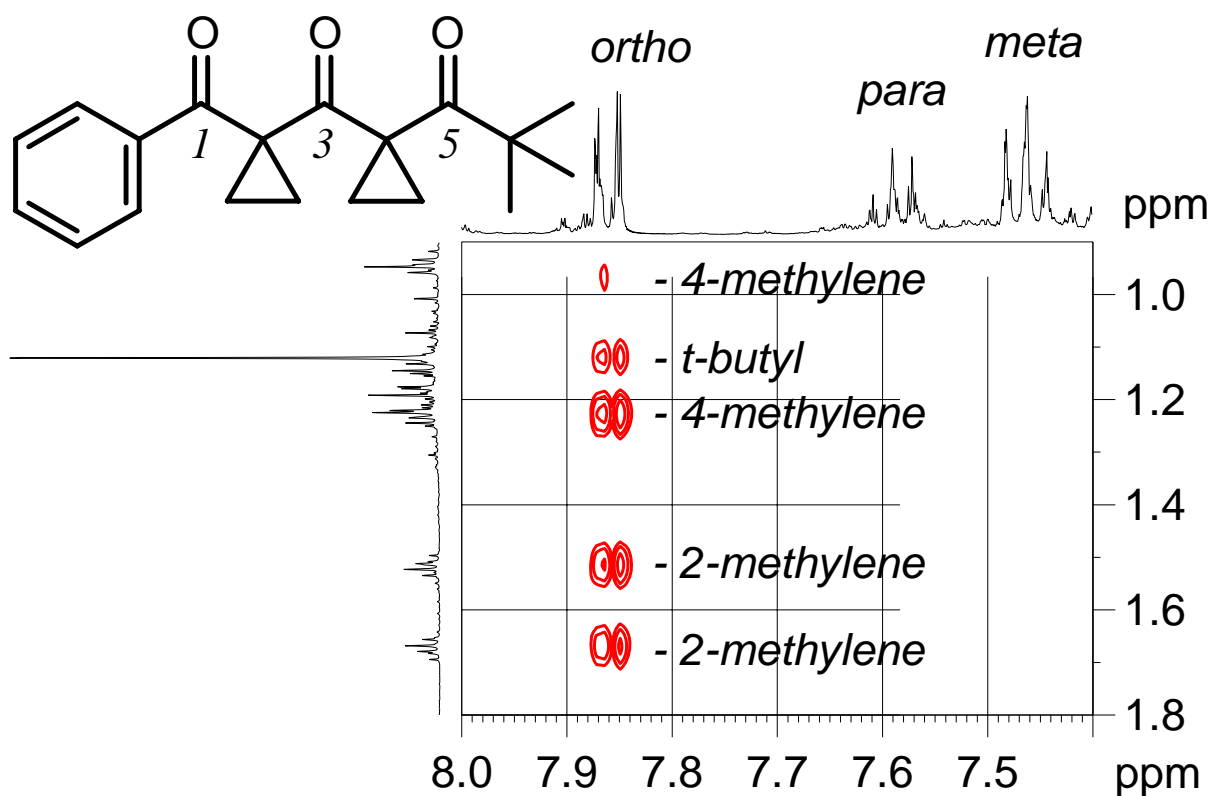
Current Data Parameters  
NAME 080801.306  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080801  
Time 17.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 21097.047 Hz  
FIDRES 0.643831 Hz  
AQ 0.7766516 sec  
RG 32768  
DW 23.700 usec  
DE 6.00 usec  
TE 296.9 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 -1.10 dB  
SFO1 75.4771825 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 19.00 dB  
PL13 21.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



**Figure S1.** Section of the <sup>1</sup>H NOESY NMR (CD<sub>2</sub>Cl<sub>2</sub>, 400.1 MHz, ambient temperature, mixing time 1.5 s) of **4c** showing the neighbourhood of the *tert*-butyl and the phenyl group.