

**Allyl *m*-Trifluoromethyldiazirine Mephobarbital: An Unusually Potent
Enantioselective and Photoreactive Barbiturate General Anesthetic**

Supporting Information

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Supporting information available: (1) Chiral chromatography of (\pm)-**14**, (2) HPLC of the mixture after hydrogenation of compound **15**, (3) determination of pK_a value of **14**, (4) NMR data for all new synthesized compounds.

Figure 1s. HPLC separation of enantiomers of compound **14**. Conditions: Daicell Chiralpack AD[®] column, 20x200 mm eluted with isocratic 15% ethanol in hexane as an eluent at 6.5 mL/min flow rate.

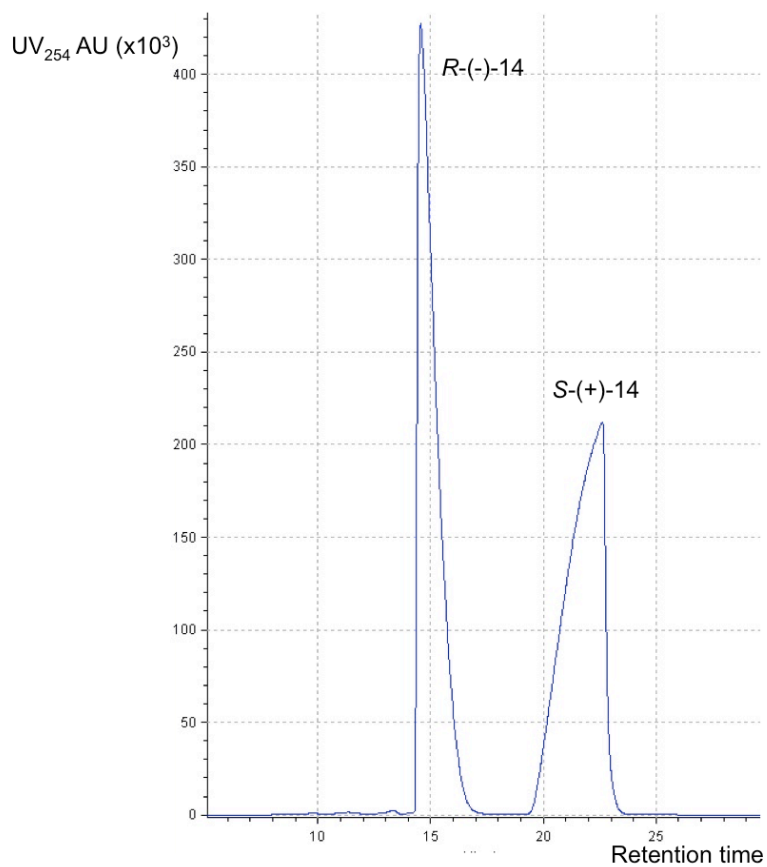
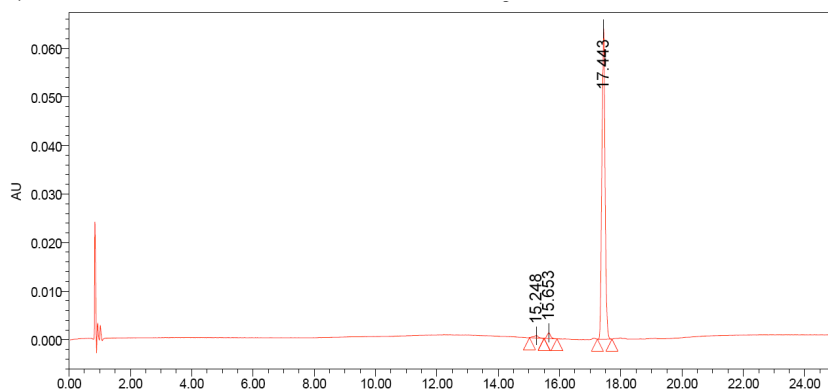
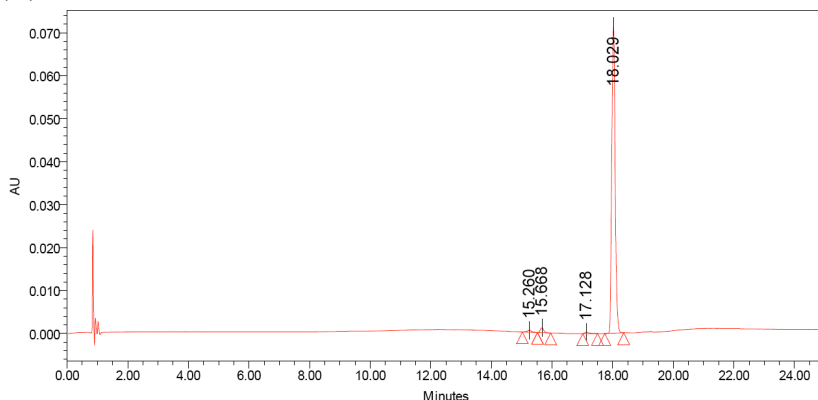


Figure 2s. Separation of compounds **14** and **15** by reverse phase HPLC. HPLC method: Luna 5 μm C18 100 \AA column, 150 x 3.00 mm from Phenomenex. During the first 2 minutes isocratic 0.05 M TFA was used as an eluent; starting at 2 min the gradient of 0.05 M TFA/MeOH (0-100%) was used to reach 100% at 17 min, and elution was continued with isocratic MeOH. Flow rate: 1 mL/min. Detection – UV array detector at 254 nm. (A) starting propargyl barbiturate **15**; (B) product allyl barbiturate **14**; (C) the mixture of **14** and **15**.

(A)



(B)



(C)

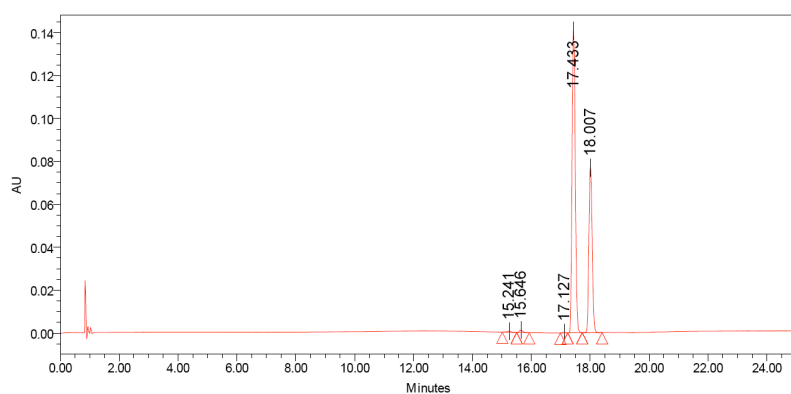


Figure 3s. Determination of pK_a of barbiturate (\pm)-14.

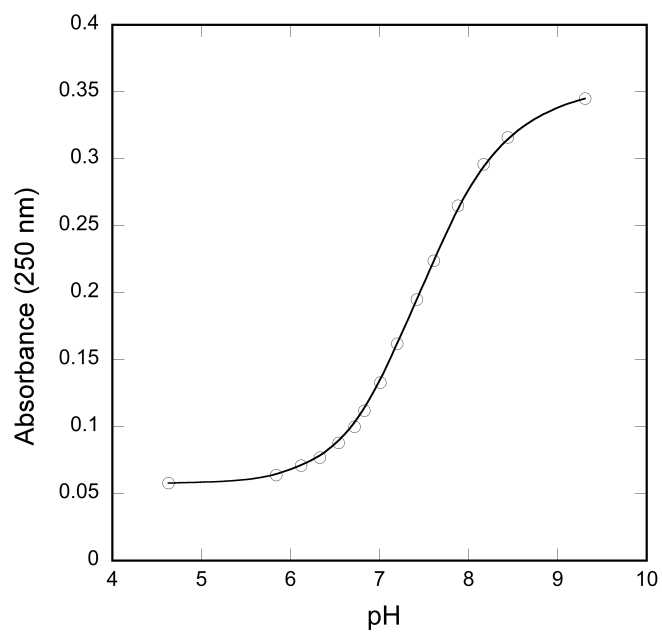
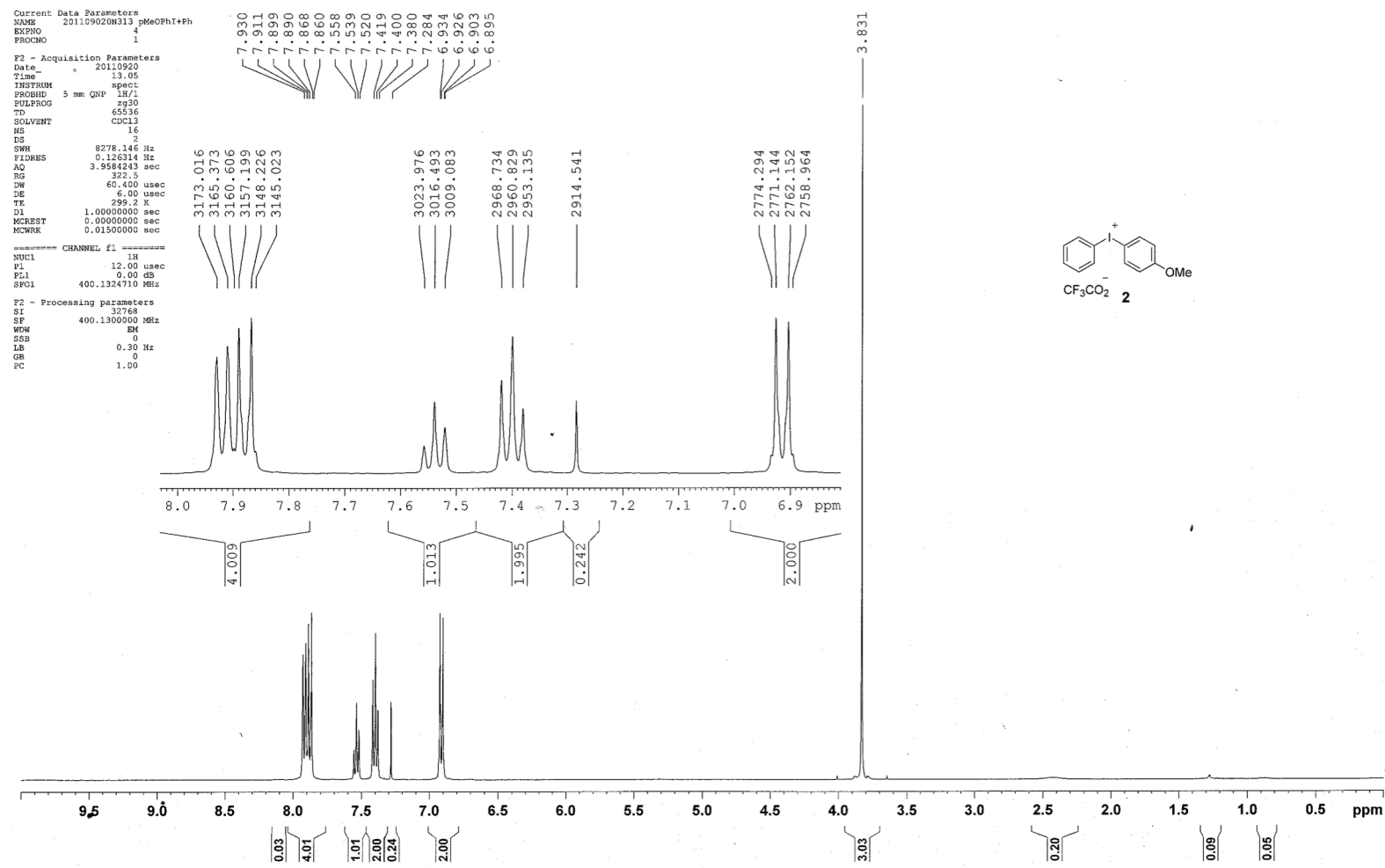


Figure 4s. NMR Data for Synthetic Intermediates and Products.



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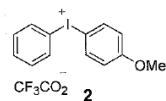
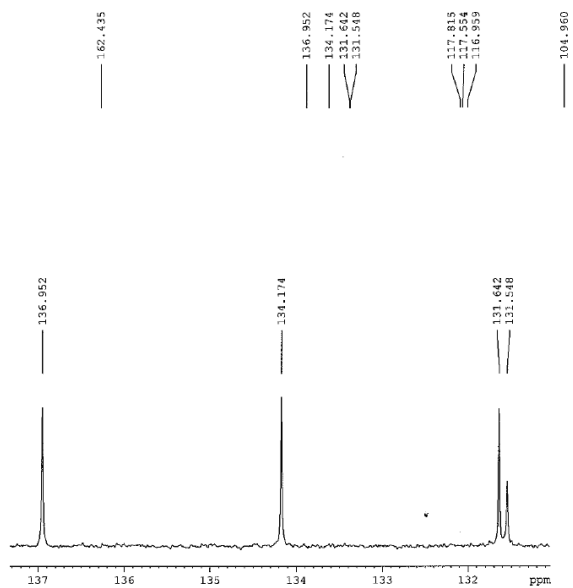
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 SOLVENT CDCl3
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 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1024
 LW 20.850 usec
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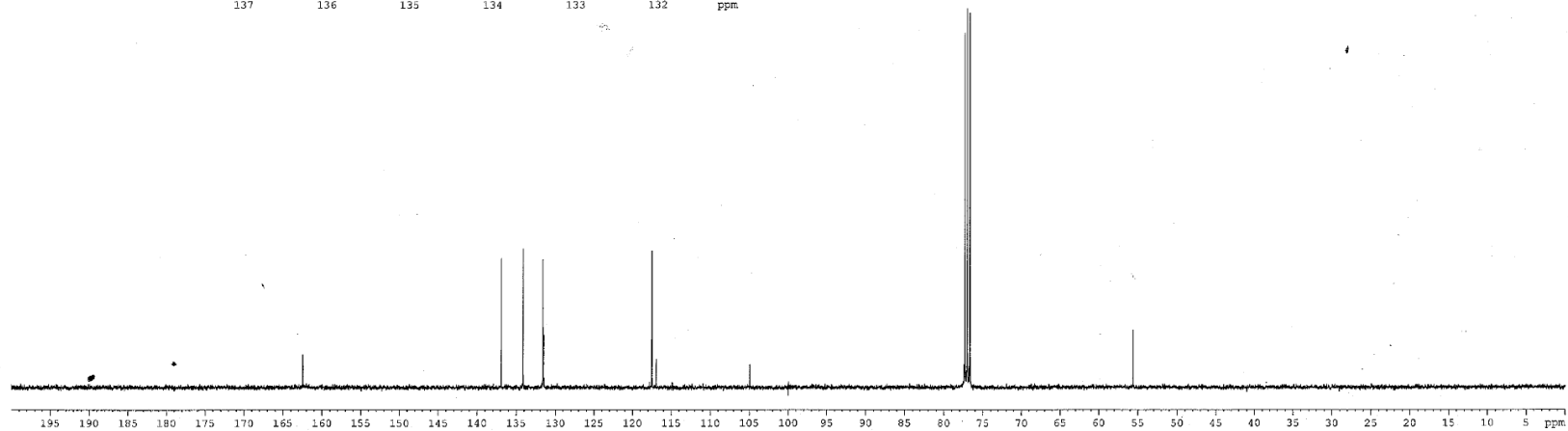
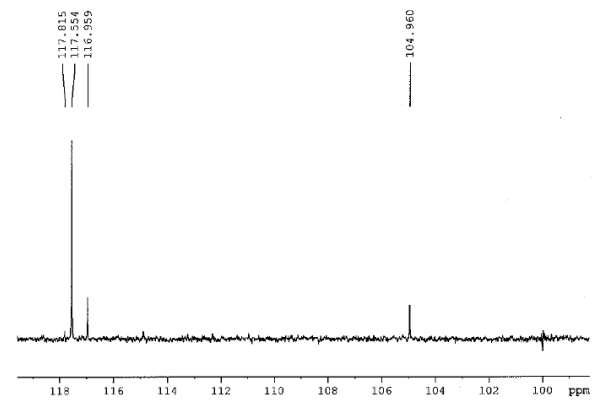
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 NU2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 400.1318005 MHz

F2 - Processing parameters
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77.000
76.758
55.622

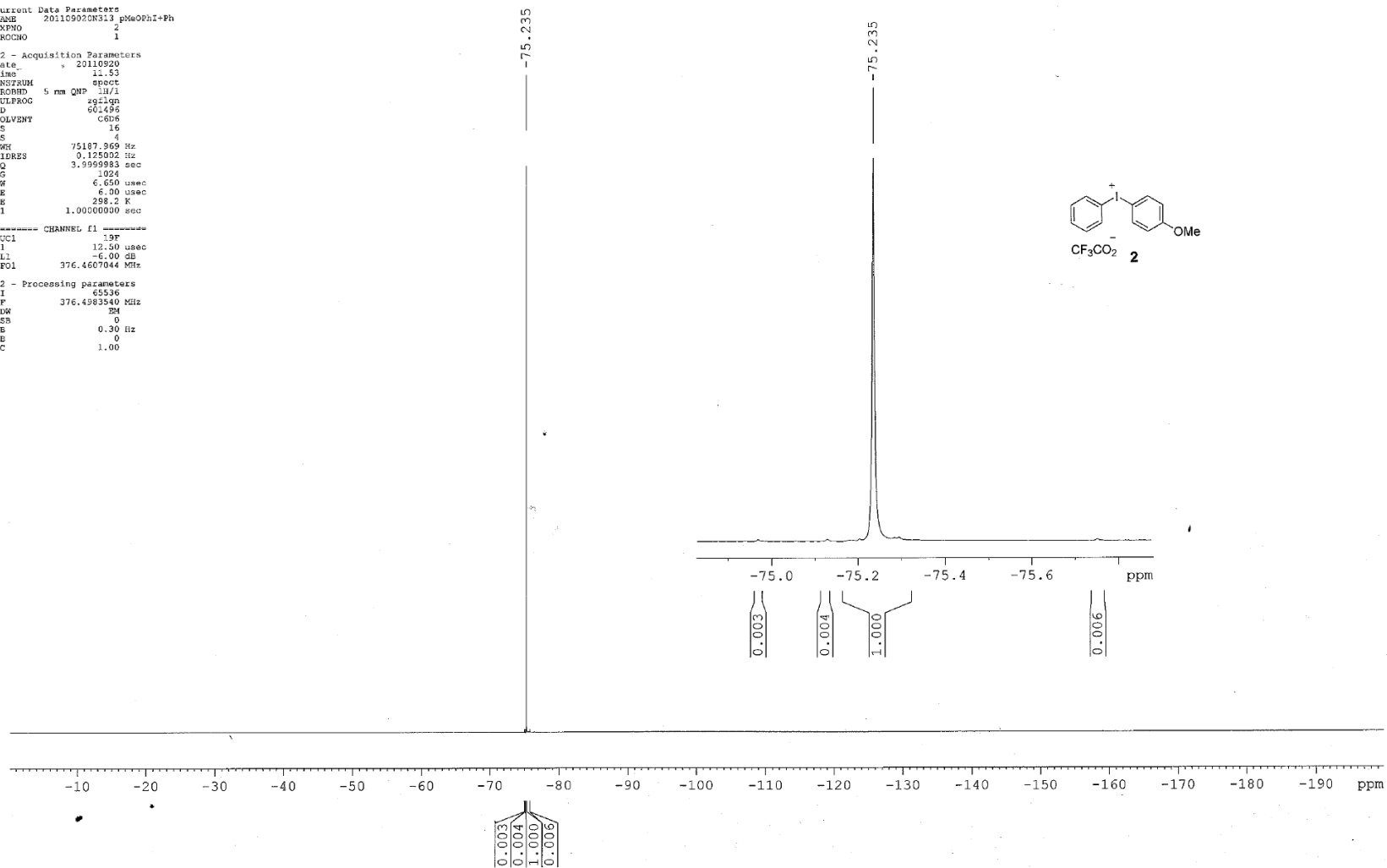


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PROCNO 1

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SOLVENT CDCl3
NS 16
DS 4
SWH 75187.969 Hz
FIDRES 0.125002 Hz
AQ 3.9999983 sec
RG 1024
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DE 6.00 usec
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NUC1 19F
P1 12.50 usec
PL1 -6.00 dB
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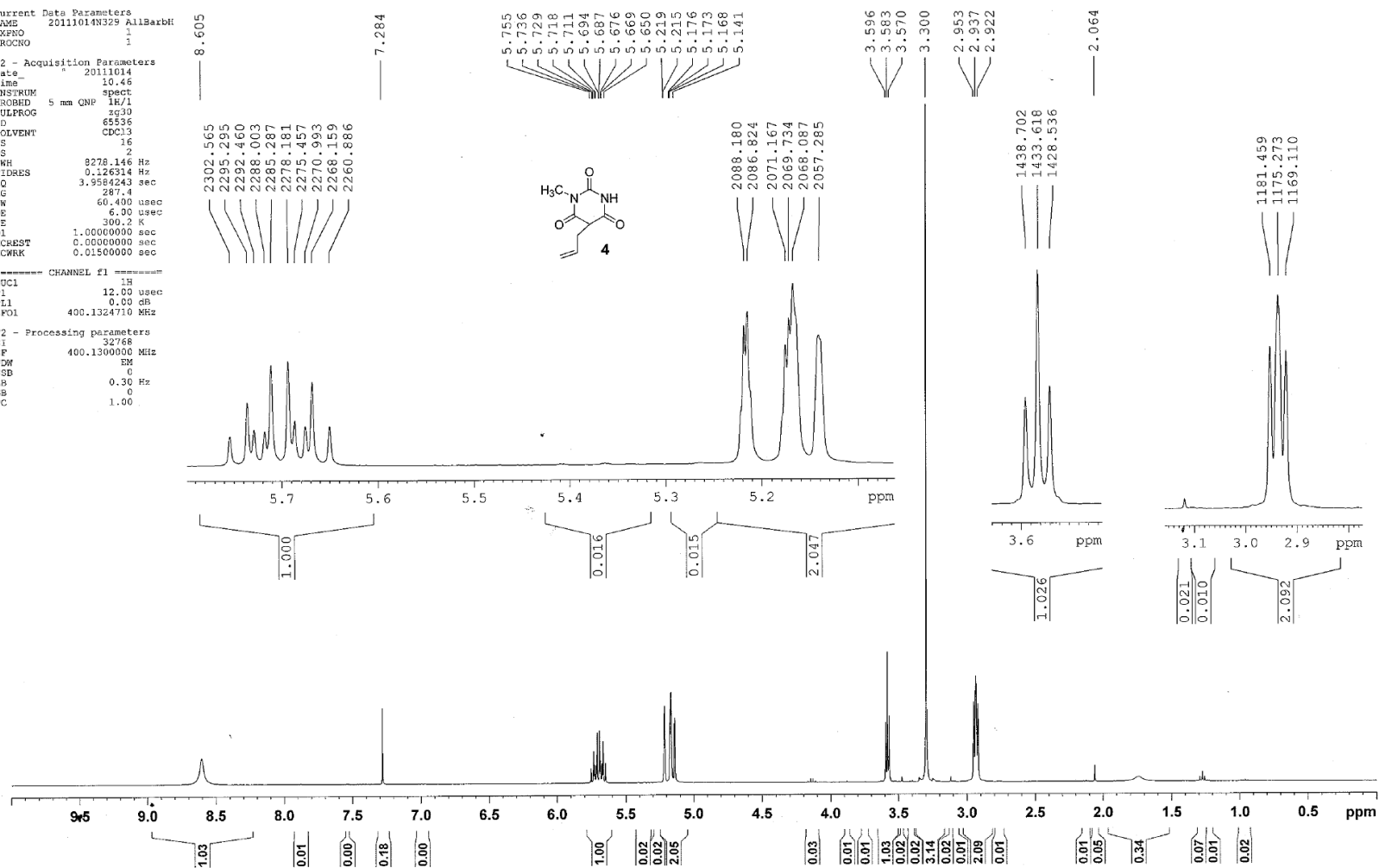


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 DE 6.90 usec
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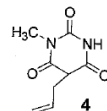
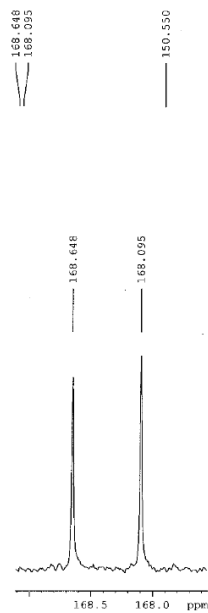
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 SOLVENT CDCl3
 NS 719
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 FIDRES 0.369918 Hz
 AQ 1.3664758 sec
 RG 912.7
 SW 20.953 usec
 DE 6.00 usec
 TE 297.4 K
 C1 2.0000000 sec
 c11 0.0300000 sec
 DELTA 1.8999999 sec
 MCMST 0.0000000 sec
 MCMRK 0.0150000 sec

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 NUC1 13C
 P1 9.50 usec
 PL1 -2.00 dB
 SFO1 100.628888 MHz

----- CHANNEL f2 -----
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 NUC2 1H
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 PL13 14.30 dB
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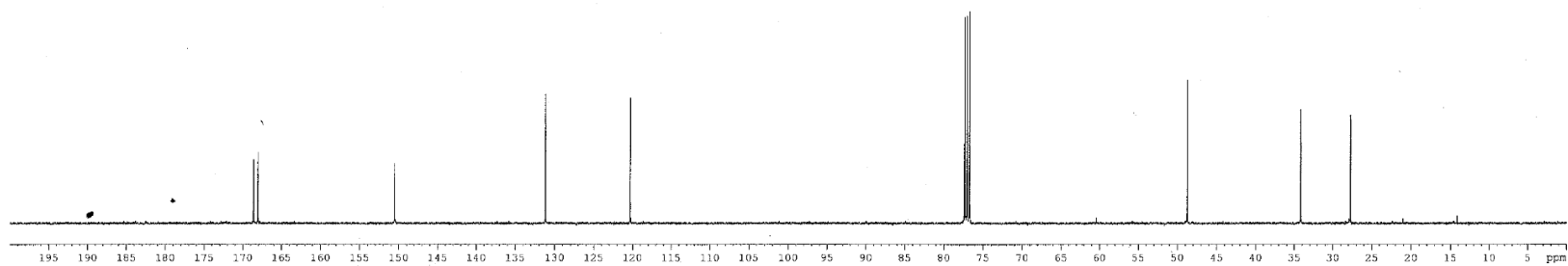
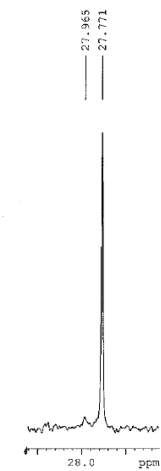
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4

SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1448.2
 DW 20.850 usec
 DE 6.00 usec
 TE 299.2 K
 DL 2.0000000 sec
 d11 0.3300000 sec
 DELTA 1.89999998 sec
 MCREST 0.0000000 sec
 MCHXK 0.01500000 sec

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 PL1 -3.00 dB
 SFO1 100.6228209 MHz

==== CHANNEL f2 =====
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 NUC2 1H
 FCPDZ 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
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 SF 100.6127690 MHz
 WDW EM
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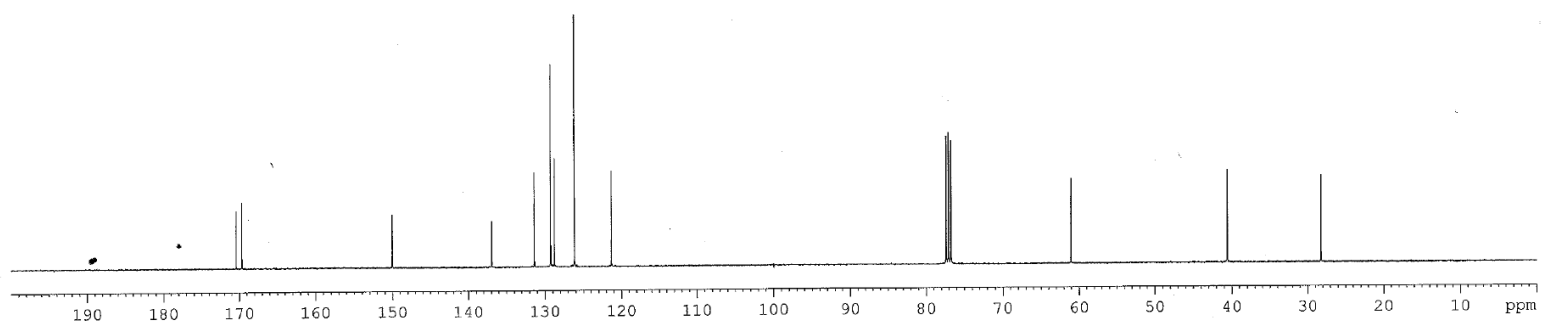
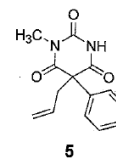
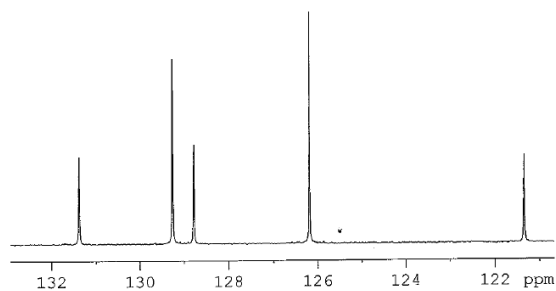
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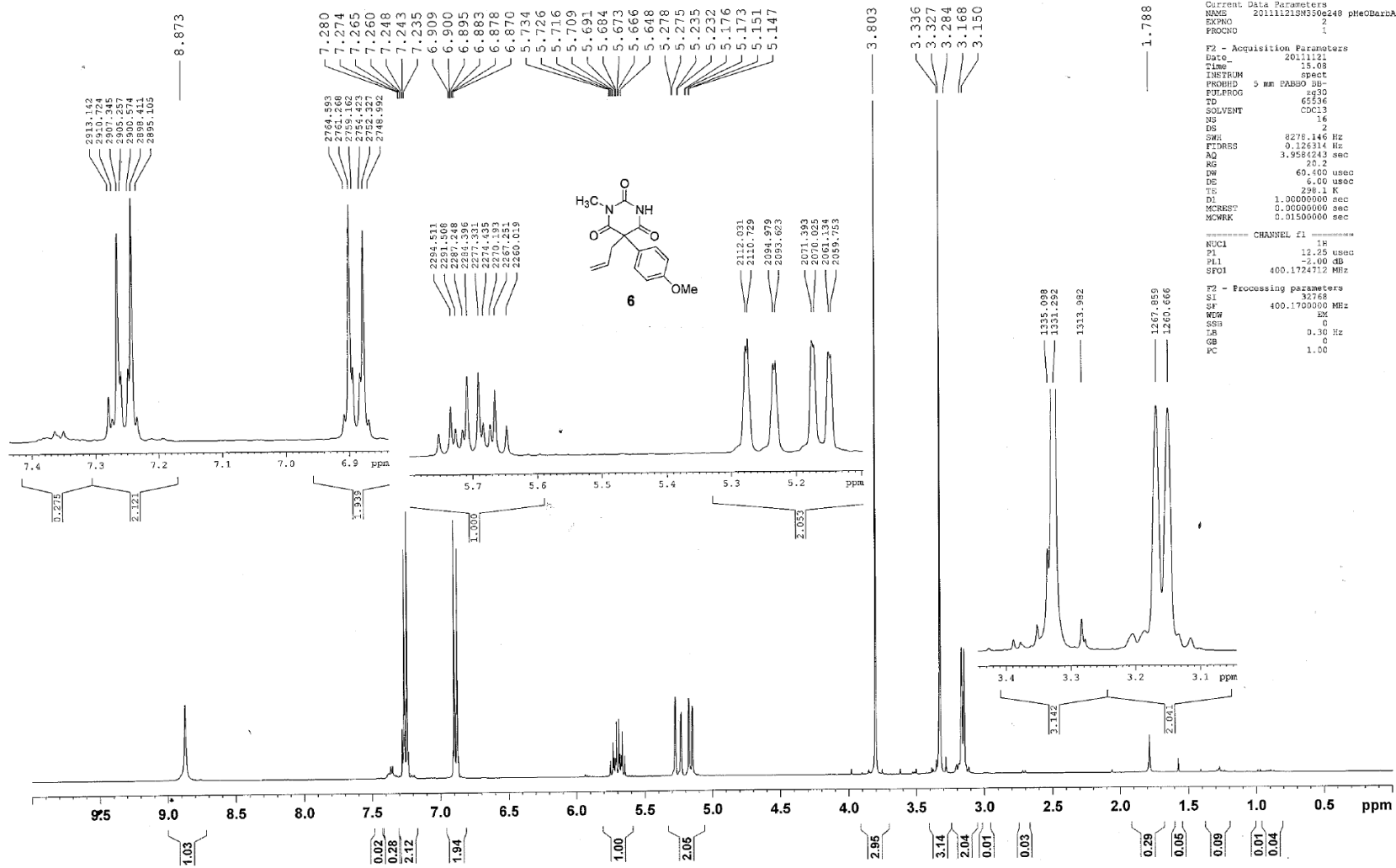
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61.074

40.622

28.250





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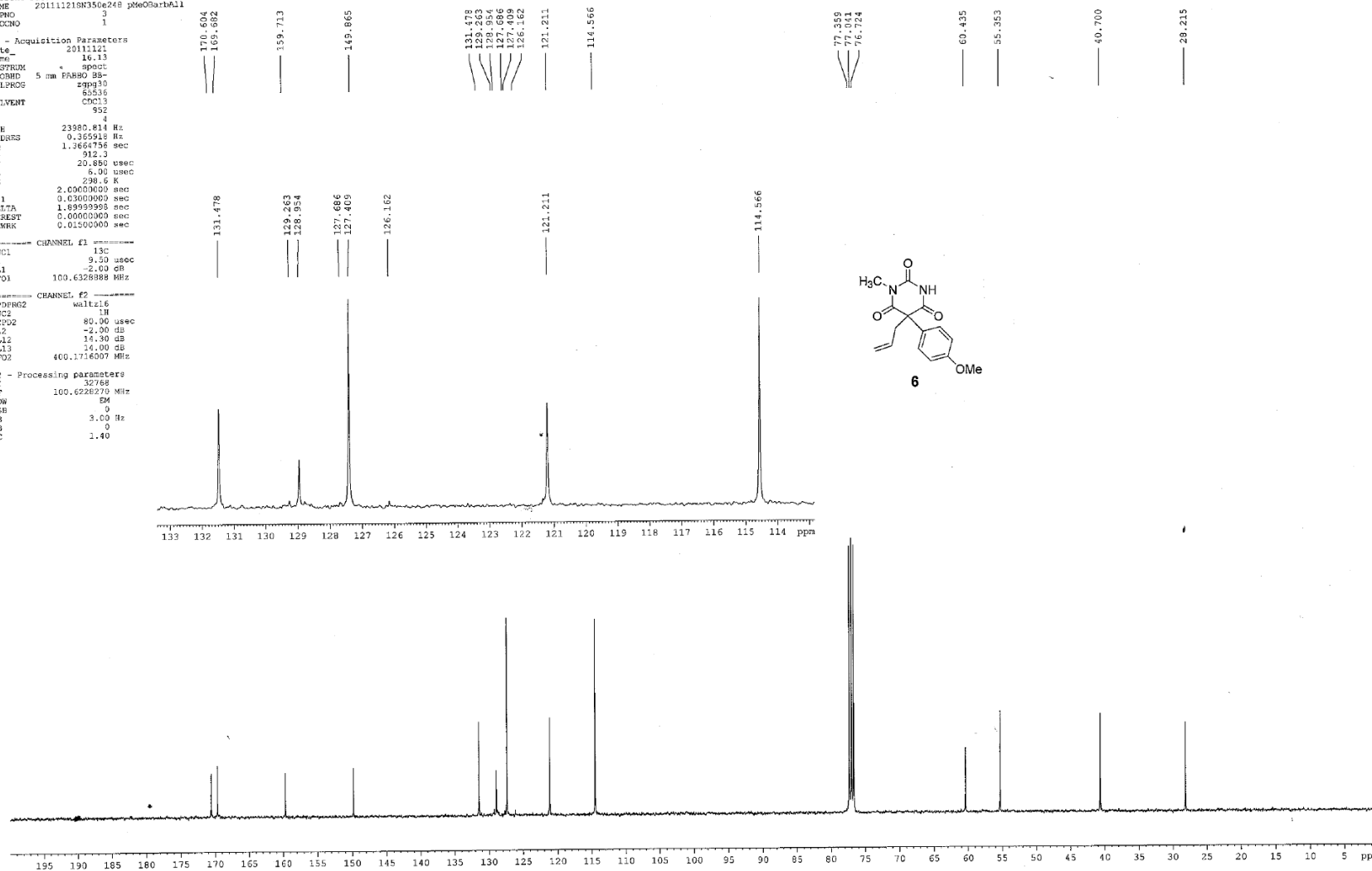
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 NS 952
 DS 4

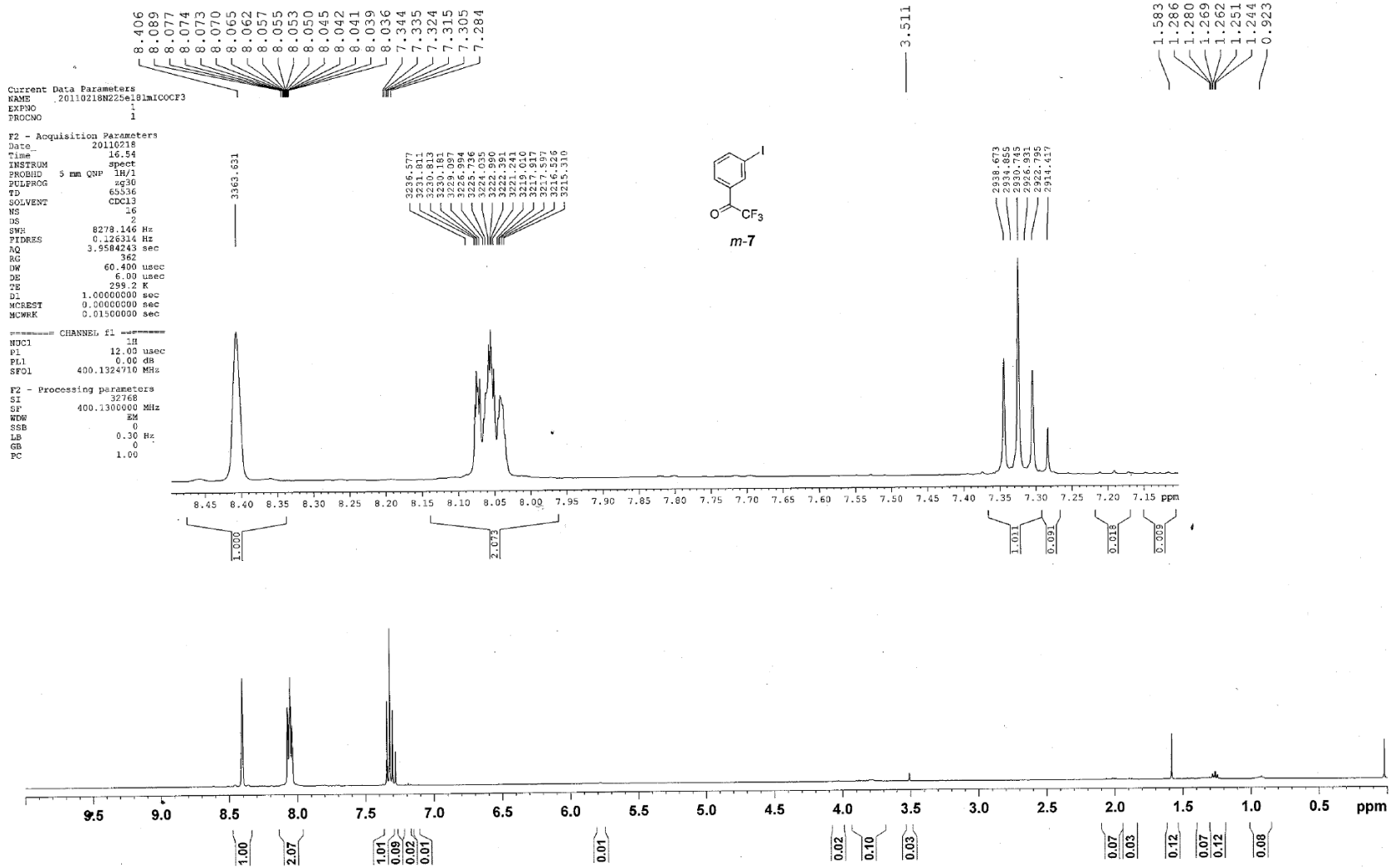
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 d11 0.0300000 sec
 DELTA 1.6999998 sec
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 MCNRES 0.0100000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 9.50 usec
 PL1 2.00 dB
 SFO1 100.628888 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.90 usec
 PL2 -2.00 dB
 PL12 16.30 dB
 PL13 16.00 dB
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 PC 1.40





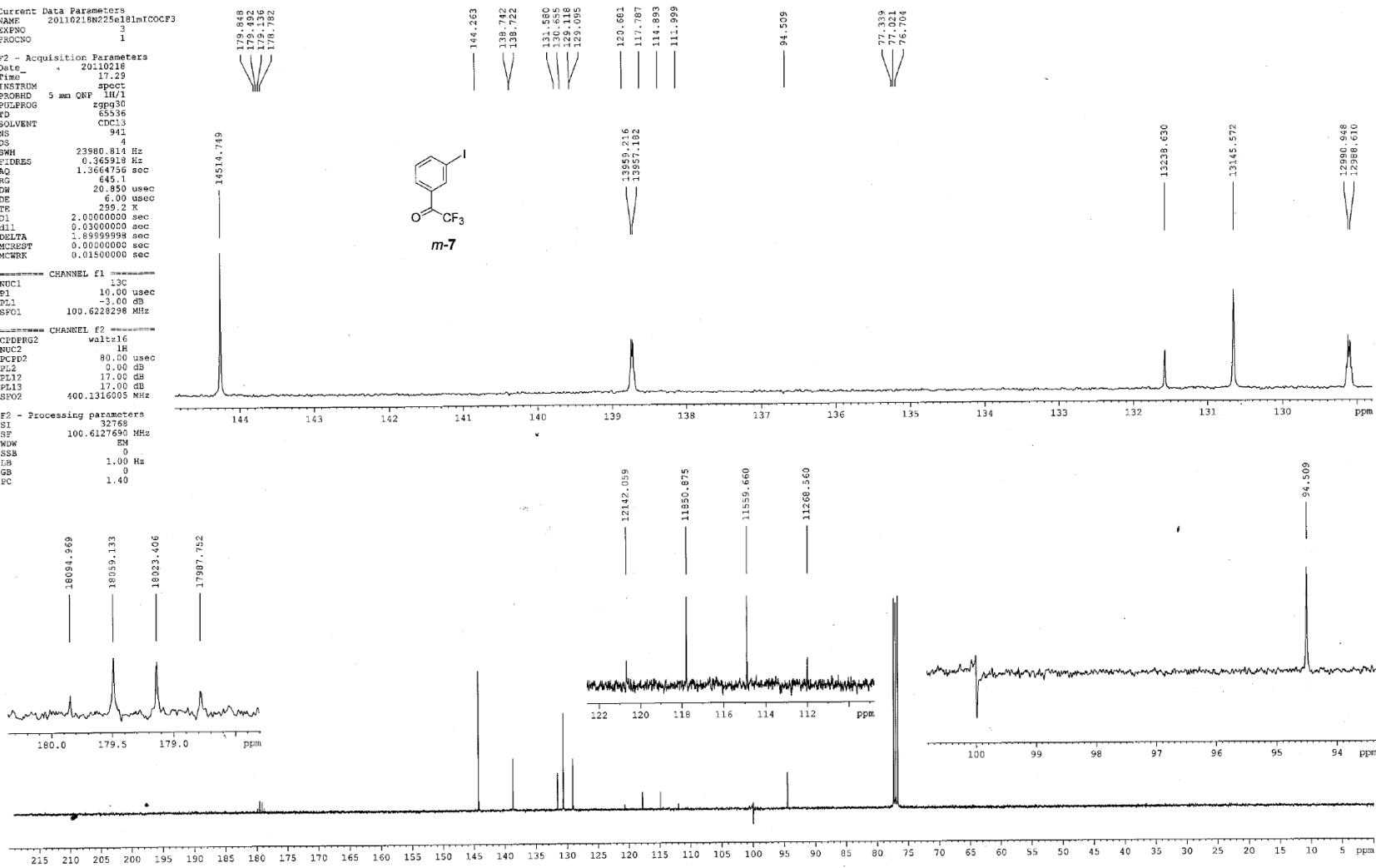
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 SOLVENT CDC13
 NS 941
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 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 645.1
 DW 20.850 usec
 DE 6.00 usec
 TK 299.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999999 sec
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 MCWRR 0.01500000 sec

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 P1 10.00 usec
 PL1 -3.00 dB
 SFO1 100.6228298 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
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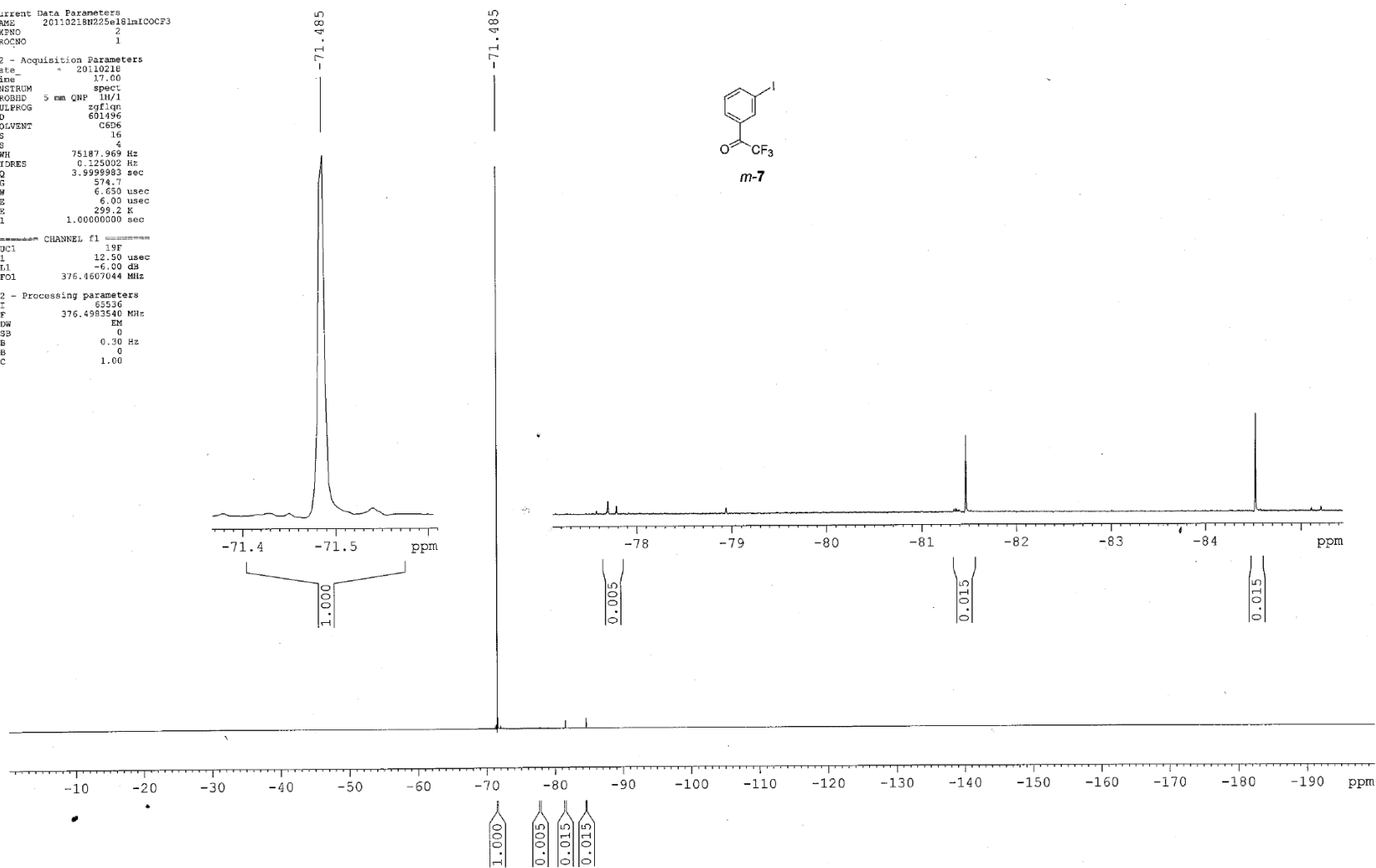
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PROCNO 1

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PULPROG zgpg30
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SOLVENT CDCl3
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DS 4
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FIDRES 0.125002 Hz
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RG 574.7
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DE 6.00 usec
TE 299.2 K
D1 1.0000000 sec

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P1 12.50 usec
PL1 -6.00 dB
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PC 1.00

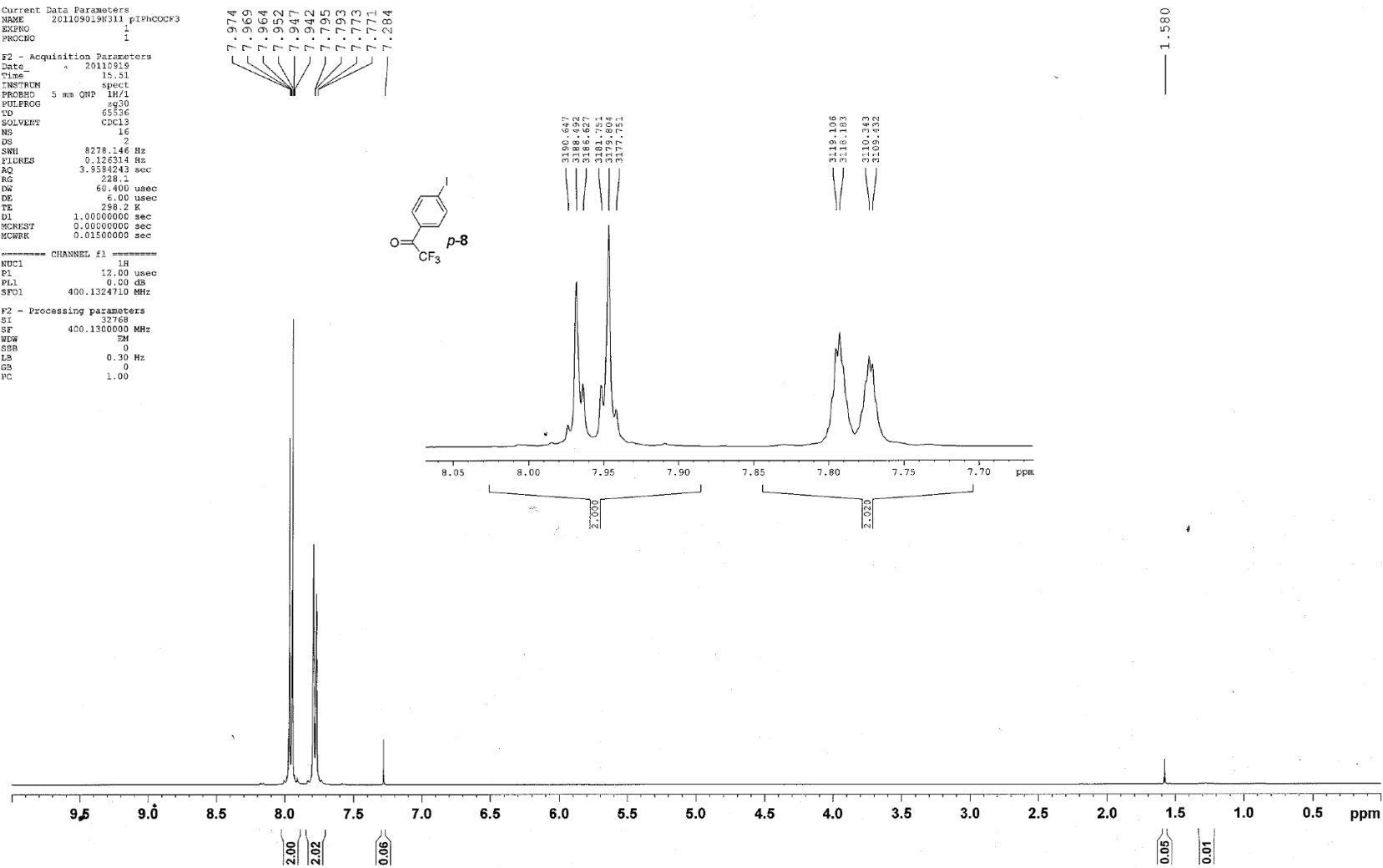


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 SOLVENT CDCl3
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 DS 2
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 FIDRES 0.126314 Hz
 AQ 3.858443 sec
 RG 228.1
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 DE 6.00 usec
 TE 298.2 K
 DL 1.00000000 sec
 MCNRET 0.00000000 sec
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CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
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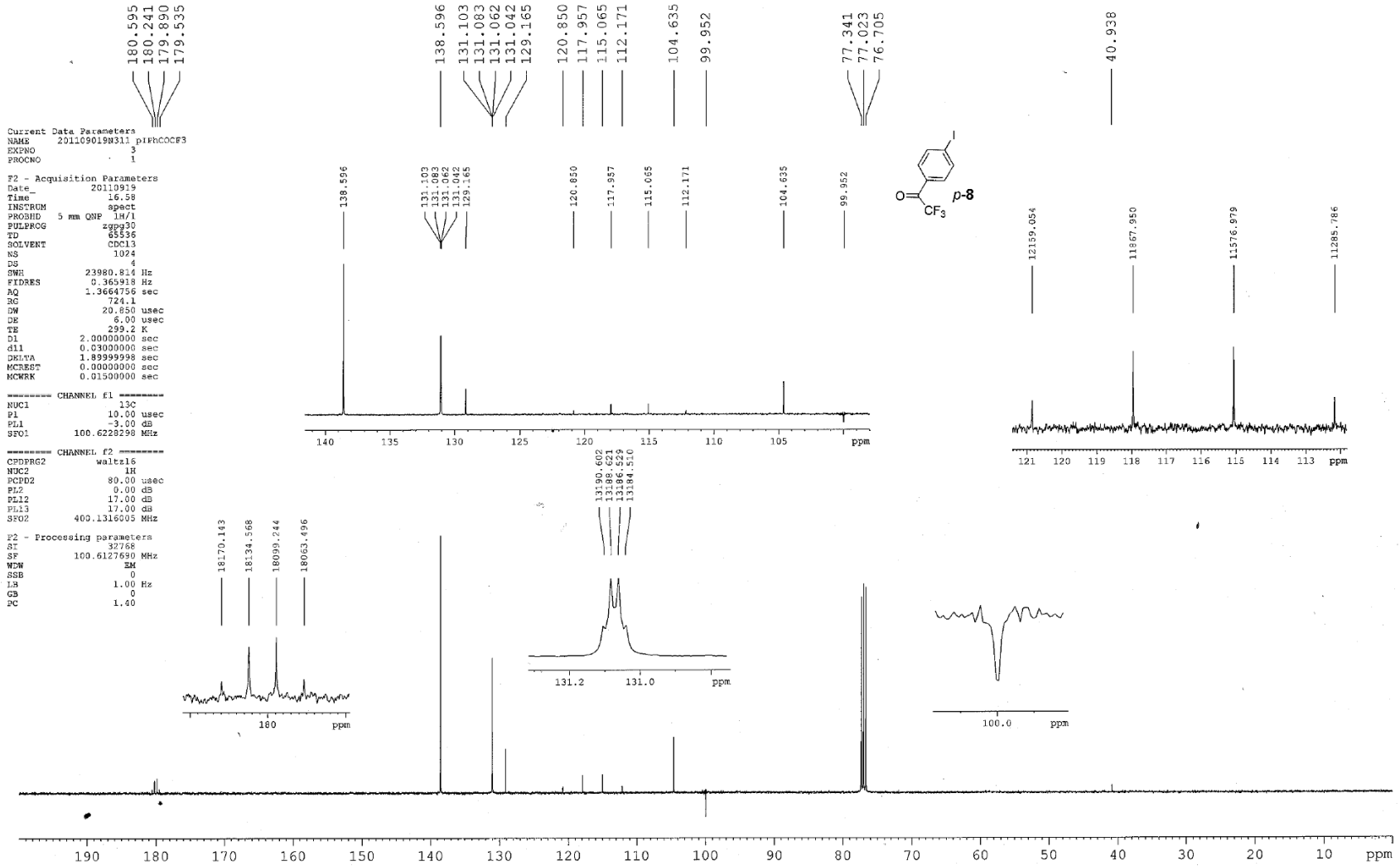
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 TD 65536
 SOLVENT cdcl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 20.850 usec
 DE 6.00 usec
 TE 299.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999999 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

CHANNEL F1
 NUC1 13C
 P1 10.00 usec
 PL1 -3.00 dB
 SFO1 100.6228298 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
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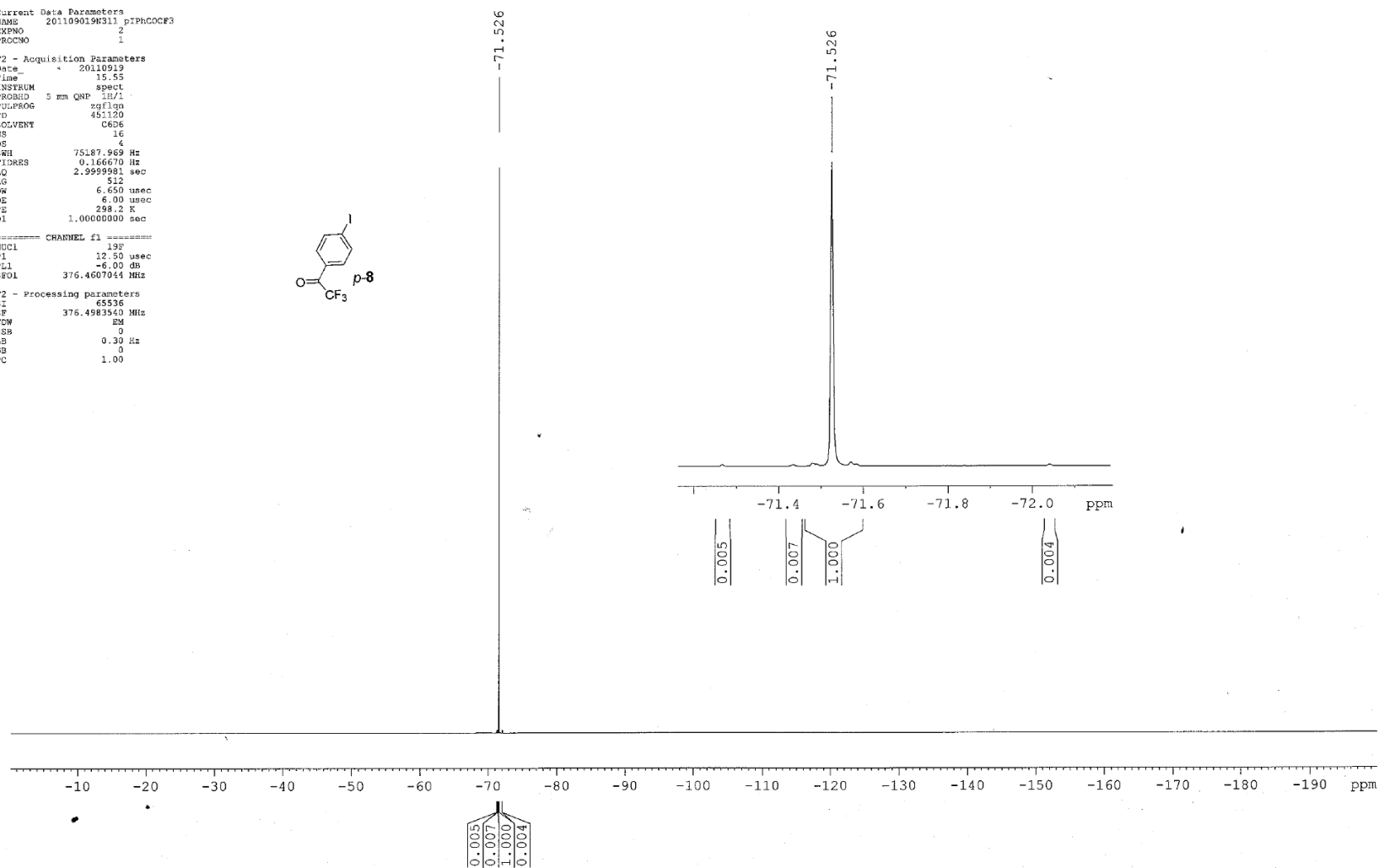
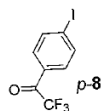


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PROCNO 1

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TD 451120
SOLVENT C6D6
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DS 4
SWH 75187.969 Hz
FIDRES 0.166670 Hz
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RG 512
DW 6.650 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec

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P1 12.50 usec
PL1 -6.00 dB
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F2 - Processing parameters
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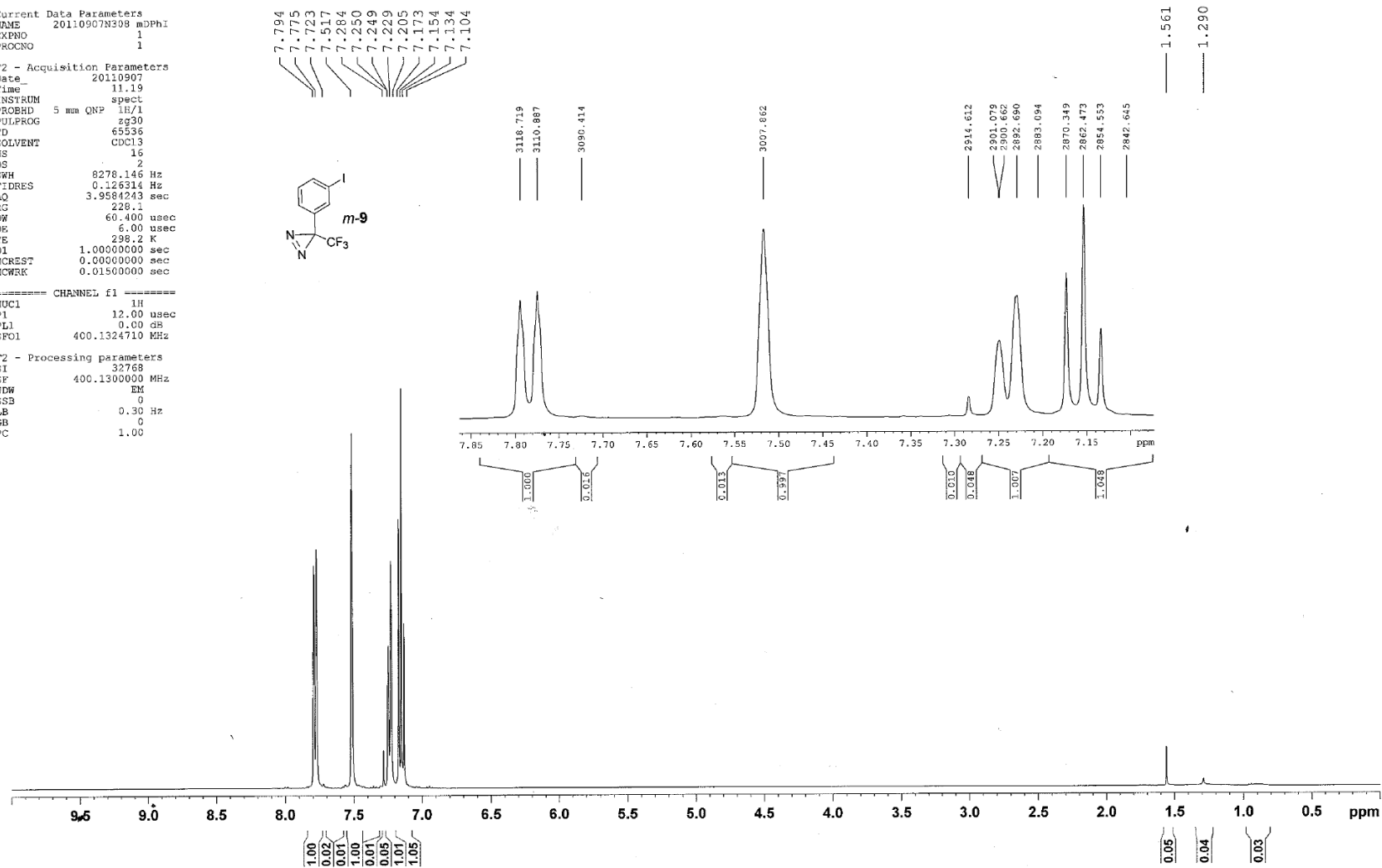
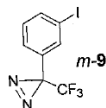
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 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.125314 Hz
 AQ 3.9584243 sec
 RG 228.1
 DW 60.400 usec
 DE 6.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.794
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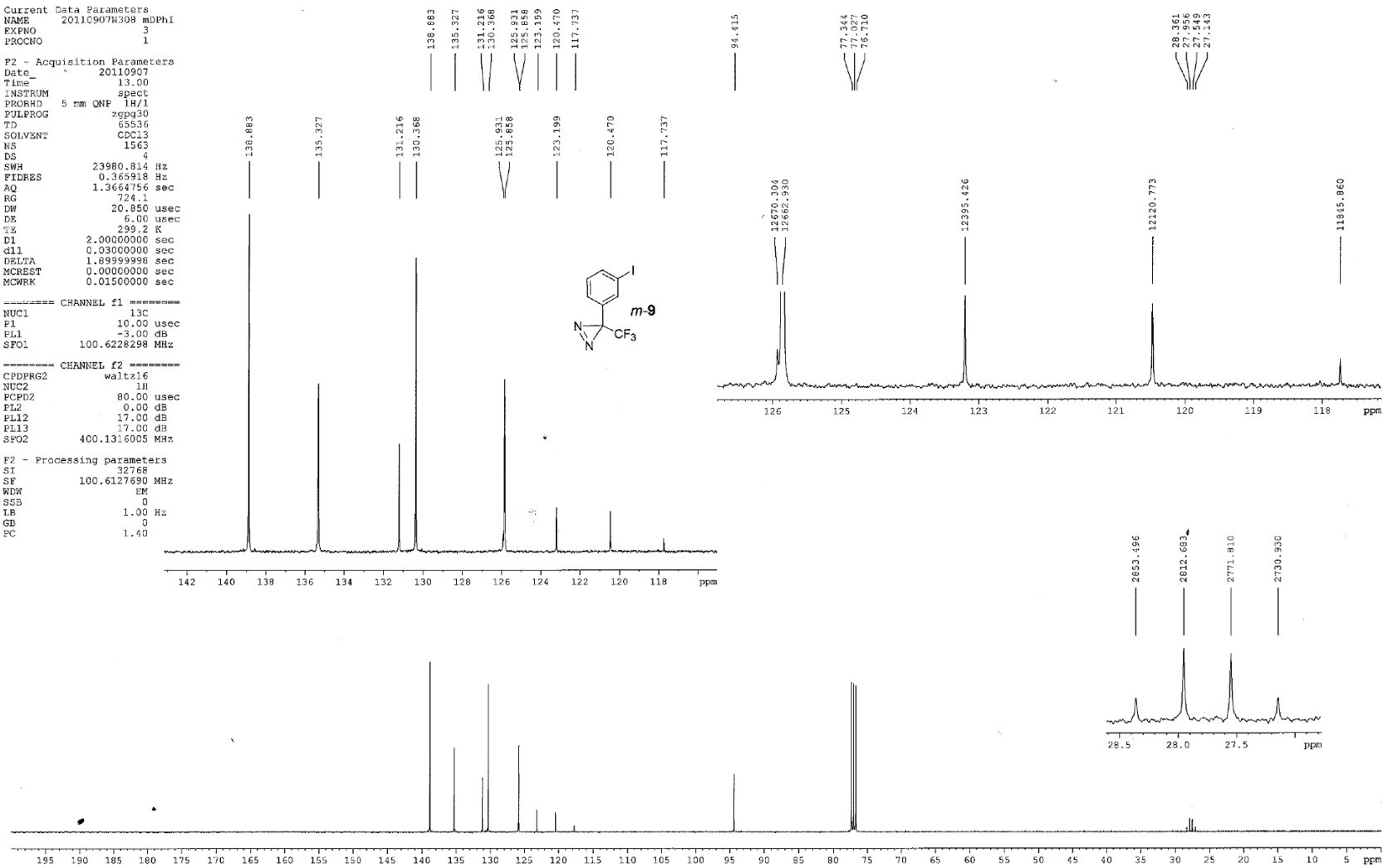
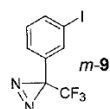
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 TD 65536
 SOLVENT CDC13
 NS 1563
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 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 20.850 usec
 DE 6.00 usec
 TE 299.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -3.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
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Current Data Parameters
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EXPNO 2
PROCNO 1

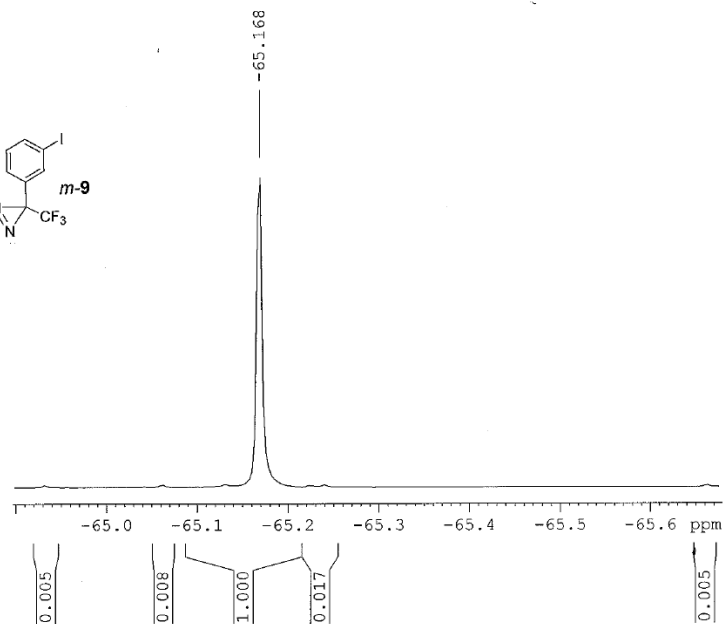
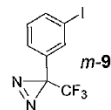
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SOLVENT C6D6
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DS 4
SWH 75187.969 Hz
FIDRES 0.250007 Hz
AQ 1.9999976 sec
RG 406.4
DW 6.650 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec

----- CHANNEL f1 -----
NUC1 19F
P1 12.50 usec
PL1 -6.00 dB
SFO1 376.4607044 MHz

F2 - Processing parameters
SI 65536
SF 376.4983540 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
EC 1.00

F19

-65.168



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

0.005
0.008
1.000
0.017
0.005

```

Current Data Parameters
NAME 201101250214 p1phCMZCF3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110125
Time 10.31
INSTRUM spect
PROBHD 5 mm PABBO S2-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 32
DN 60.400 usec
DE 6.00 usec
TE 297.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCNKK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 12.25 usec
PL1 -2.00 dB
SFO1 400.1724712 MHz

F2 - Processing parameters
SI 32768
SP 400.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```

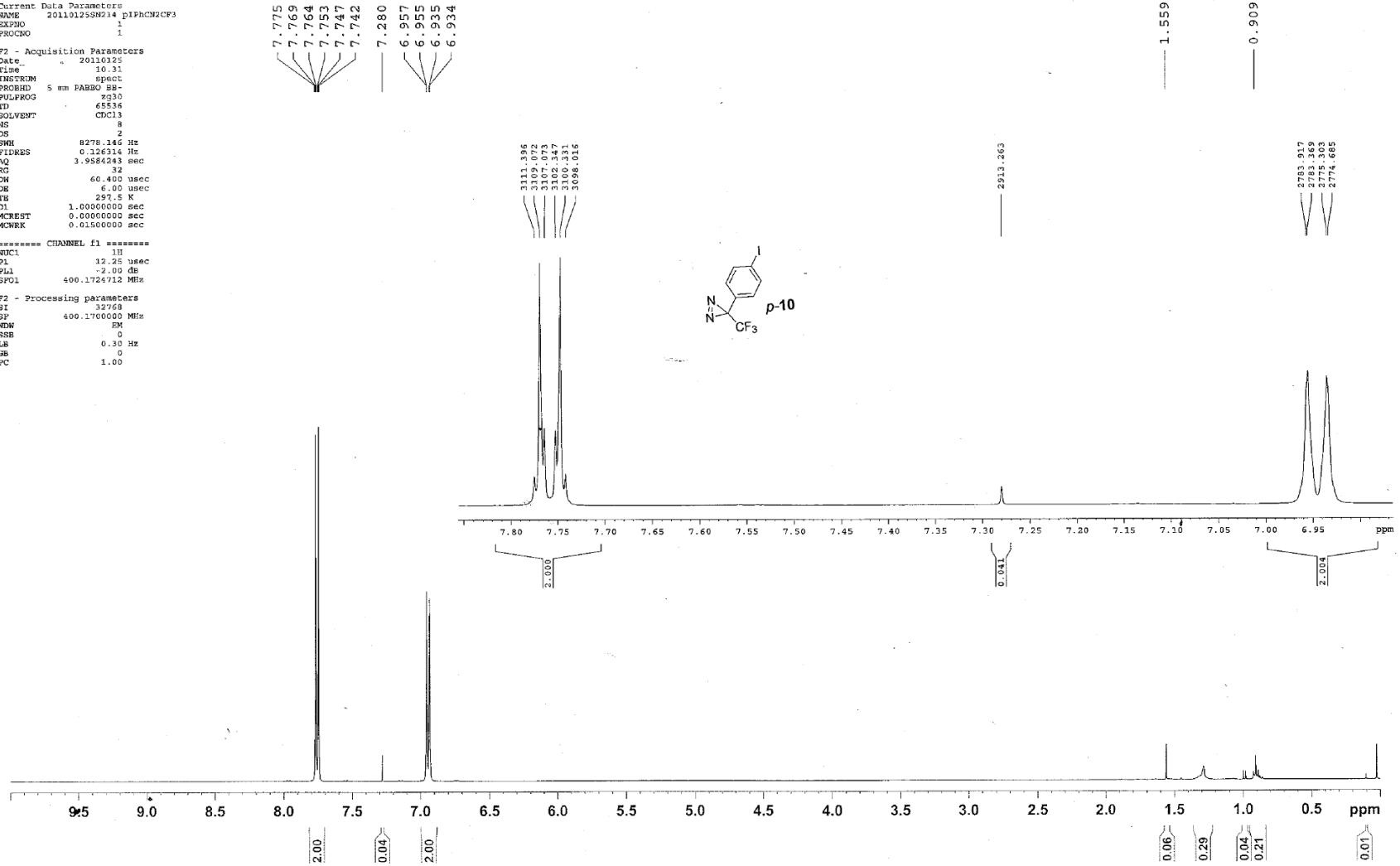
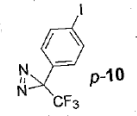
7.775
7.769
7.764
7.753
7.747
7.742
7.280
6.957
6.955
6.935
6.934

3111.396
3107.072
3102.347
3100.331
3098.016

2913.263

2783.917
2783.369
2775.303
2774.685

1.559
0.909



Current Data Parameters
 NAME 20110125SN214_p1PhCN2CF3
 EXPNO 2
 FREQC0 1

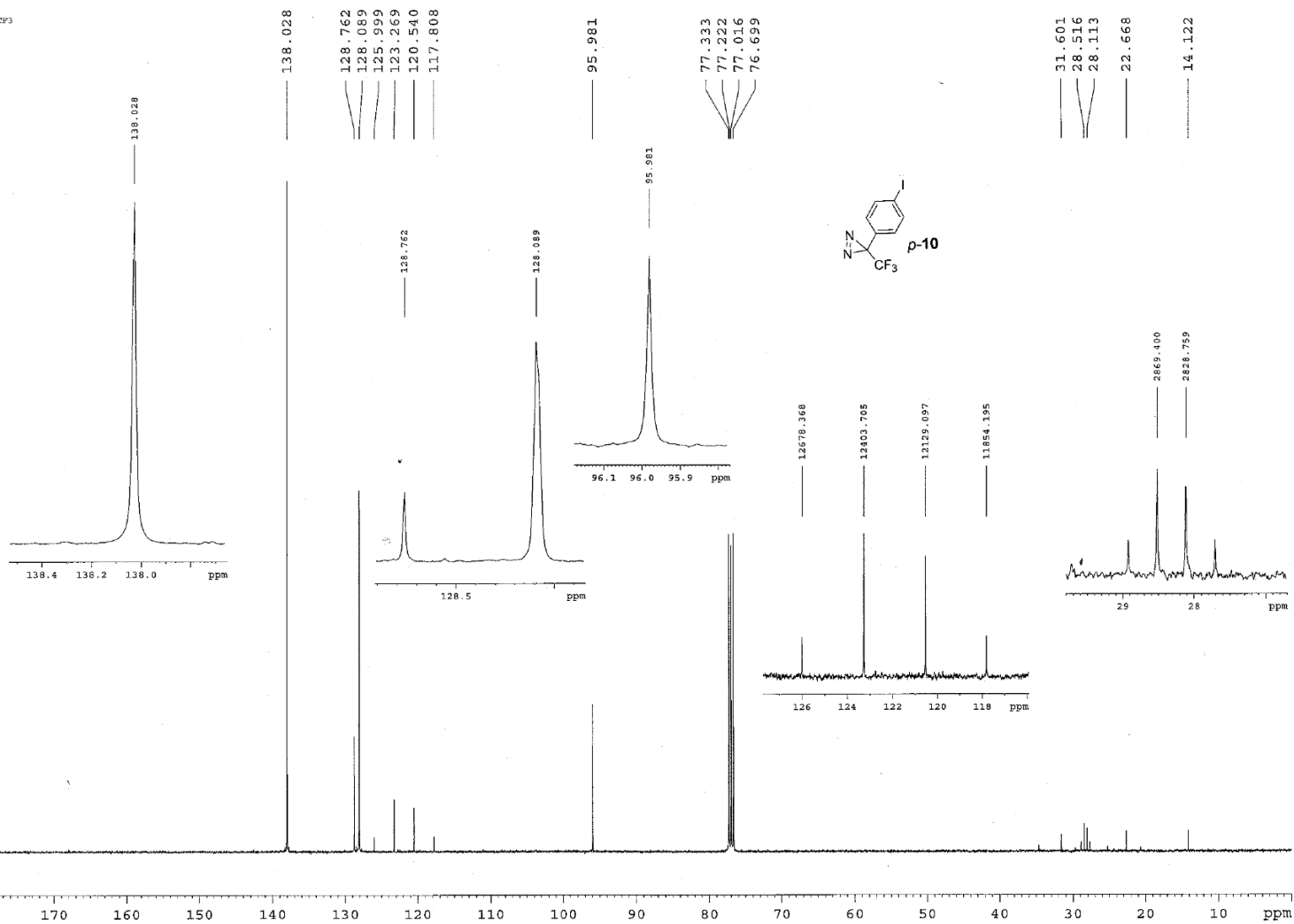
F2 - Acquisition Parameters
 Date 20110125
 Time 12.28
 INSTRUM spect
 PULPROG 5 mm PABBO H1-
 PULPROG zpg30
 TD 65536
 SOLVENT CCl3
 NS 1934

DS 4
 SWH 23960.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3660786 sec
 RG 1290.2
 EW 20.850 usec
 DS 6.00 usec
 TE 297.9 K
 DL 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 MCREST 0.0000000 sec
 MCMRK 0.0250000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 9.50 usec
 PL1 -2.00 dB
 SF01 100.6228888 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.30 dB
 PL13 14.00 dB
 SFO2 400.1716007 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6228270 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



```

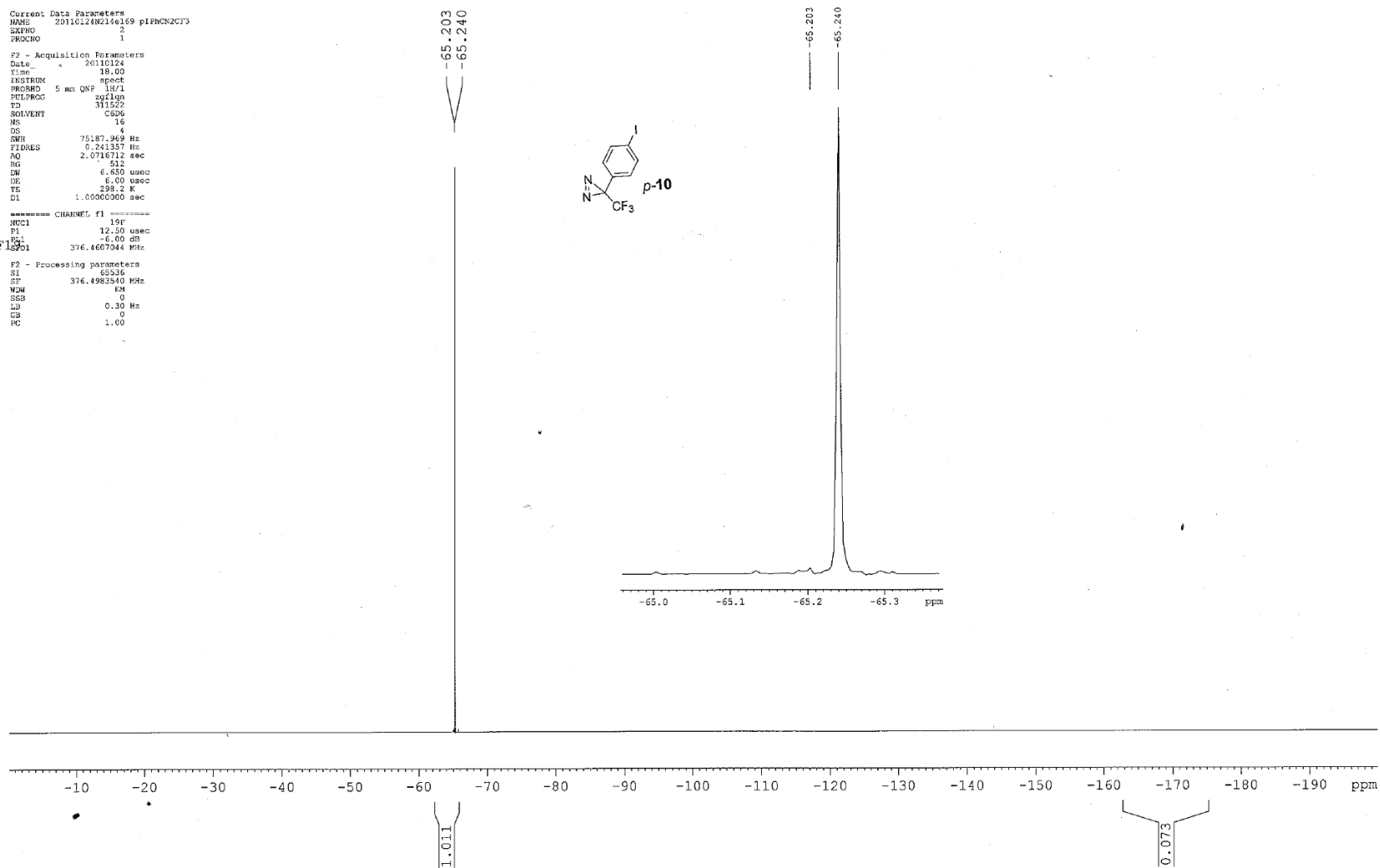
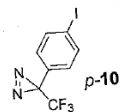
Current Data Parameters
NAME      2011012402196169 p1PNCN2CF3
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20110124
Time     18.00
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD       311522
SOLVENT  CDCl3
NS       16
DS       4
SWH      75187.369 Hz
FIDRES   0.241357 Hz
AQ       2.0714713 sec
RG       512
DM       6.850 usec
DE       6.00 usec
TE       298.2 K
D1       1.00000000 sec

===== CHANNEL f1 =====
NUC1     19F
P1       12.50 usec
PL1     -6.00 dB
FREQ    376.4607044 MHz

F2 - Processing parameters
SI       62536
SF       376.4983540 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
CB       1.00

```



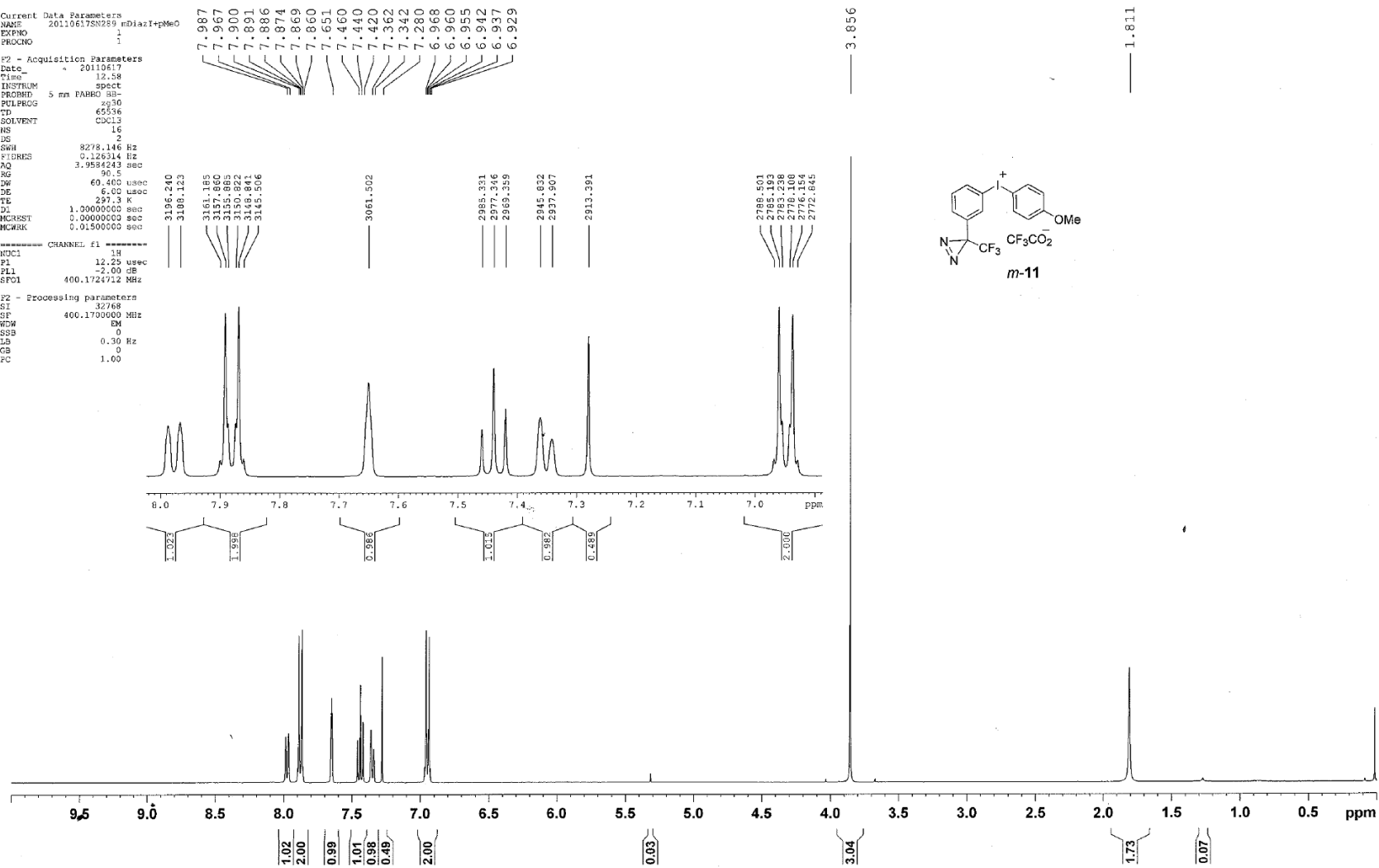
Current Data Parameters
 NAME 20110617SN2829 mDiazI+pMeO
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20110617
 Time 12.58
 INSTRUM spect
 PROBRD 5 mm FAPRO sb-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SSB 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.00 usec
 TE 297.3 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWAK 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.25 usec
 PL1 -2.00 dB
 SFO1 400.1724712 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1700000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 C 1.00



Current Data Parameters
 NAME 201103170242e194mbiaz1+pMeO maj
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date 20110317
 Time 12.54
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 ID 65536
 SOLVENT CDCl3
 NS 362
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 2048
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

CHANNEL f1

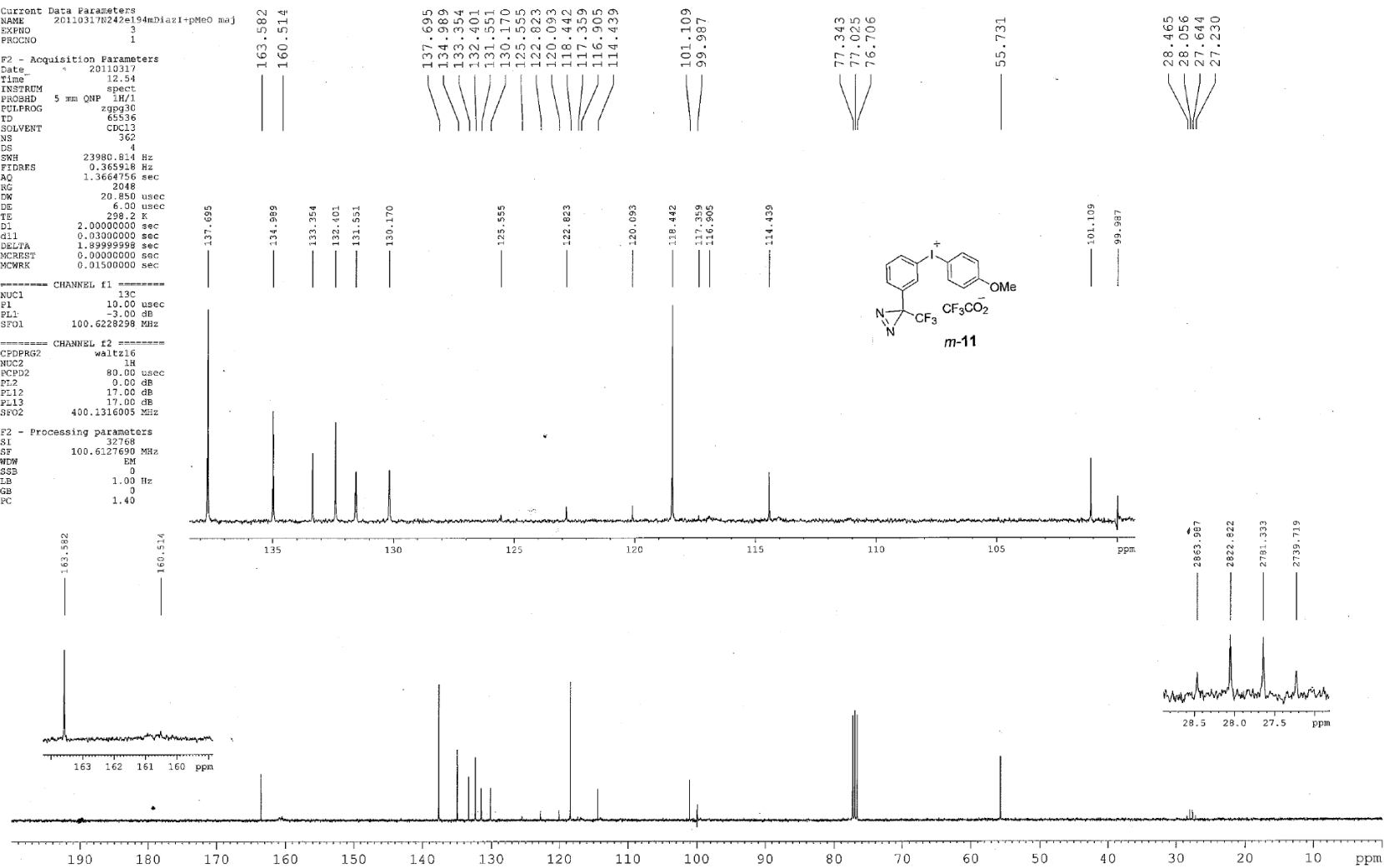
NUC1 13C
 P1 10.00 usec
 PL1 -3.00 dB
 SFO1 100.6228298 MHz

CHANNEL f2

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
 SF 100.6127690 MHz
 WMW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



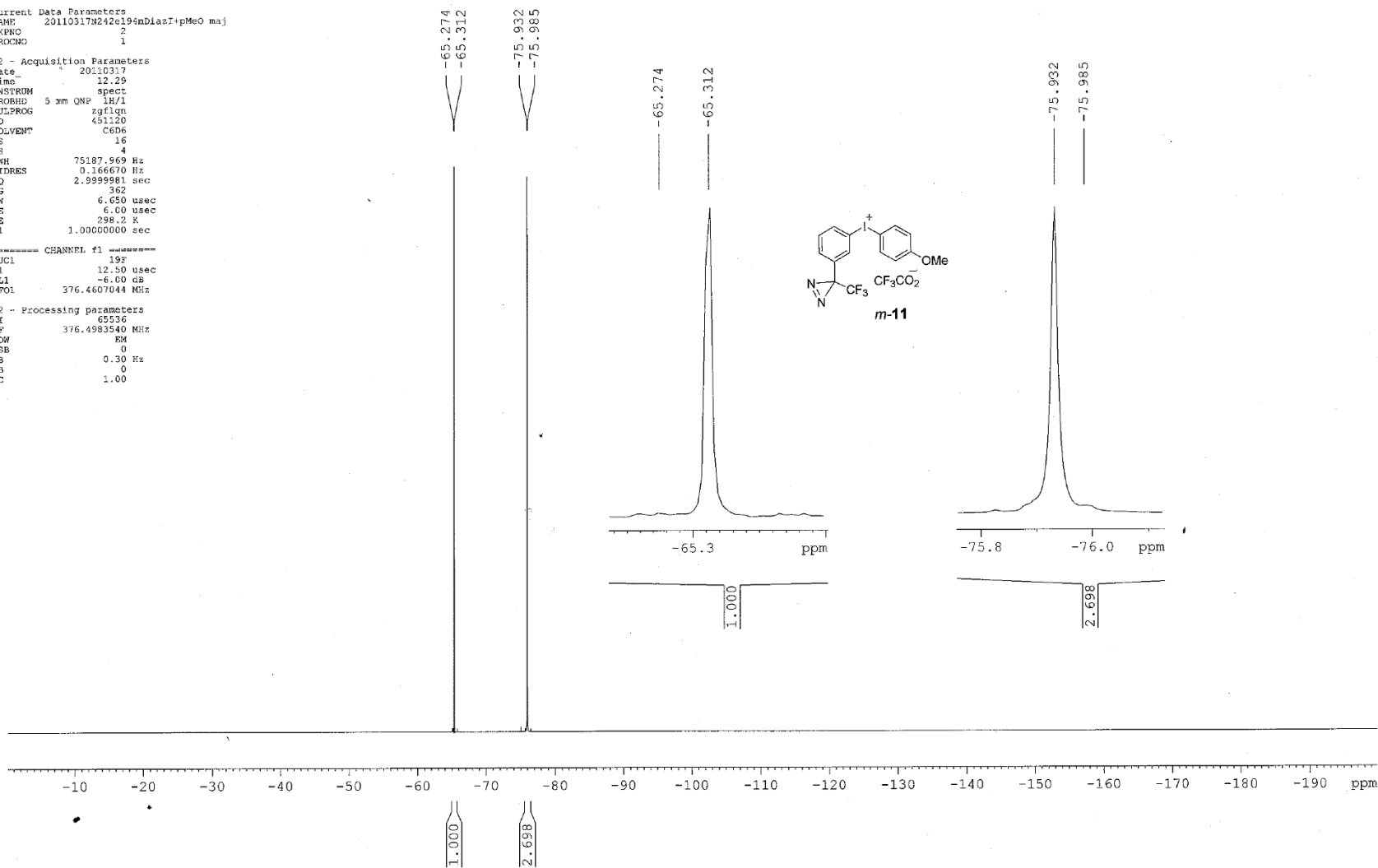
F19

Current Data Parameters
 NAME 20110317N242e19mDiazI+pMeO maj
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110317
 Time 12.29
 INSTRUM spect
 PROBRD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 451120
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 75187.969 Hz
 FIDRES 0.166570 Hz
 AQ 2.9999981 sec
 RG 362
 DW 6.650 usec
 DE 6.00 usec
 TE 298.2 K
 D1 1.0000000 sec

----- CHANNEL f1 -----
 NUC1 19F
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 376.4607044 MHz

F2 - Processing parameters
 SI 65536
 SF 376.4983540 MHz
 RDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

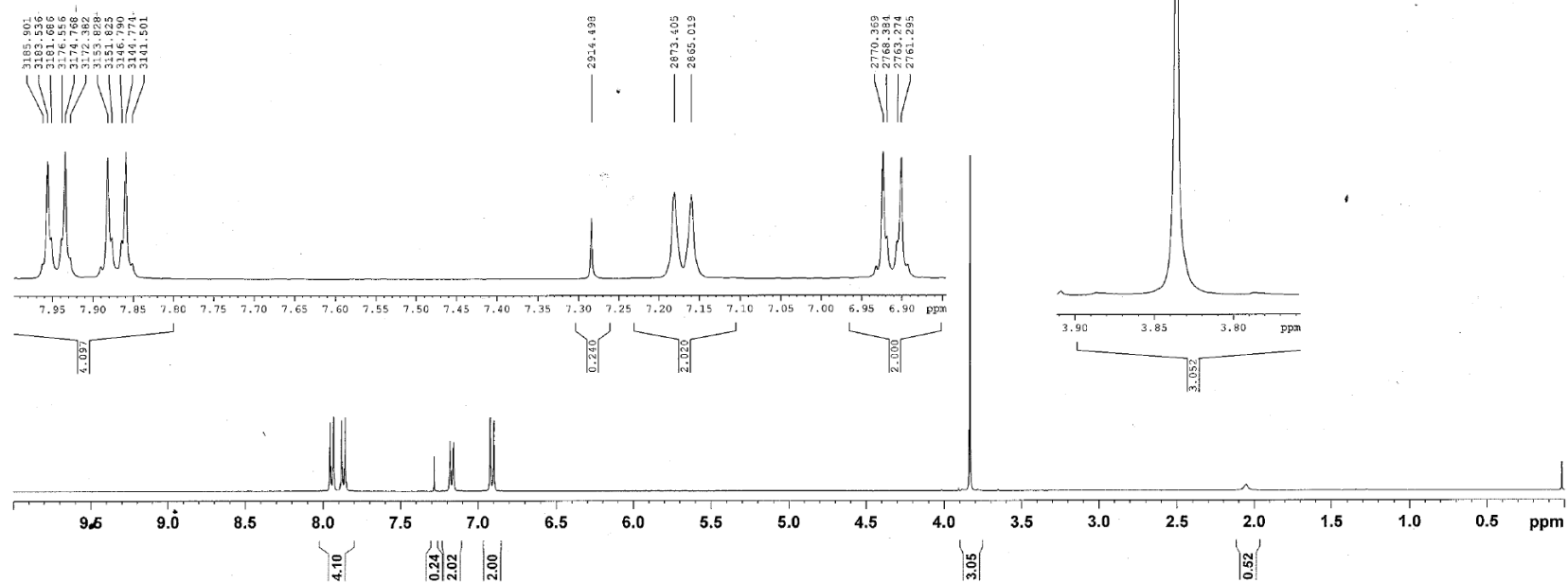
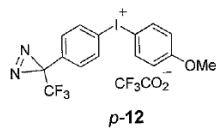


Current Data Parameters
 NAME 20100506N276e213 p01a21-pMeC
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110505
 Time 15:27
 INSTRUM spect
 FREQHD 5 cm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 352
 LW 60.400 usec
 DE 6.00 usec
 VE 299.2 K
 DI 1.00000000 sec
 MCREST 0.00000000 sec
 MCHRG 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 6
 RC 1.00

7.962
7.956
7.952
7.939
7.934
7.928
7.882
7.877
7.864
7.859
7.851
7.284
7.181
7.160
6.924
6.919
6.906
6.901



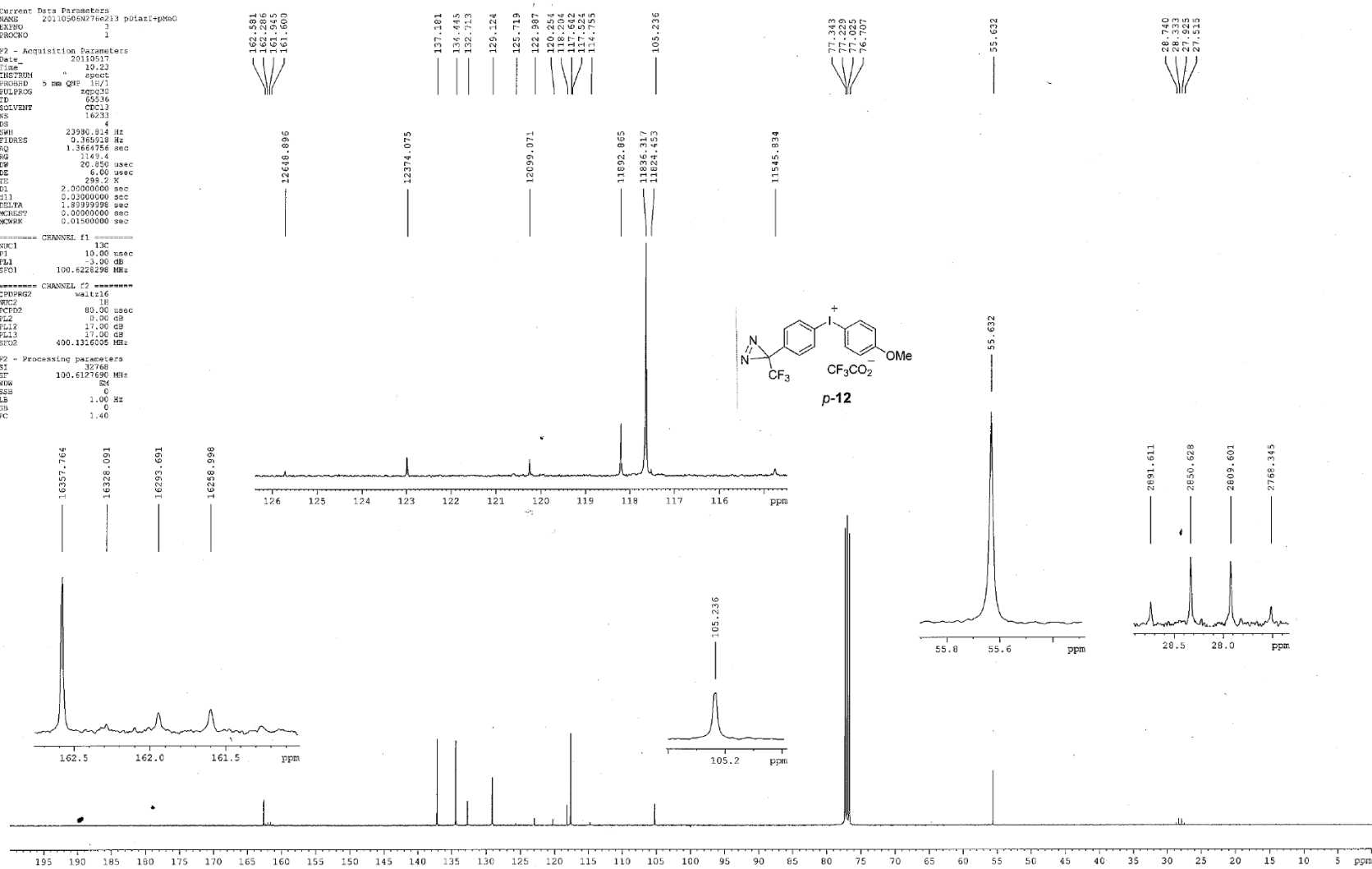
Current Data Parameters
 NAME 20110506N276213 p01asi-pms0
 EXPRD 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110517
 Time_ 19:21
 INSTRUM spect
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16233
 DS 4
 SWH 23986.814 Hz
 FIDRSS 0.365918 Hz
 RG 1.5664756 sec
 SG 1149.4
 DW 20.850 usec
 DE 6.40 usec
 TE 295.2 K
 D1 2.30000000 sec
 d11 0.03000000 sec
 DELTA 1.87999998 sec
 MEAS1 0.00000000 sec
 MEAS2 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -3.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 0.00 dB
 SFO2 400.1316102 MHz

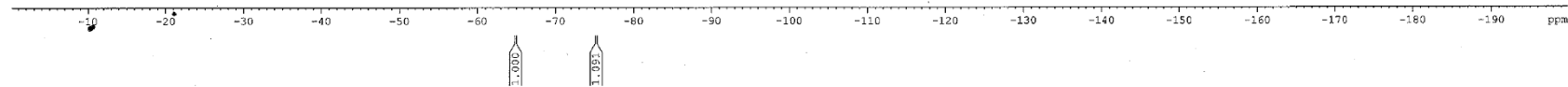
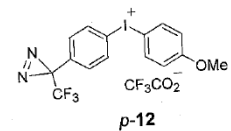
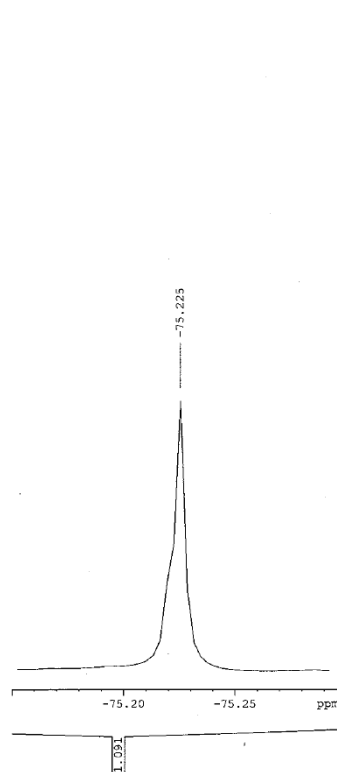
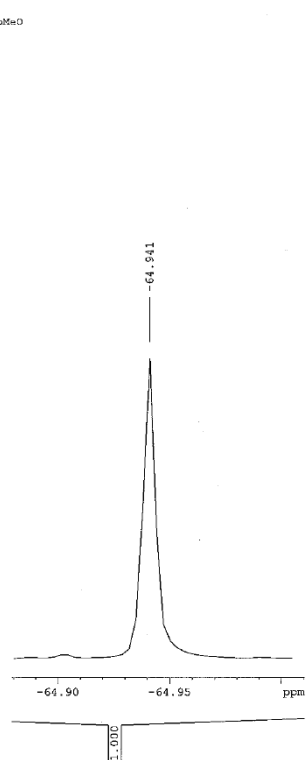
F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WU 24
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

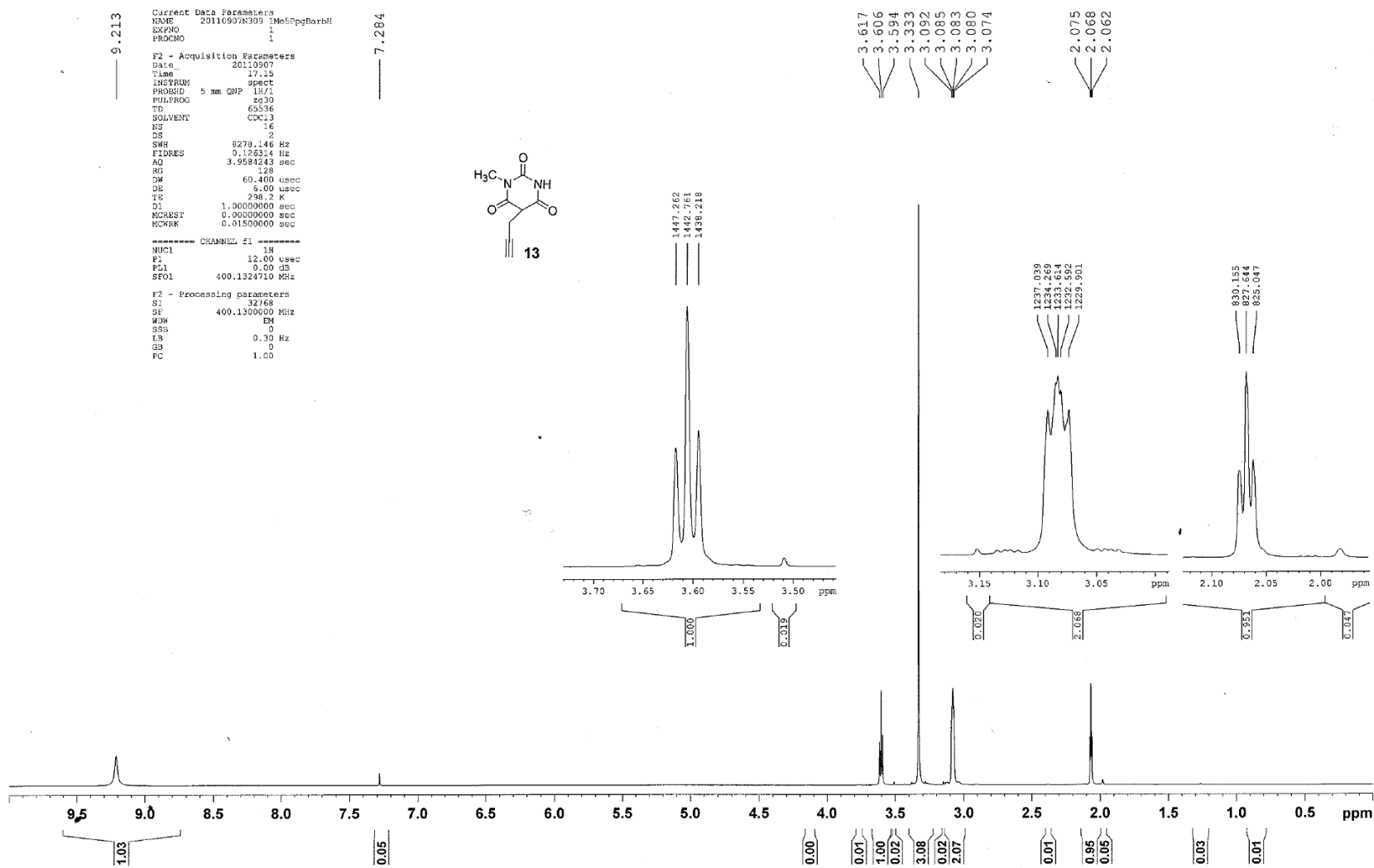


Current Data Parameters
 NAME 20110506276e213 pDiazI-pMeO
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110517
 Time 10.40
 INSTRUM spect
 PROBRD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 300744
 SOLVENT C6D6
 NS 64
 DS 4
 SWH 75187.869 Hz
 FIDRES 0.250007 Hz
 AQ 1.9999976 sec
 RG 812.7
 DW 6.650 usec
 DE 6.00 usec
 TE 299.2 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 19F
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 376.4607044 MHz
 F2 - Processing parameters
 SI 65536
 SF 376.4903540 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





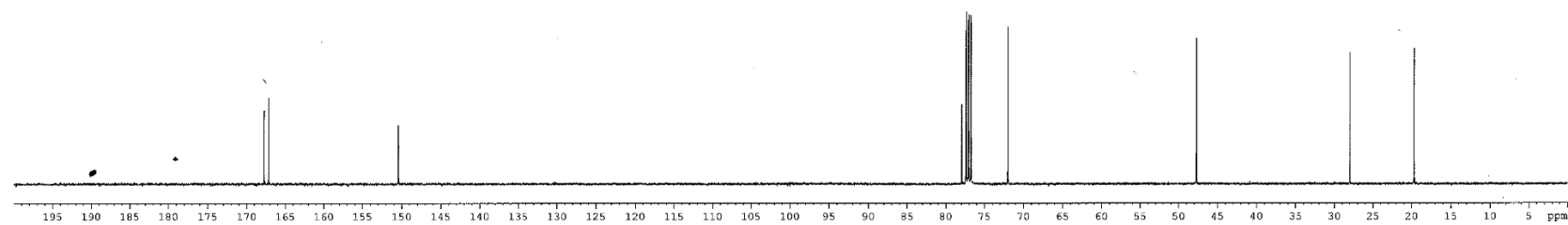
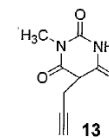
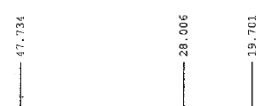
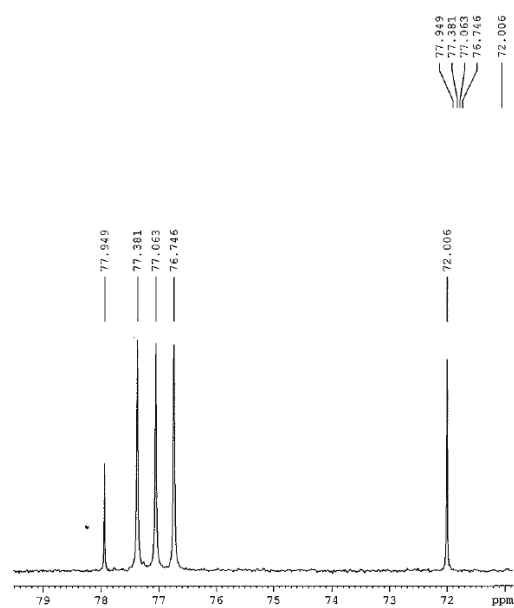
Current Data Parameters
 NAME 20110907N309 1Me5PpgbarbH
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110907
 Time_ 17.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 513
 DS 4
 SWH 23980.614 Hz
 FIDRES 0.355916 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 20.850 usec
 DE 6.00 usec
 TE 299.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 MCHYST 0.0000000 sec
 MCHRK 0.0150000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 10.00 usec
 PL1 -3.00 dB
 SFO1 100.6228298 MHz

----- CHANNEL f2 -----
 CDDEG2 waltz16
 NUC2 1H
 DCEG2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SP 100.6127690 MHz
 WDW DM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

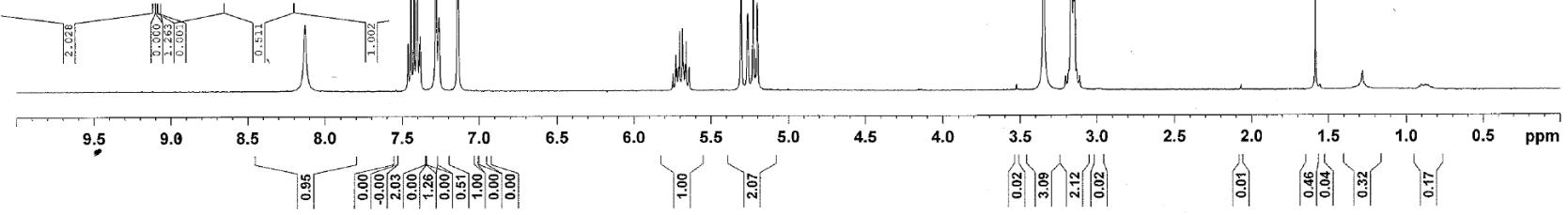
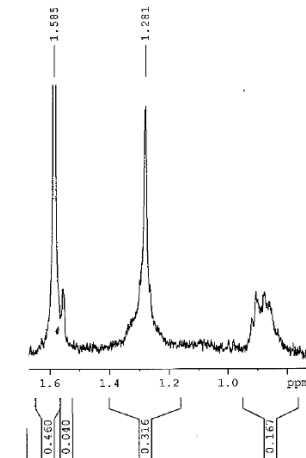
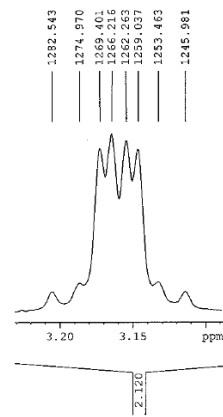
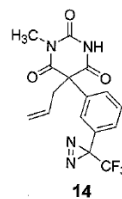
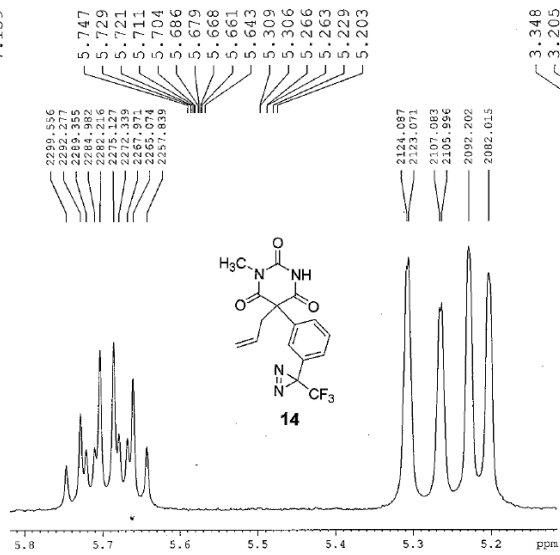
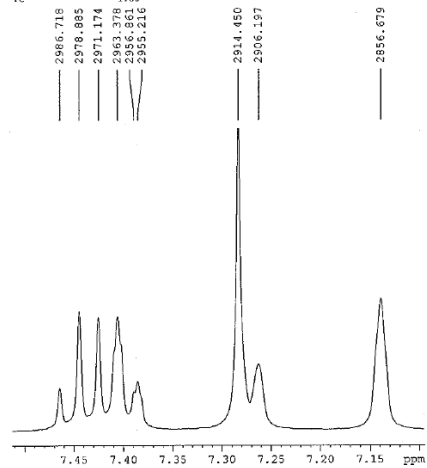


Current Data Parameters
 NAME: 211200700007.HMBarball rec per
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20120207
 Time: 14.12
 INSTRUM: spect
 PULPROG: zgpg30
 FIDRES: 5 mm QNP
 ID: 65534
 SOLVENT: CDCl3
 NS: 16
 DS: 4
 SFO: 8278.146 Hz
 FIDRES: 0.126314 Hz
 AQ: 3.534915 sec
 RG: 315
 EN: 60.420 usec
 DE: 6.20 usec
 TE: 299.2 K
 DL: 1.0000000 sec
 MEKREF: 0.0000000 sec
 MARRS: 0.0150000 sec

CHANNEL F1
 NU1: 1H
 P1: 12.00 usec
 PL1: 0.00 dB
 SFO1: 400.124710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300000 MHz
 NQ: 1H
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

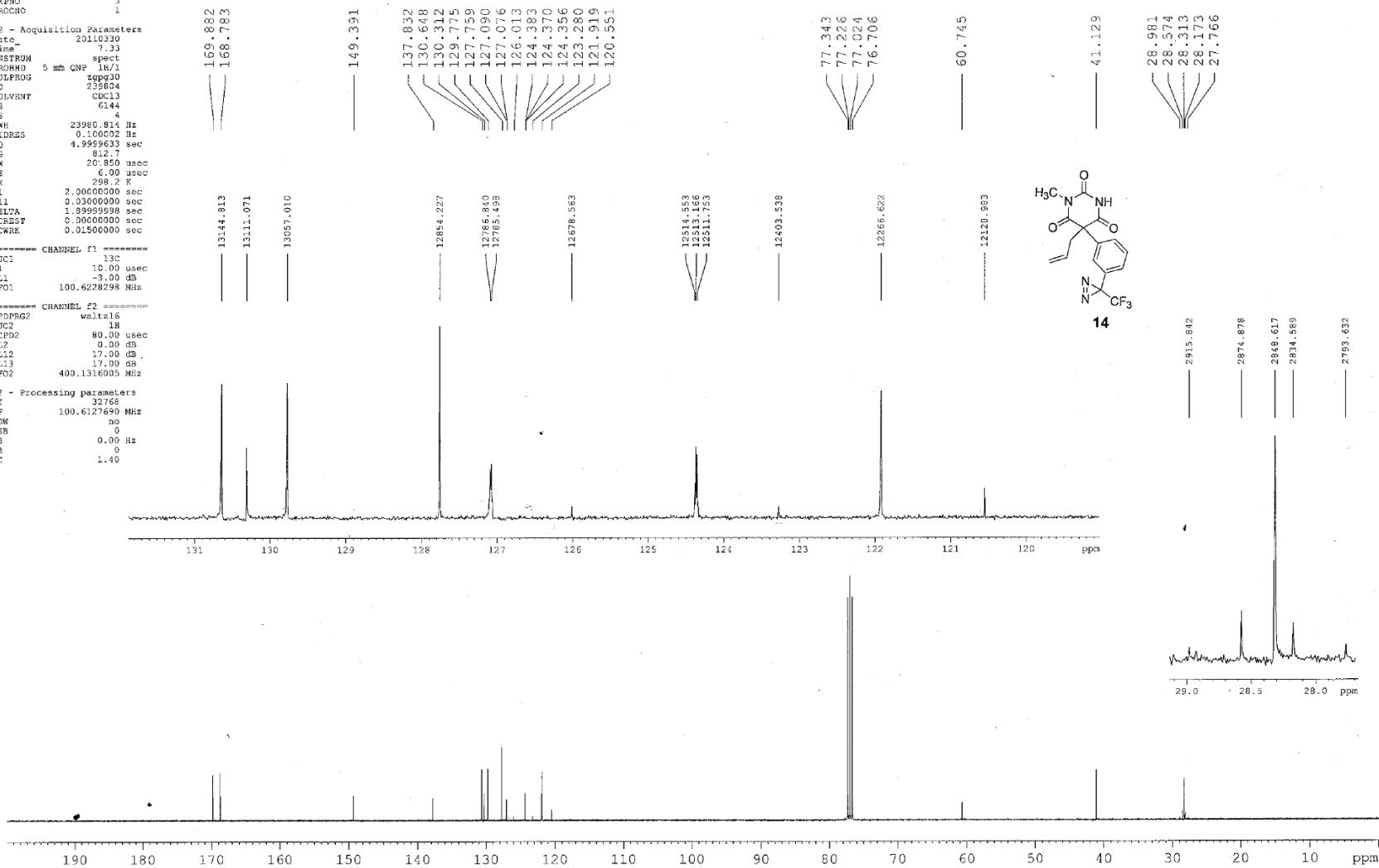


Current Data Parameters
 NAME F0110329M1508aruDiaz repur
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110330
 Time_ 7.33
 INSTRUM spect
 PROBM 5 MHz QNP 1H/1
 PULPROG zgpg30
 TD 239804
 SOLVENR CDCl3
 NS 6144
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.100002 Hz
 AQ 4.9989633 sec
 RG 812.7
 BW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8989998 sec
 MCREST 0.5000000 sec
 KWARK 0.0150000 sec

----- CHANNEL f1 -----
 NUC1 13C
 P1 10.00 usec
 PL1 -3.00 dB
 SFO1 100.6228298 MHz
 ----- CHANNEL f2 -----
 CDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

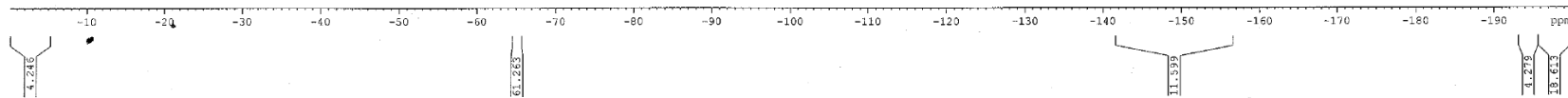
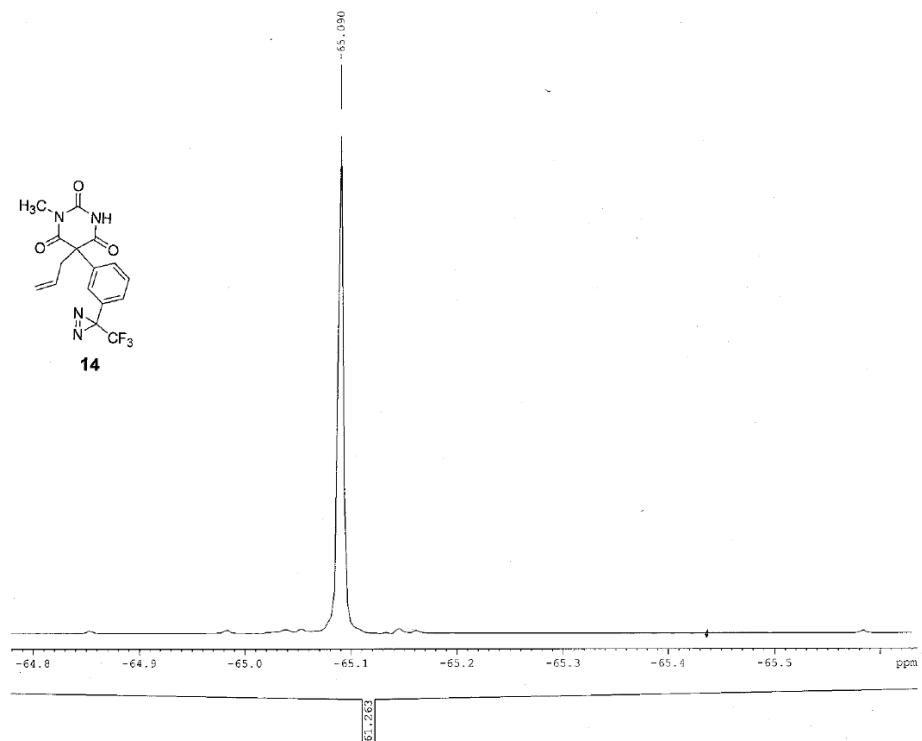
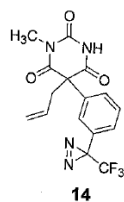


Current Data Parameters
 NAME 20110329N250HarDiaz repur
 EXFNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20110329
 Time 19.26
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 451120
 SOLVENT C6D6
 NS 16
 DS 4
 SWH 75187.969 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999981 sec
 RG 912.3
 DW 6.650 usec
 DE 6.00 usec
 TE 298.2 K
 D1 1.00000000 sec

----- CHANNEL f1 -----
 NUC1 19F
 P1 12.50 usec
 PL1 -6.00 dB
 SF01 376.4607044 MHz

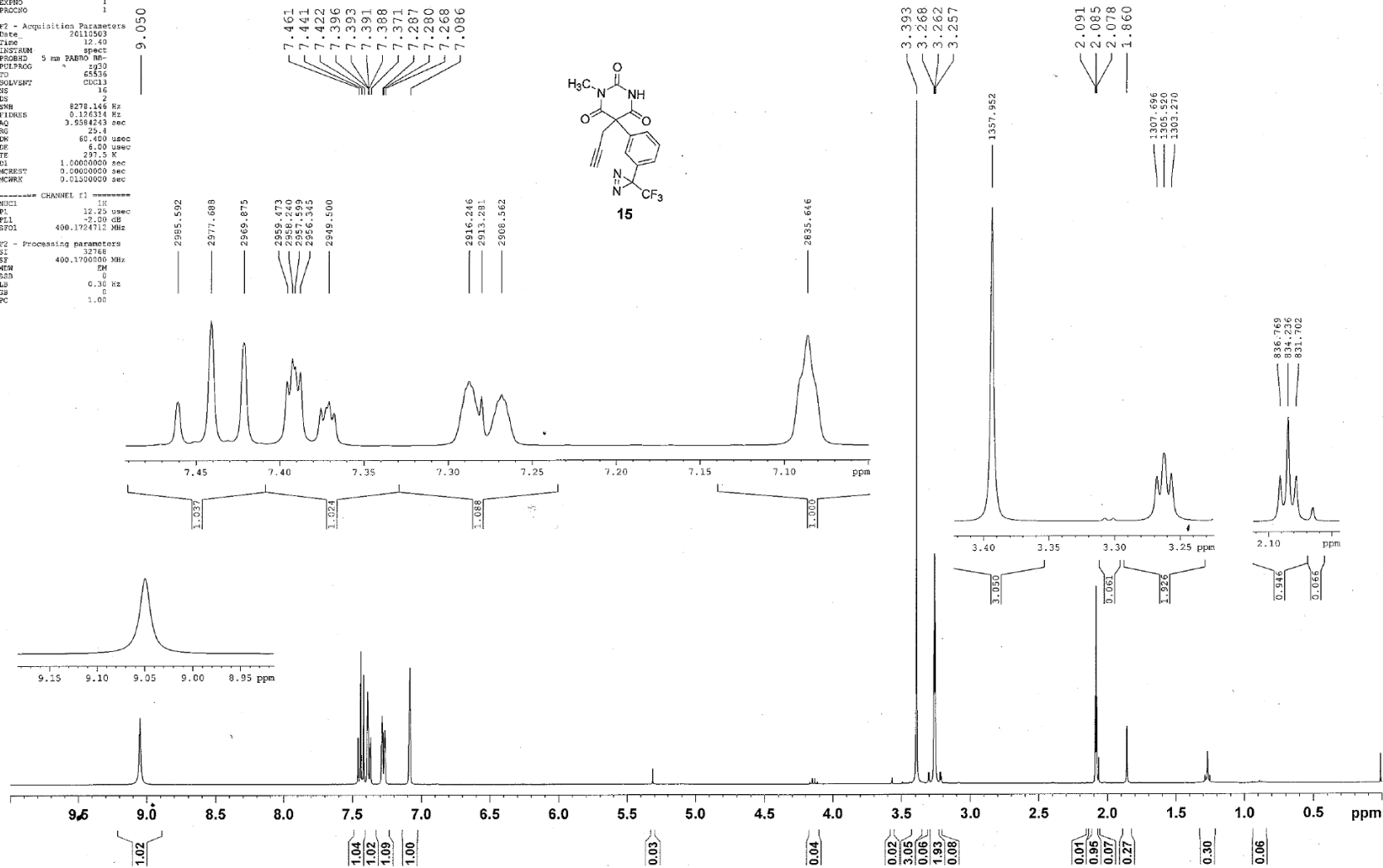
F2 - Processing parameters
 SI 65336
 SF 376.4983540 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 20110503N271e209 FpgBarb-mDias
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110503
 Time 12.40
 INSTRUM spect
 PROBRD 5 mm PABBO WB-
 PULPROG zgpg30
 TO 65536
 SOLVENT ccdcl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.176314 Hz
 AQ 3.9594243 sec
 RG 25.4
 DW 60.460 usec
 DE 6.00 usec
 TE 297.5 K
 D1 1.0000000 sec
 MCREST 0.0000000 sec
 MCWRR 0.01500000 sec

CHANNEL f1
 NUC1 13C
 P1 12.25 usec
 PL1 -2.00 dB
 SFO1 400.172417 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1700000 MHz
 WHW 8M
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



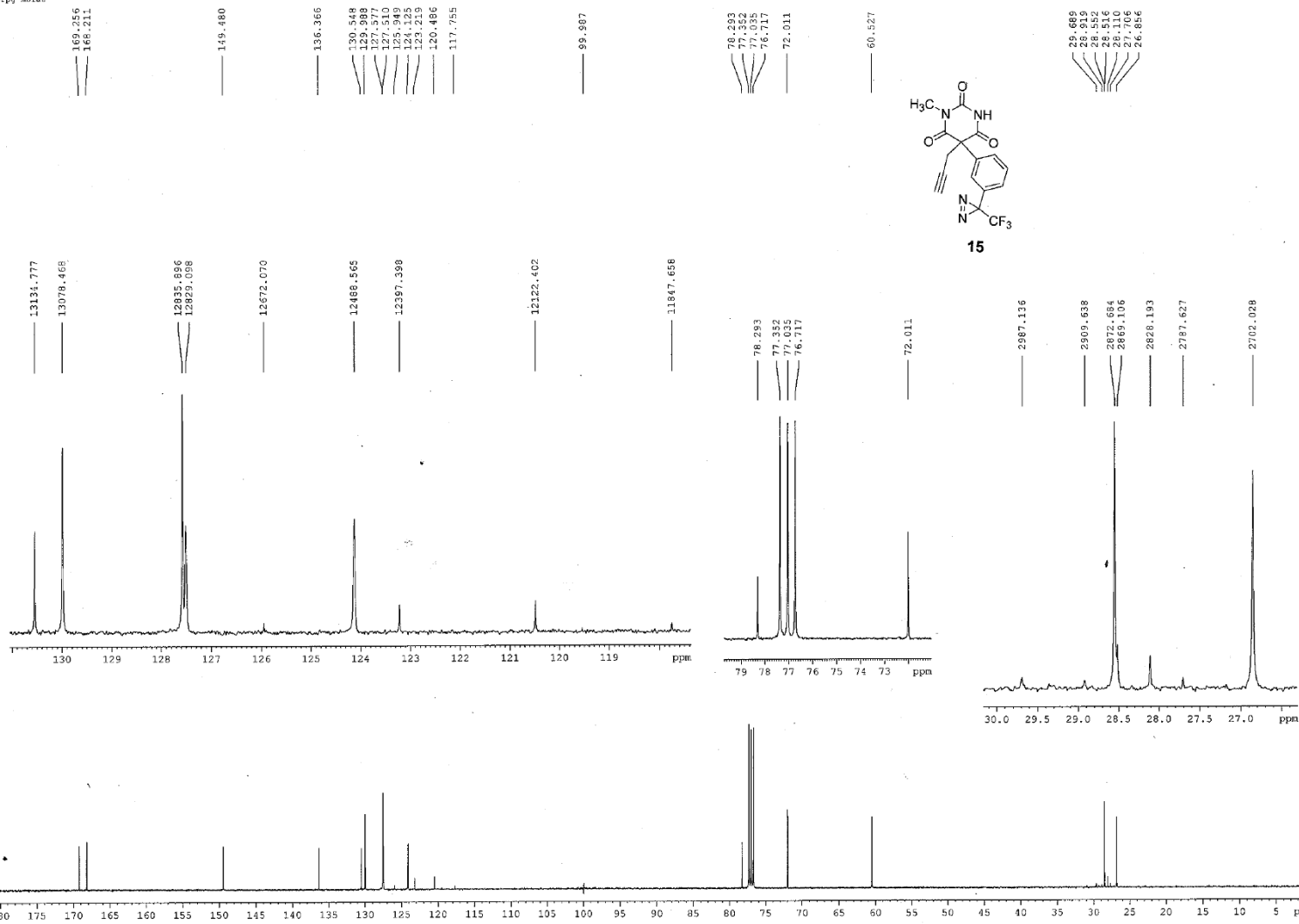
Current Data Parameters
 NAME 201205180271a209 MeBarbDpp-mDias
 EXPR0 2
 PROC00 3

F2 - Acquisition Parameters
 Date 20110518
 Time 16.04
 INSTRUM spect
 PROC00 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWE 22980.814 Hz
 FIDRES 0.395938 Hz
 AQ 1.3664756 sec
 WC 724.1
 EM 20.850 usec
 DE 8.00 usec
 TE 303.2 K
 D1 2.00000000 sec
 d11 0.33000000 sec
 DELTA 1.89999998 sec
 MCH001 0.00000000 sec
 MCH002 0.31000000 sec

CHANNEL f1
 NUC1 13C
 P1 10.00 usec
 PL1 3.00 dB
 SFO1 100.628298 MHz

CHANNEL f2
 CDP002 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SP 100.6127689 MHz
 RMW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



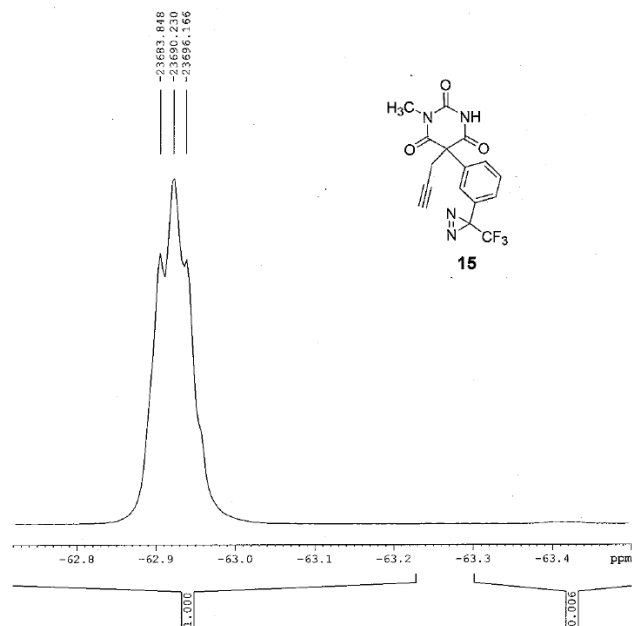
Current Data Parameters
 NAME 20110518N271e209 MeBarbPp-sDiaz
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20110519
 Time 12.03
 INSTRUM spect
 PROBRD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 390784
 SOLVENT C6D6
 NS 16
 DS 4
 SWH 75107.969 Hz
 FREQSS 0.250007 Hz
 AQ 1.9999976 sec
 RG 645.1
 DW 6.650 usec
 DE 6.00 usec
 TE 299.2 K
 D1 1.0000000 sec

----- CHANNEL f1 -----
 NUC1 19F
 P1 12.00 usec
 PL1 -6.00 dB
 SFO1 376.4607044 MHz

F2 - Processing parameters
 SI 65536
 SF 376.4983540 MHz
 WCW 6K
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

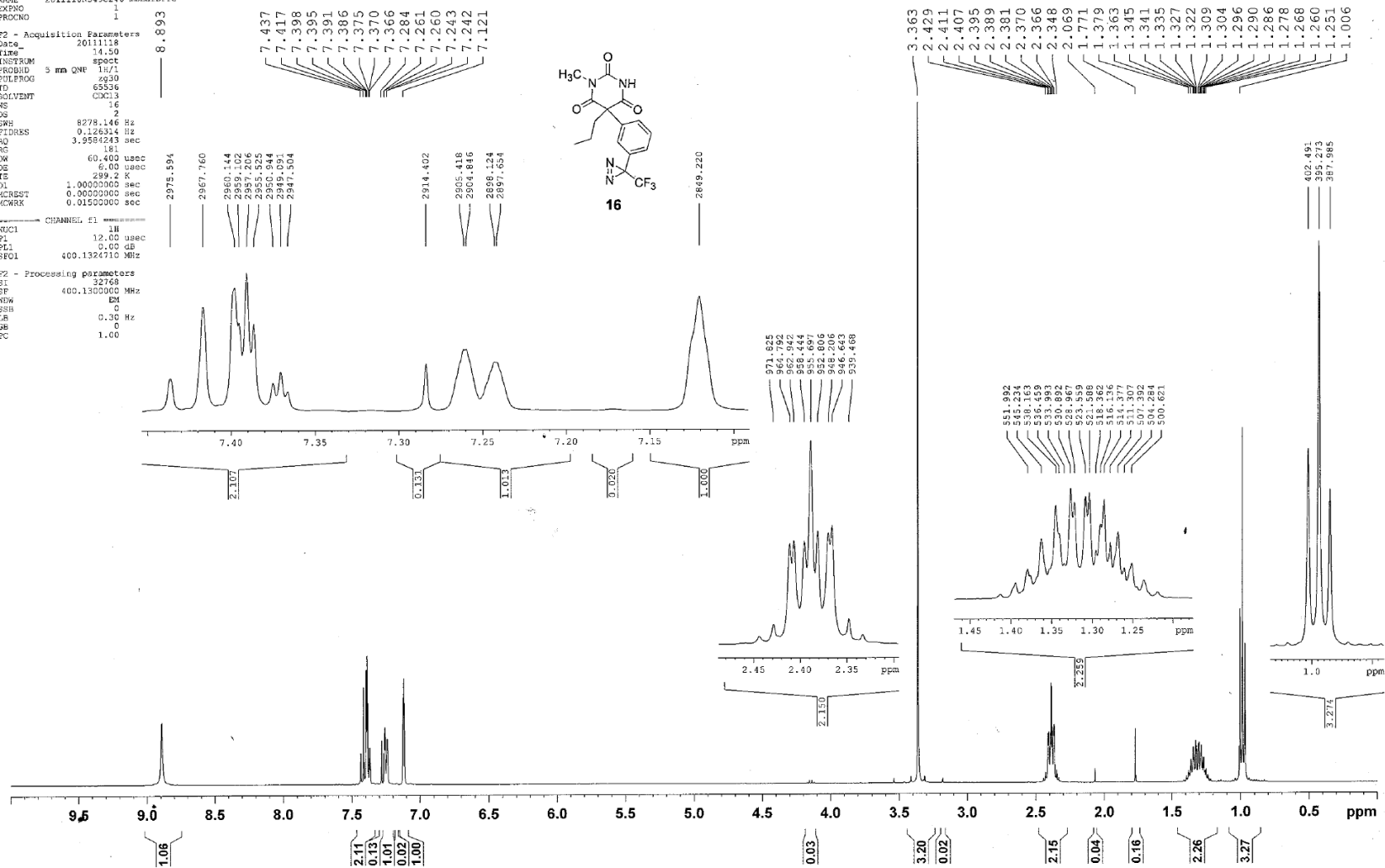
62.926
 62.922
 62.918



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

62.926
 62.922
 62.918

Current Data Parameters
 NAME 2011118349246 sHBarbPro
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20111118
 Time 14.59
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 CQX13
 SOLVENT
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 161
 DW 60.400 usec
 DB 6.00 usec
 TS 299.2 K
 D1 1.00000000 sec
 NUC1 1H
 NUC2 13C
 NUC3 19F
 NUC4
 NUC5
 NUC6
 NUC7
 NUC8
 NUC9
 NUC10
 NUC11
 NUC12
 NUC13
 NUC14
 NUC15
 NUC16
 CHANDEL f1
 MUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.1324510 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 REW 64
 SSI 0
 LB 0.30 Hz
 GB 0
 PC 1.00



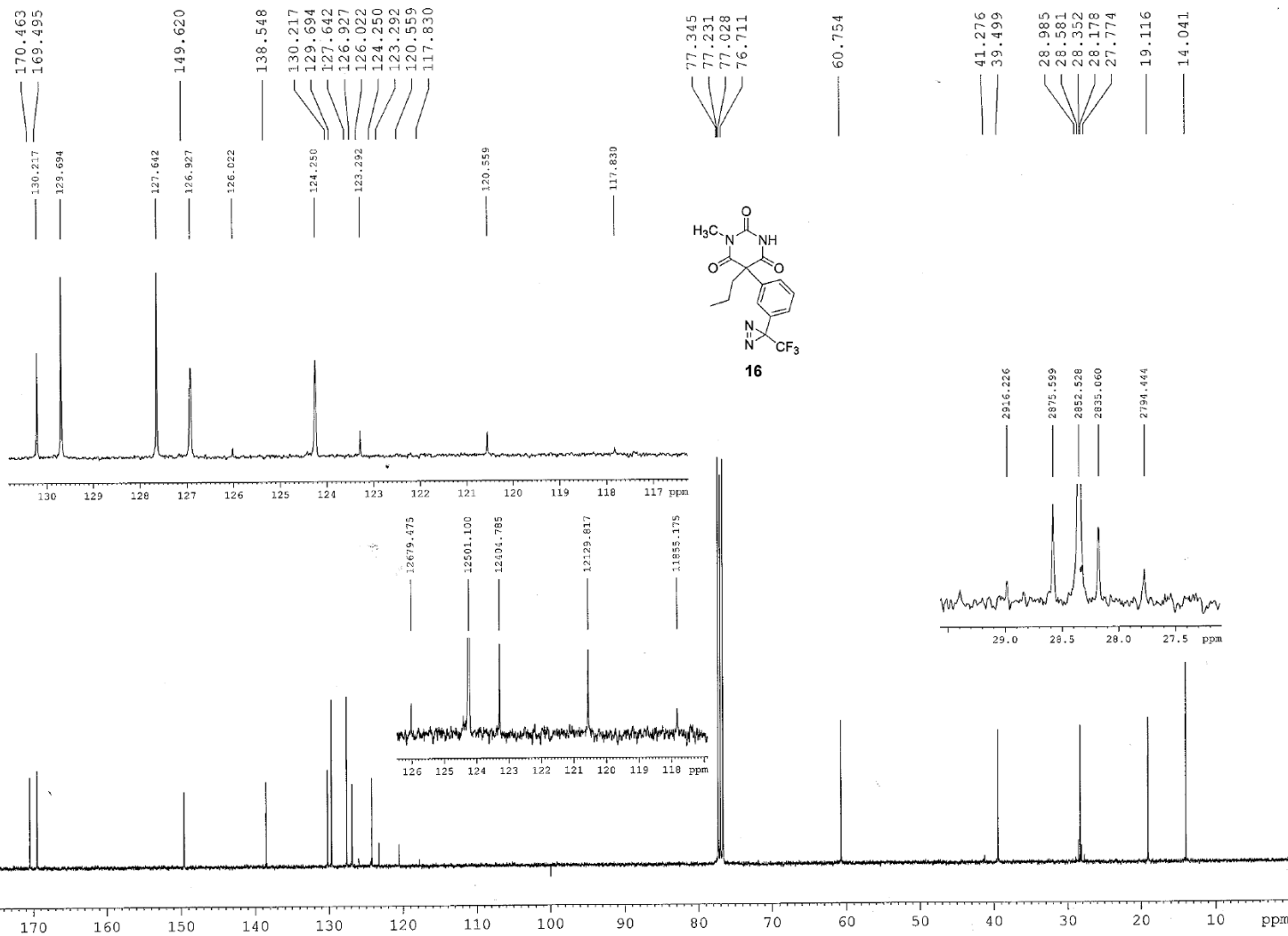
Current Data Parameters
 NAME 201118N349246 mDBarbPro
 EXNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20111118
 Time 15.14
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 724.1
 DW 20.850 usec
 DE 6.00 usec
 TE 299.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.39999999 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

CHANNEL F1
 NDC1 13C
 P1 10.00 usec
 PL1 -9.00 dB
 SFO1 100.6228298 MHz

CHANNEL F2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 400.1315005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



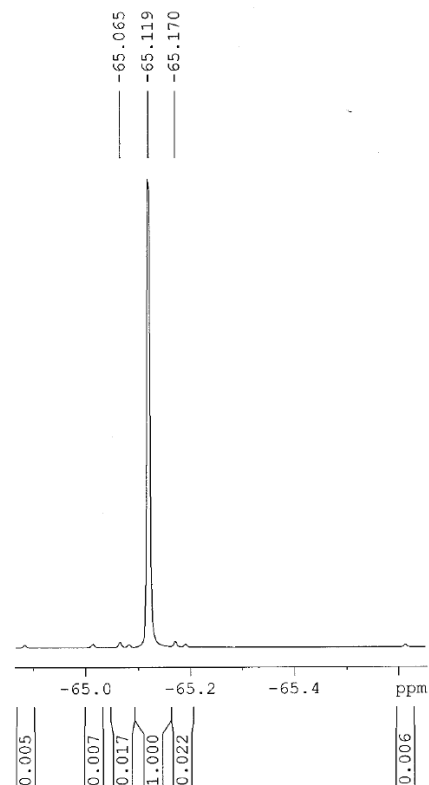
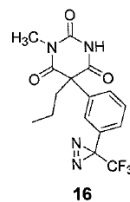
Current Data Parameters
 NAME 201118R349e246 mDBarbPro
 EXPRNO 2
 PRGNO 1

F2 - Acquisition Parameters
 Date_ 20111118
 Time 14.57
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 451120
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 75187.969 Hz
 FIDRES 0.166670 Hz
 AQ 2.990981 sec
 RG 645.1
 DW 6.650 usec
 DE 6.00 usec
 TE 299.2 K
 D1 1.0000000 sec

----- CHANNEL f1 -----
 NDC1 19F
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 376.4607044 MHz

F2 - Processing parameters
 SI 65536
 SF 376.4983400 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

-65.065
 -65.119
 -65.170



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

0.005
 0.007
 0.017
 1.000
 0.022
 0.006

