

Supporting Information

A 1,3-Carbonyl Shift in the Platinum-catalyzed Aromatization of 2-Epoxy-1-(methoxyalk-2-ynyl)benzenes

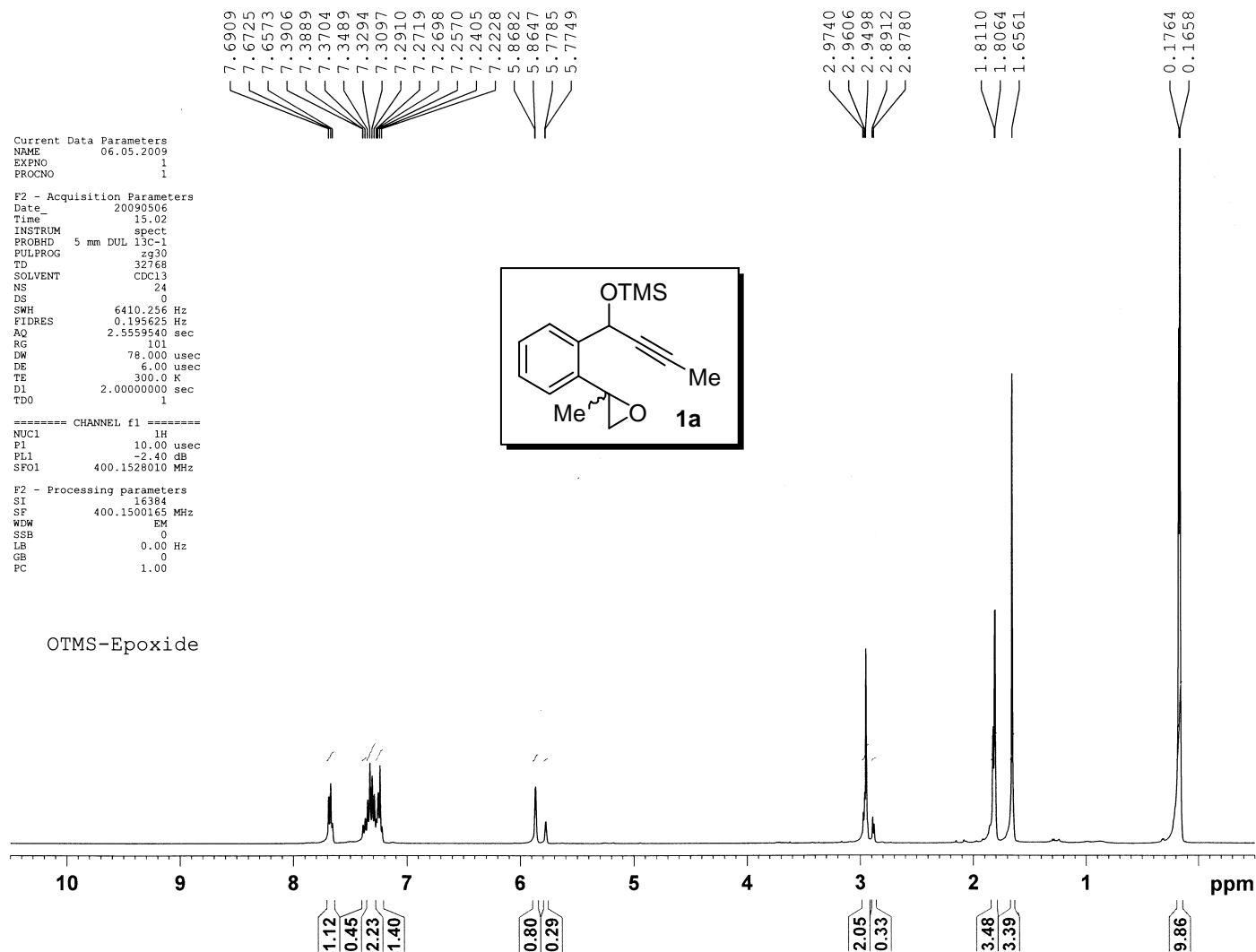
Rupsha Chaudhuri, Arindam Das, Hsin-Yi Liao and Rai-Shung Liu*

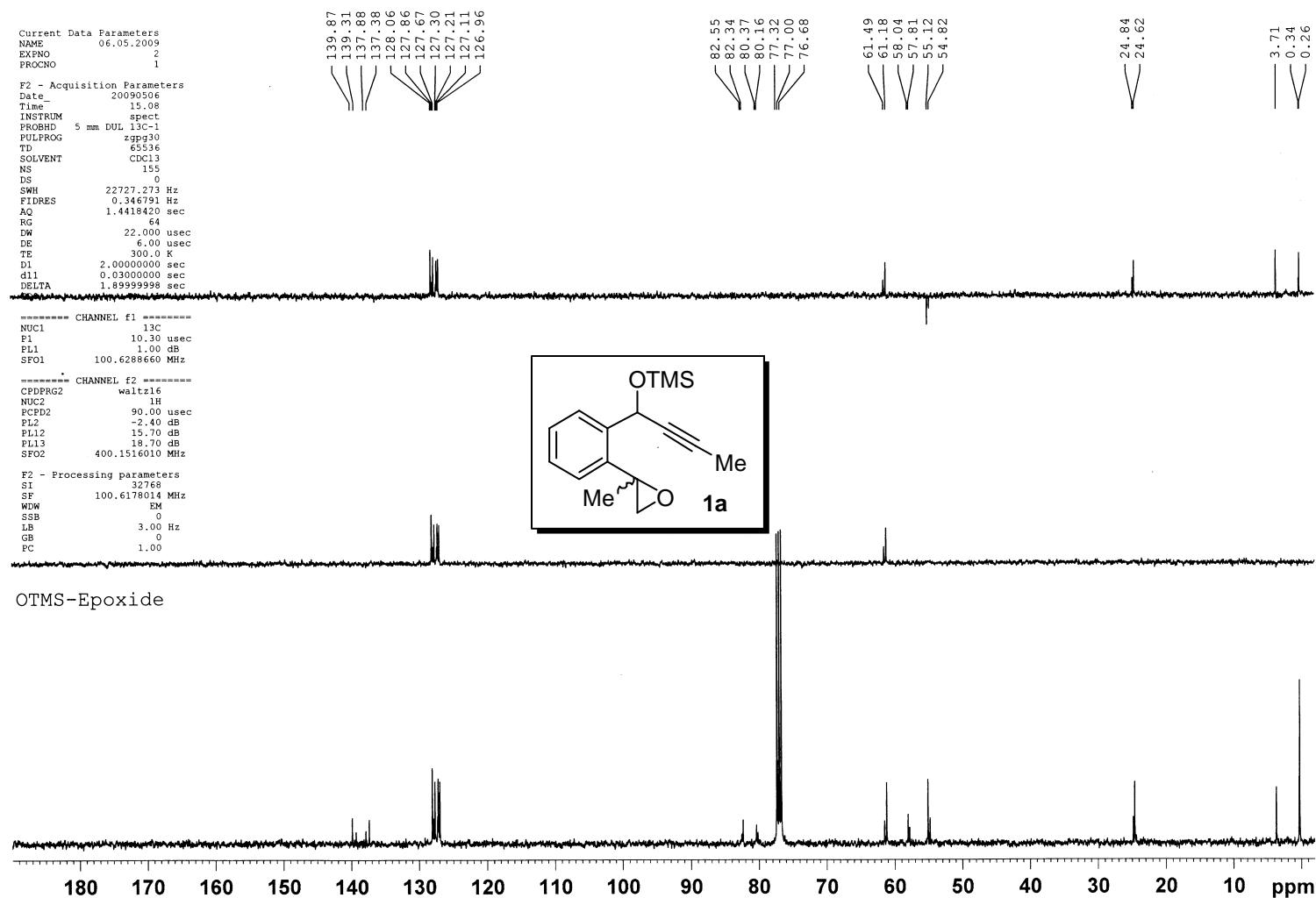
**Department of Chemistry, National Tsing-Hua University, Hsinchu, Taiwan, ROC and ‡Department of Science Education, National
Taipei University of Education, Taipei, Taiwan, ROC*

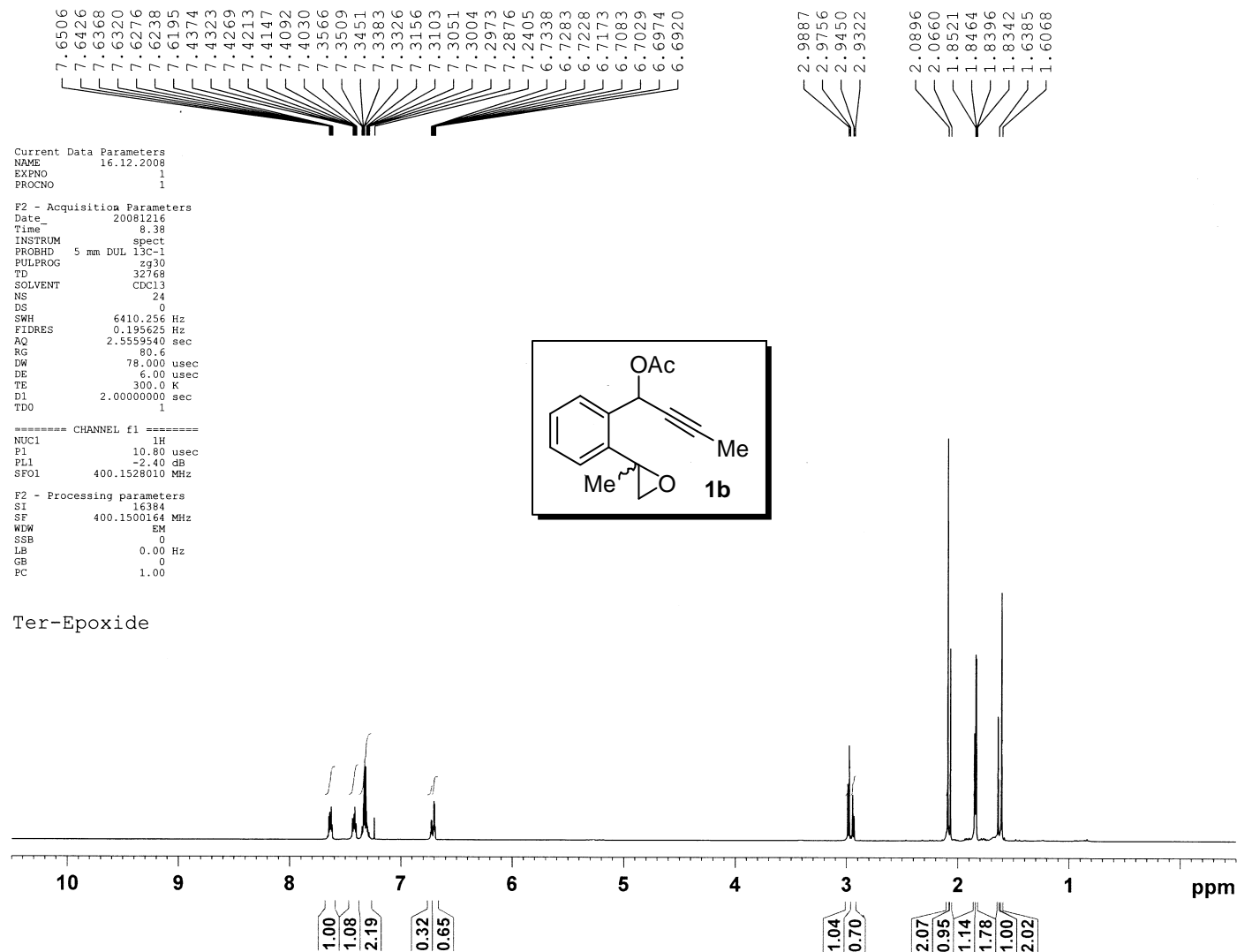
----- *rsliu@mx.nthu.edu.tw*

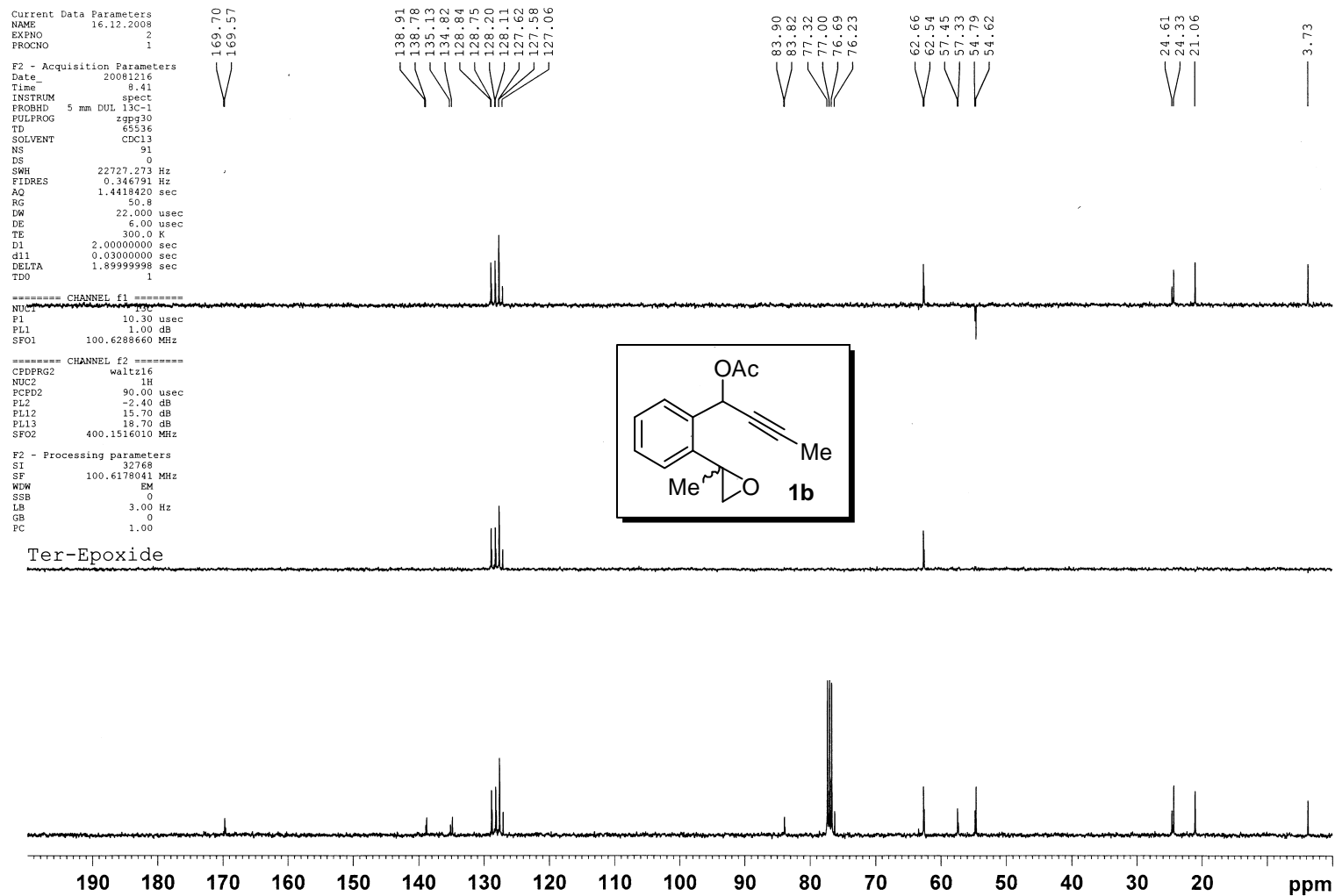
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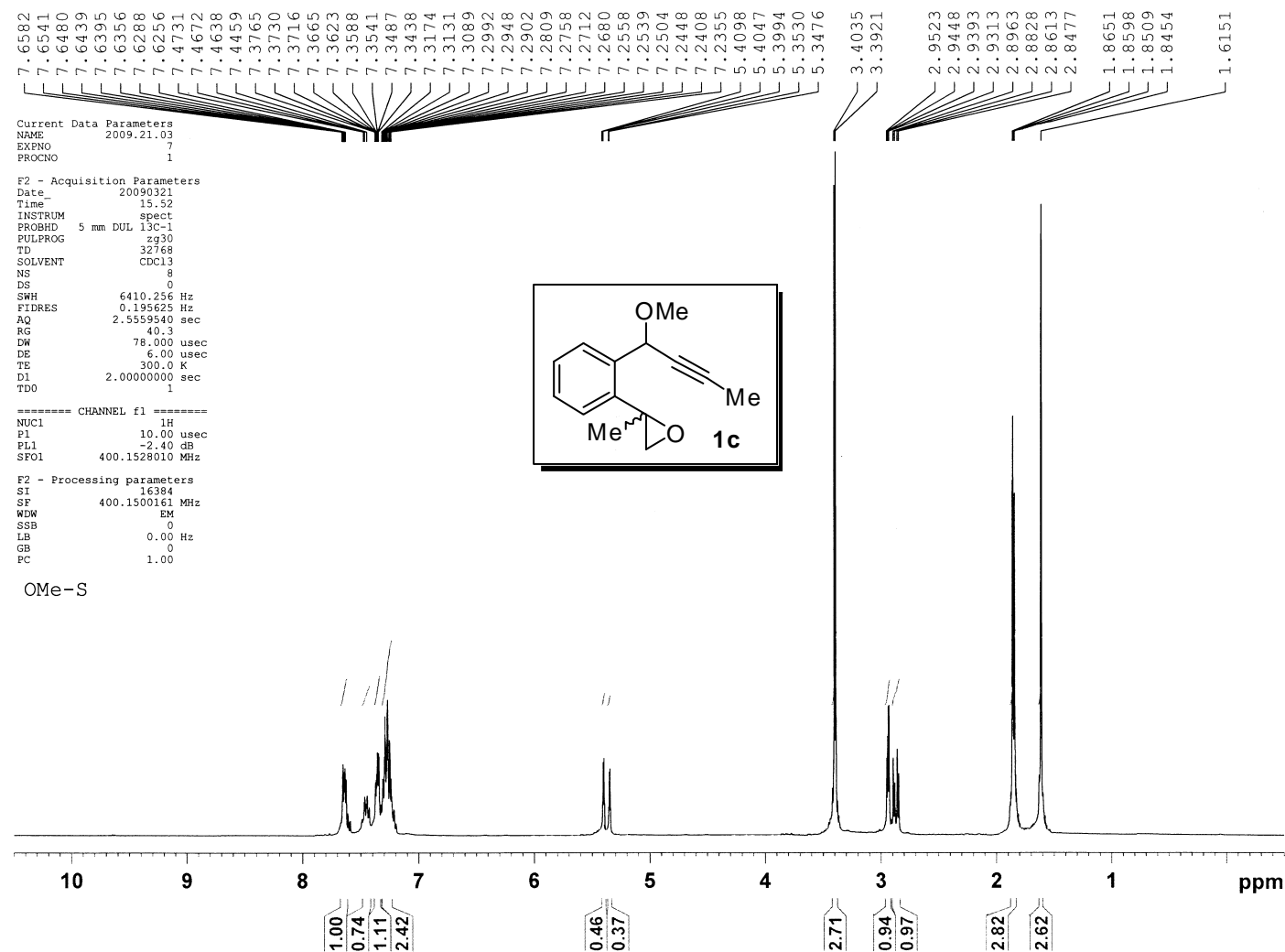
- (1) ^1H & ^{13}C spectra of compounds **1a-8** -----S 2- S 91.
- (2) NOE spectra of compounds **6g, 6h, 6i, 6l, 6o & 6p**-----S 92 – S 117.

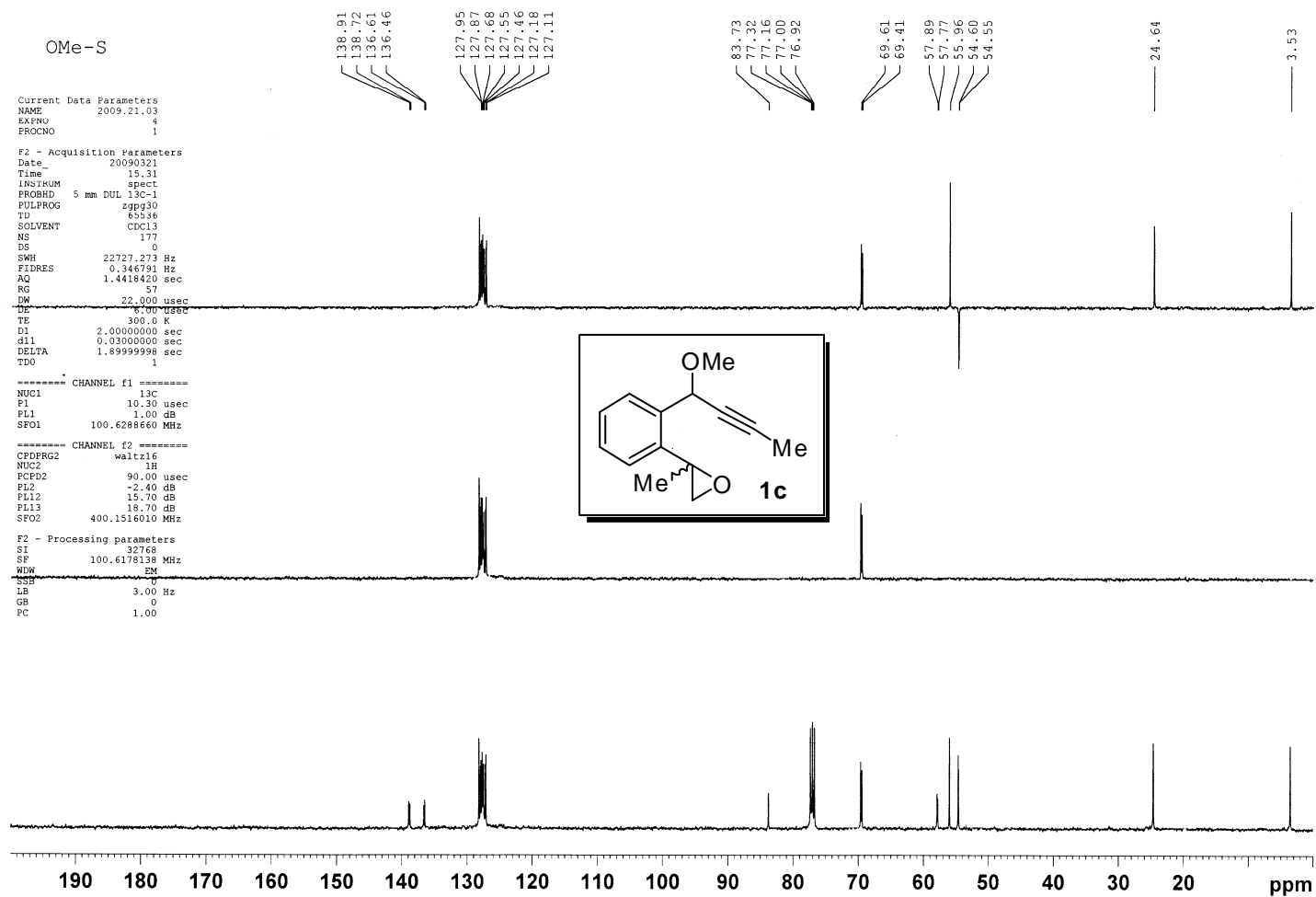


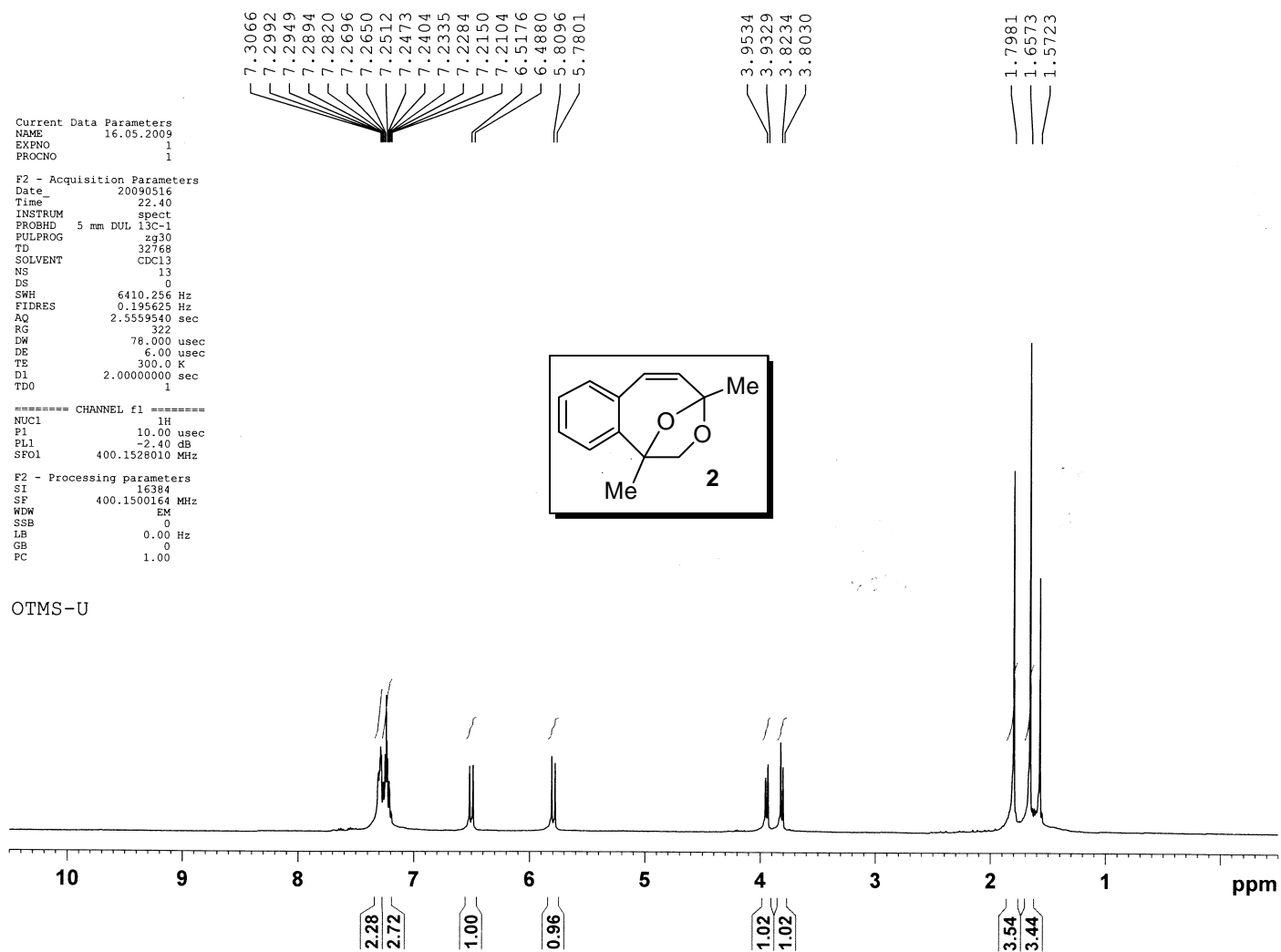


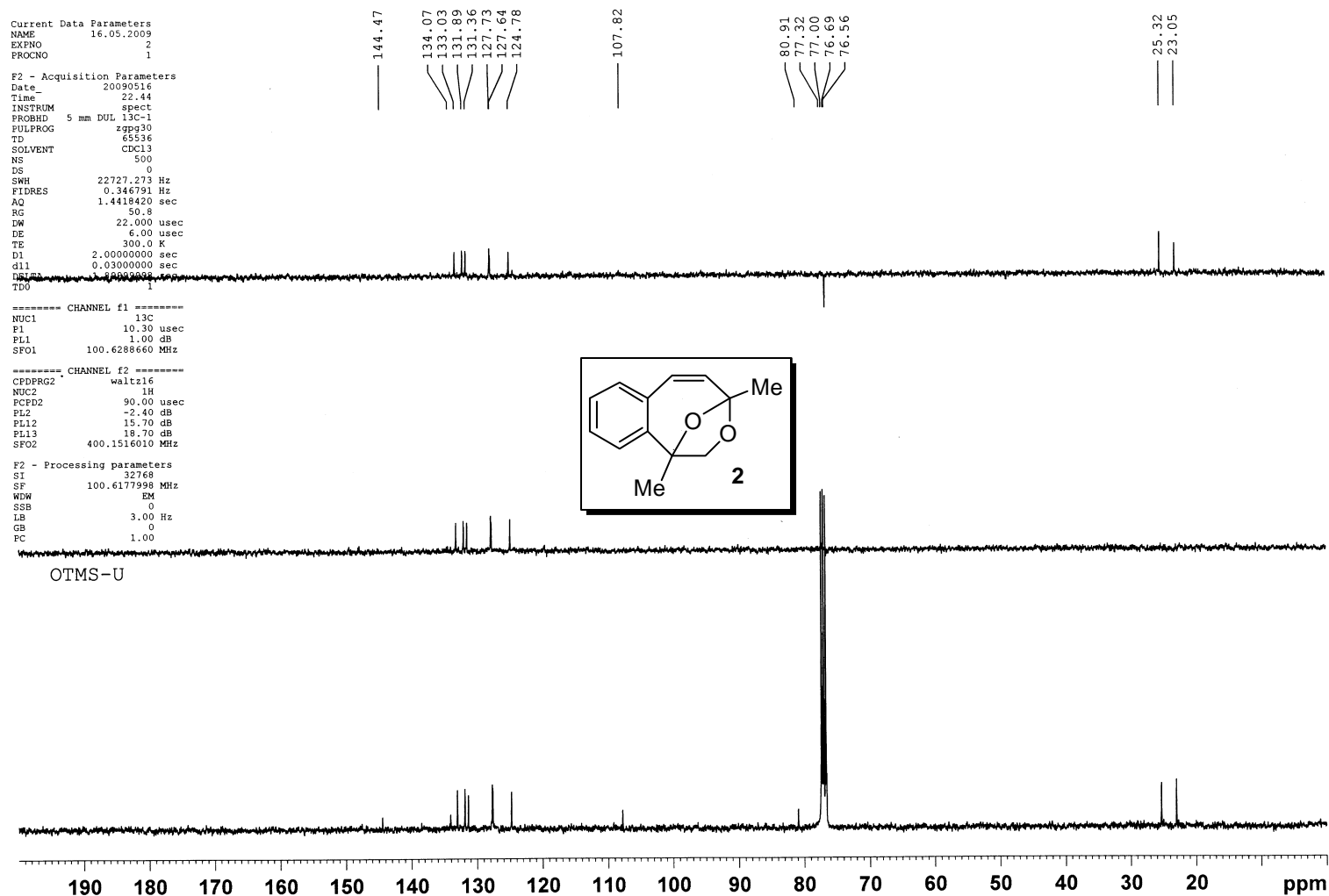


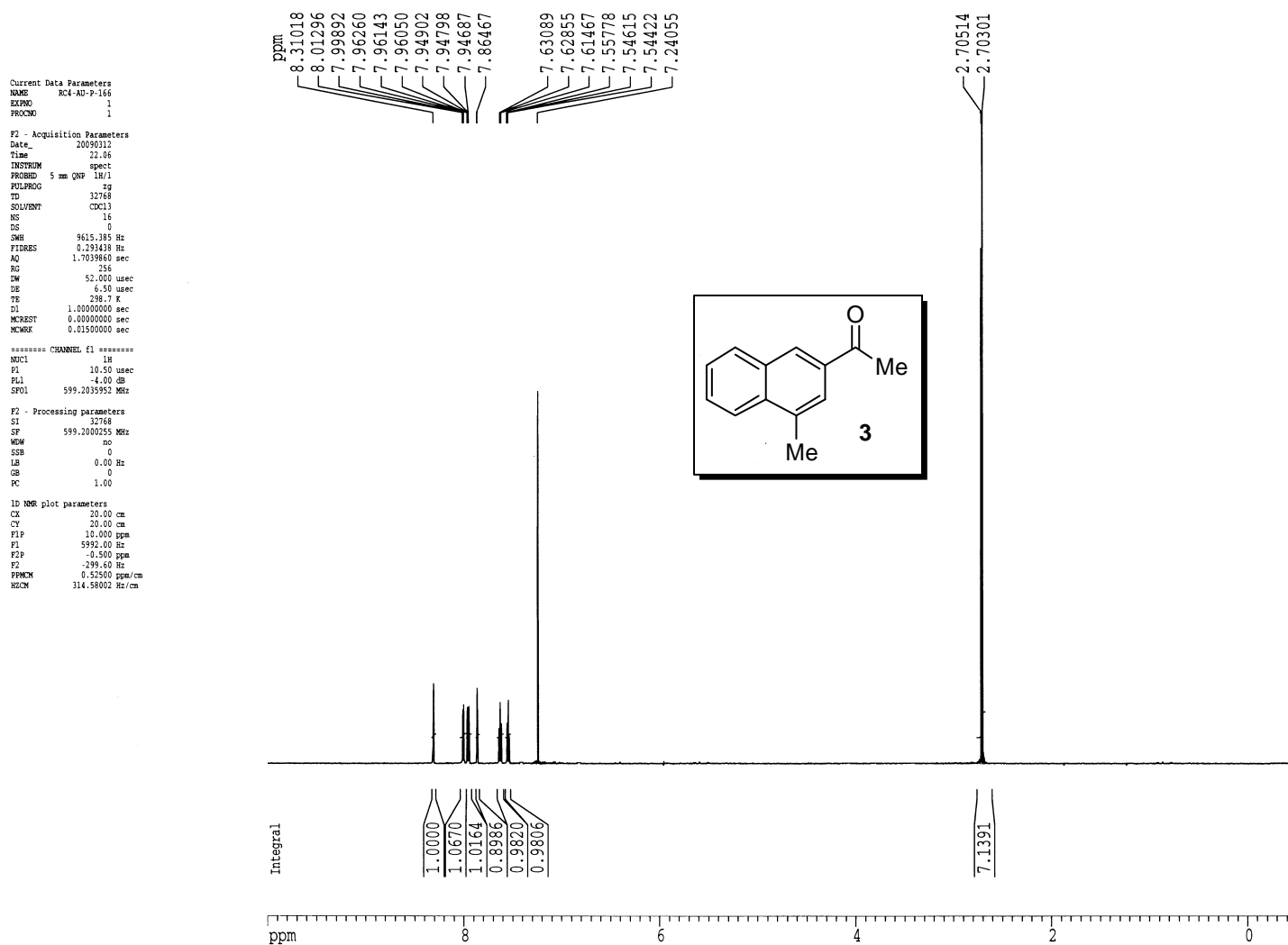


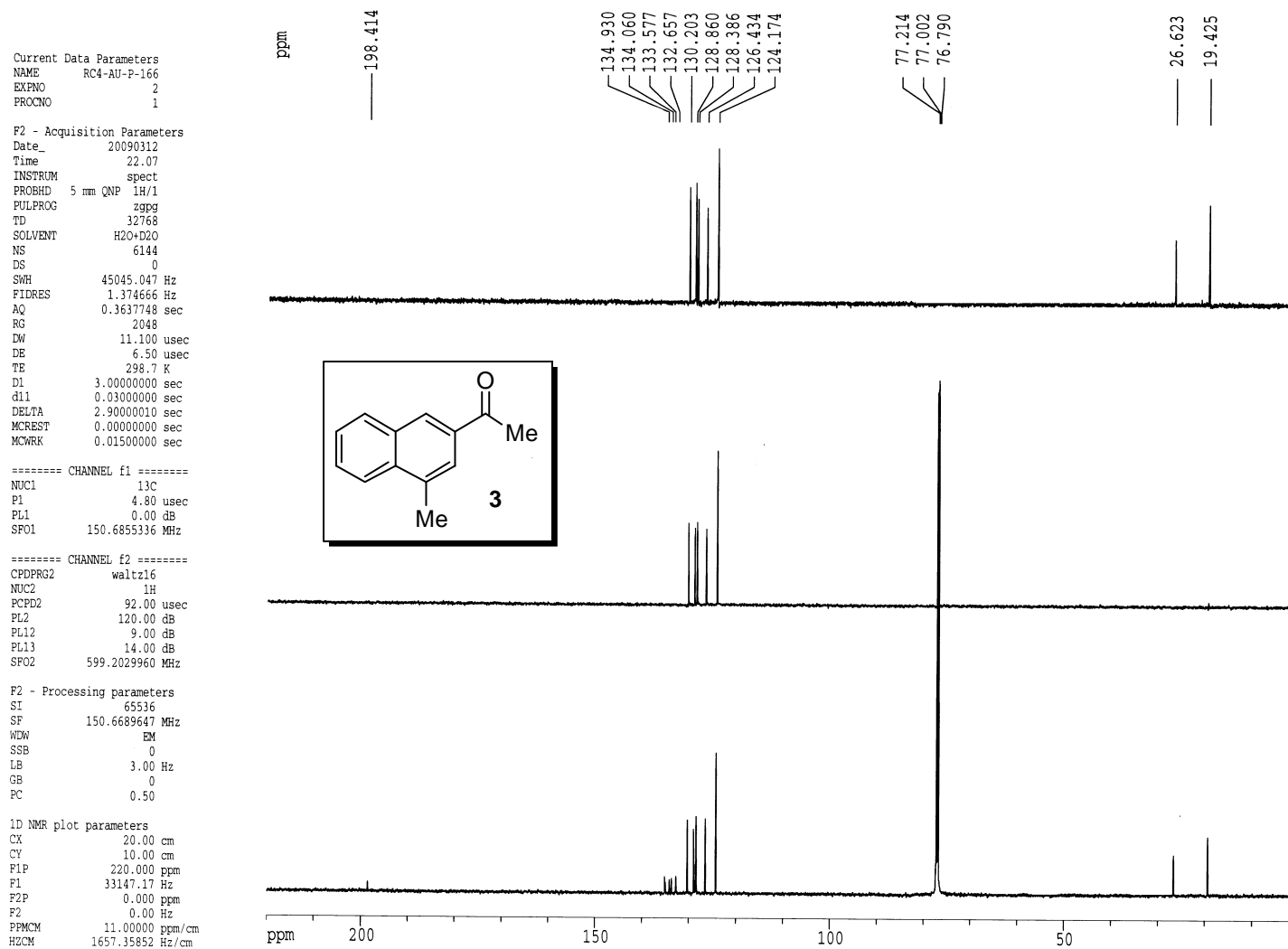


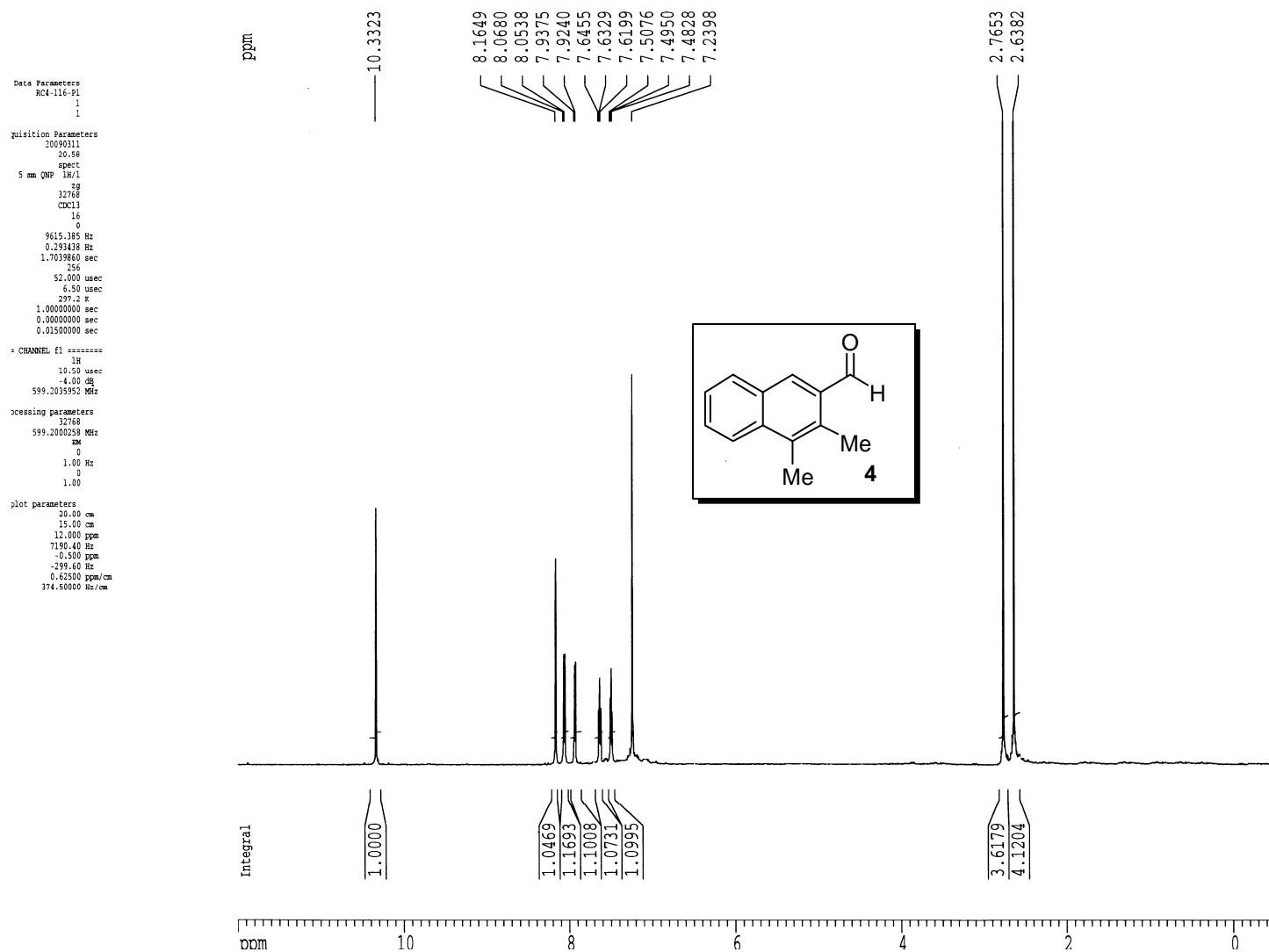


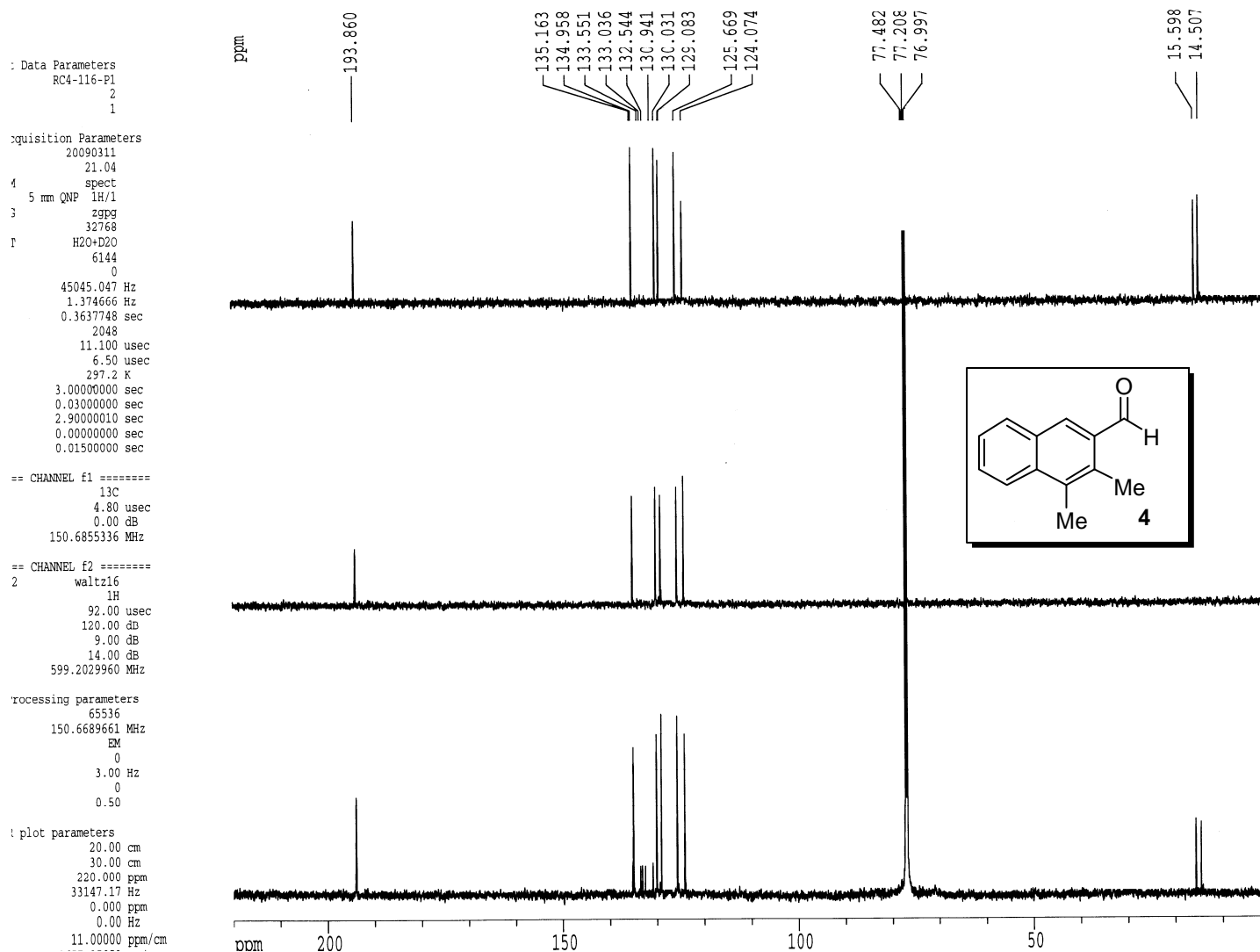


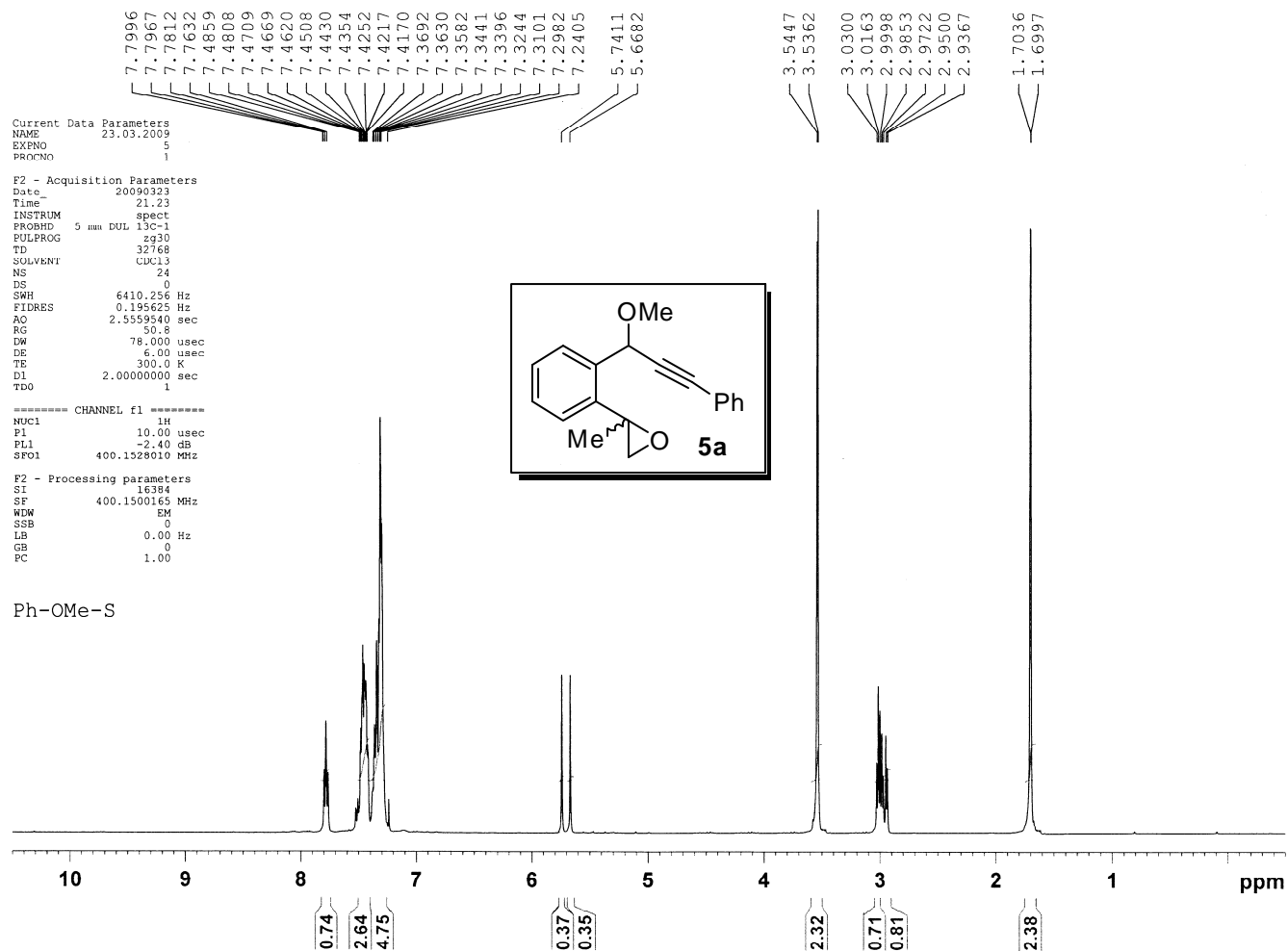


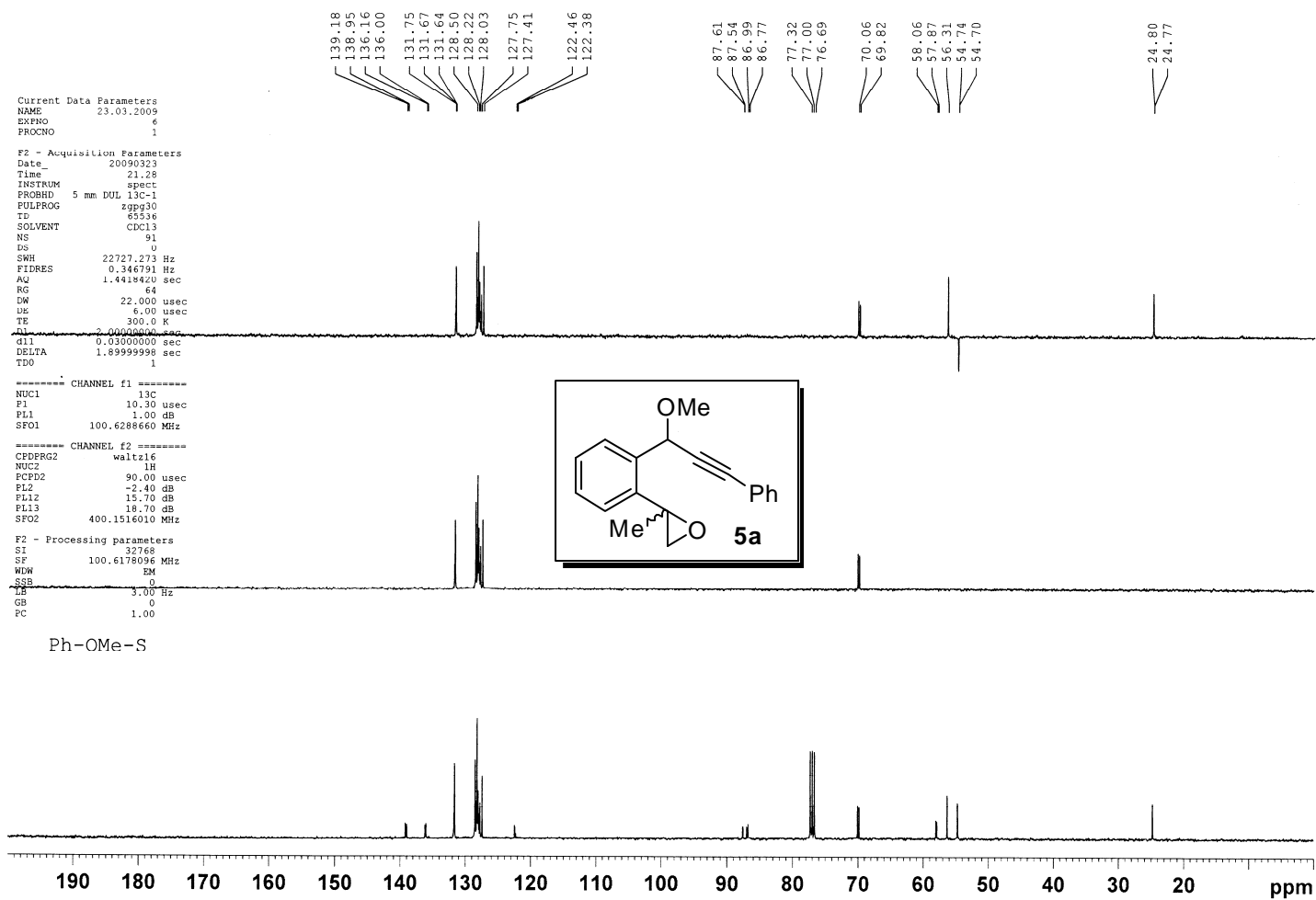


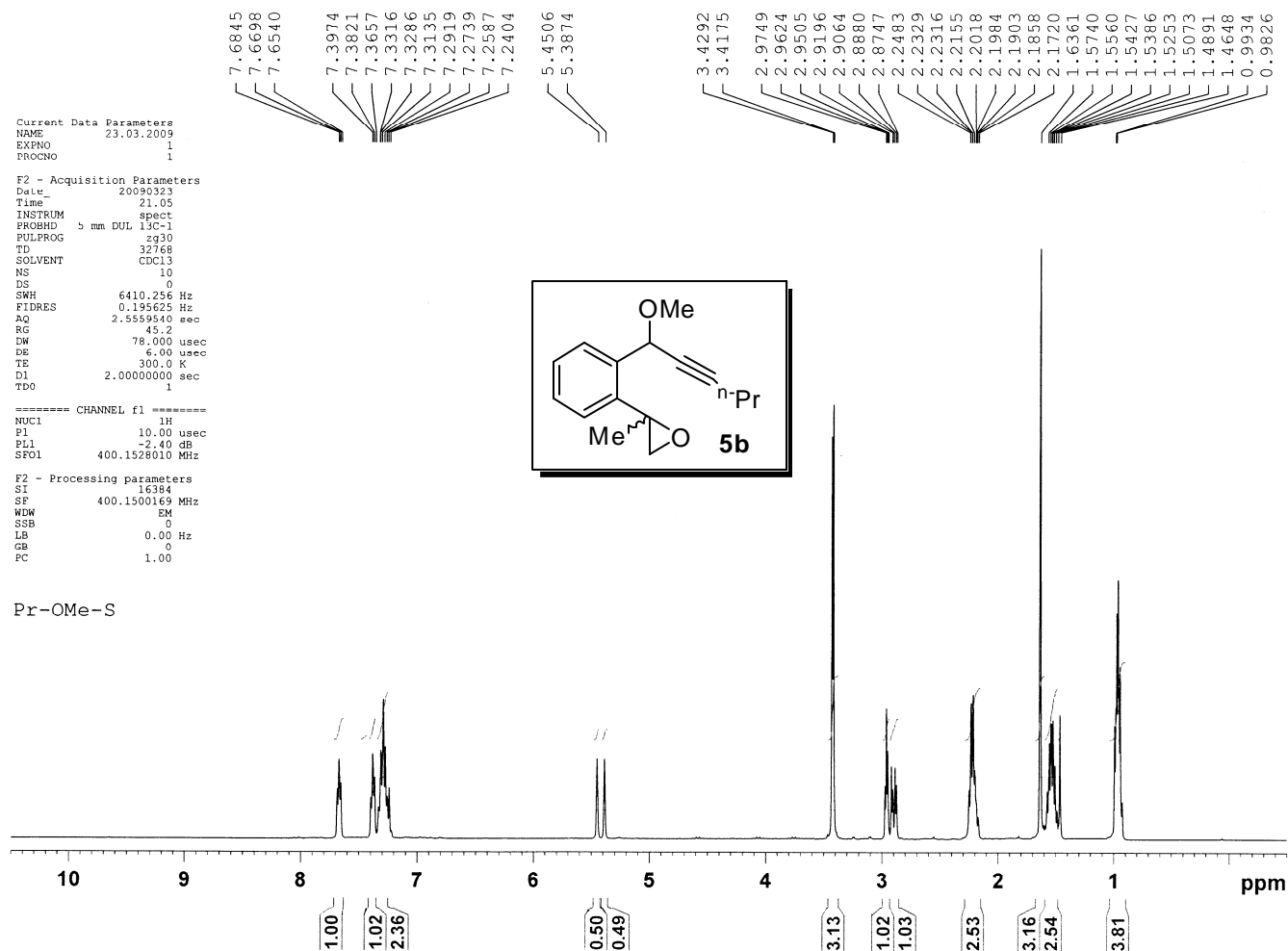


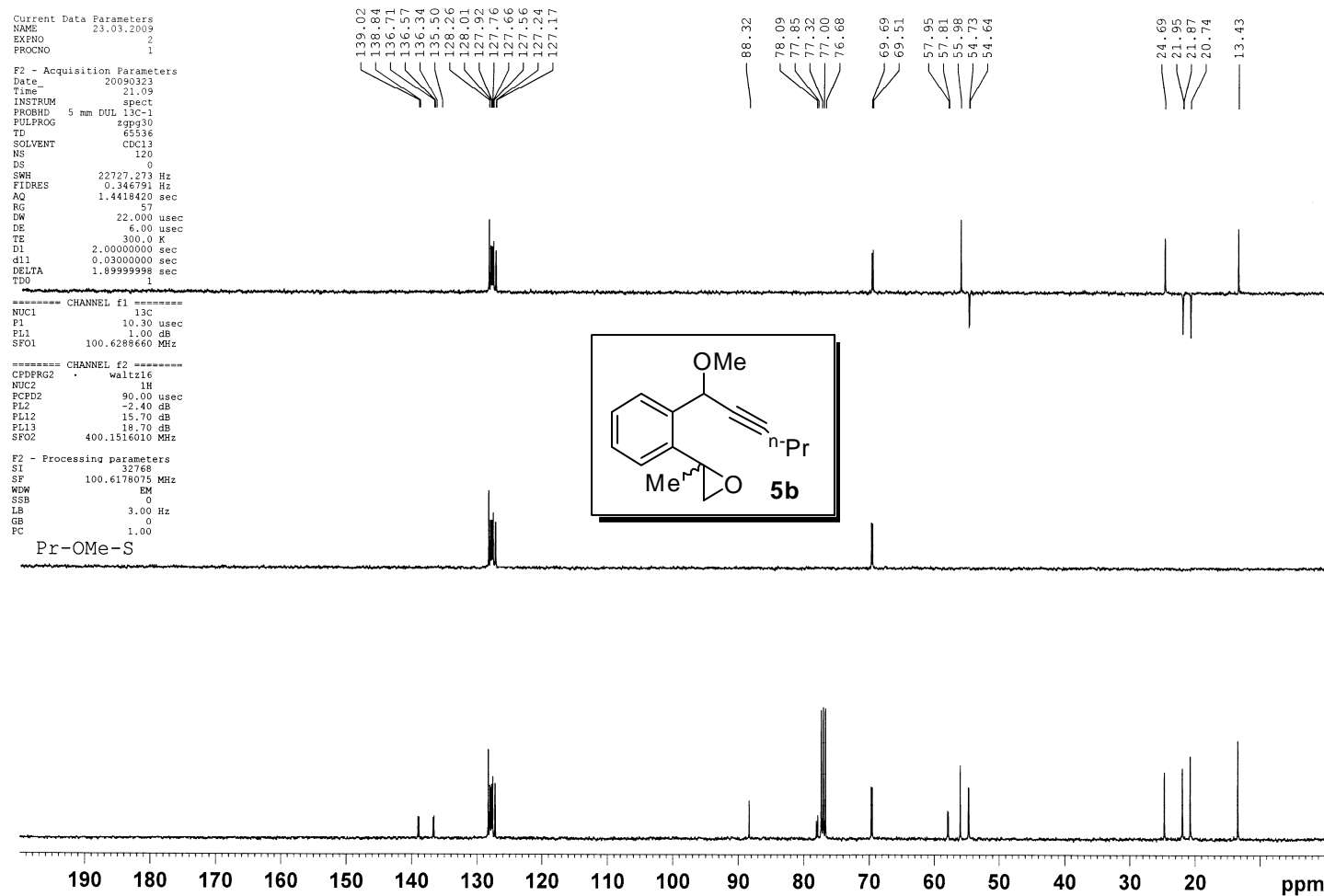












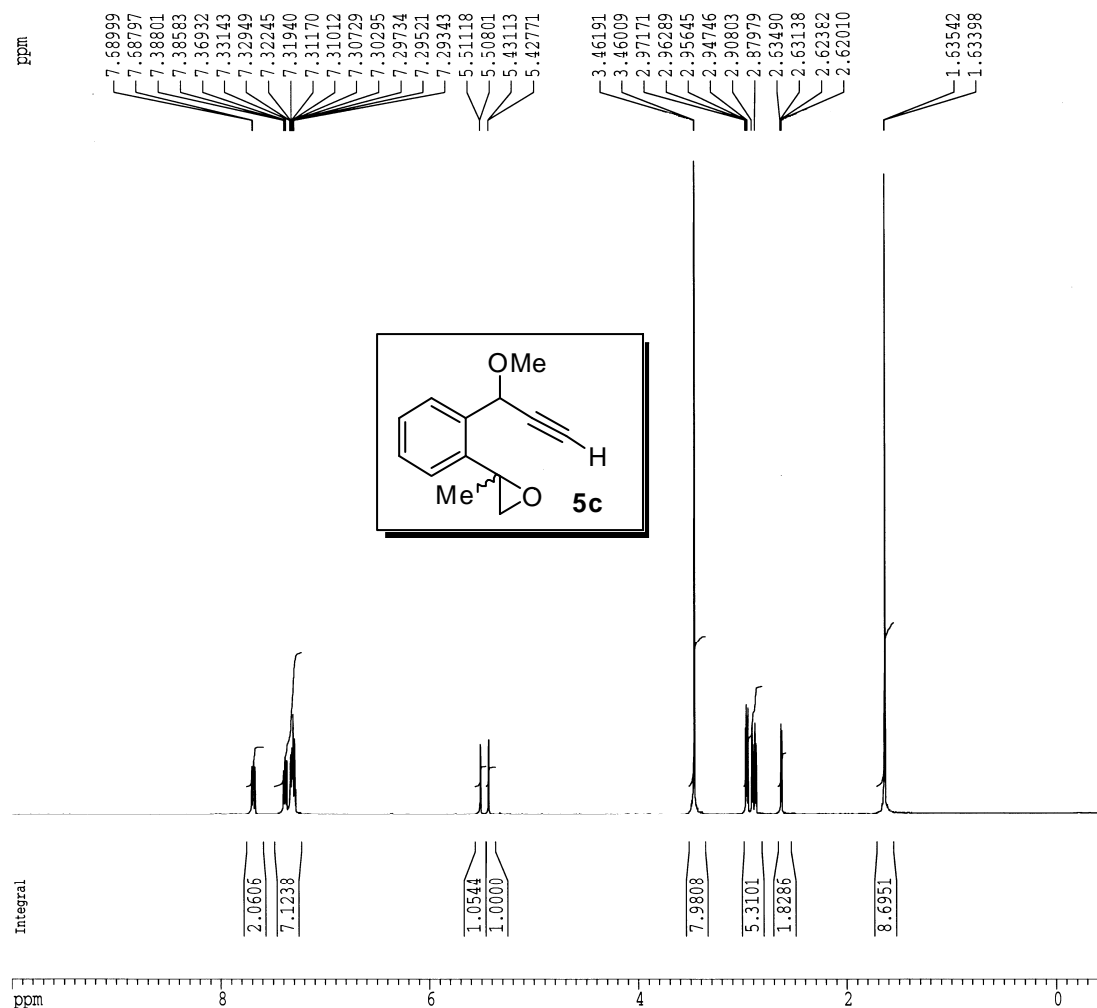
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XCNO 1

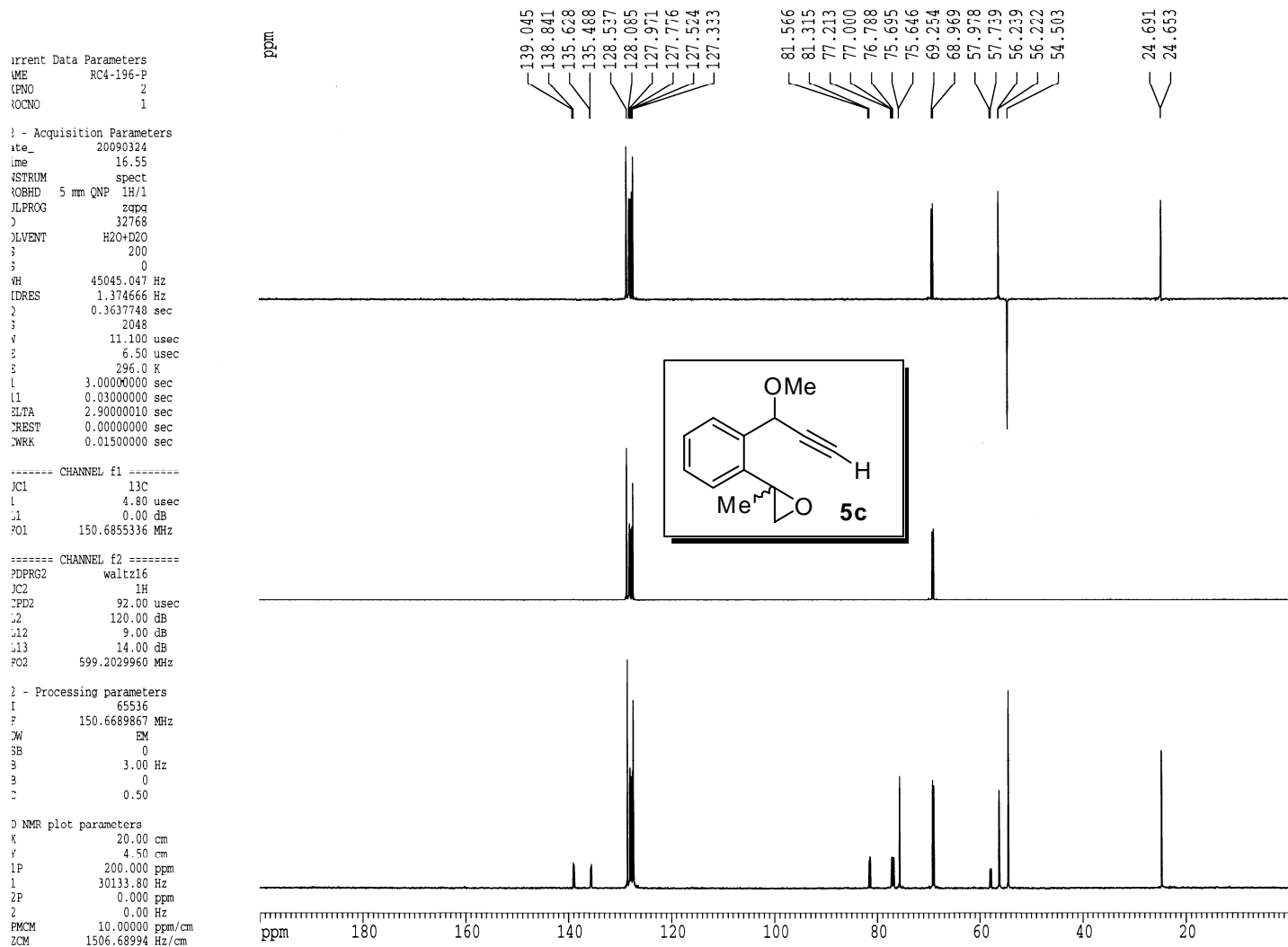
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Time 18.11
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PROBHD 5 mm QNP 1H/1
JLPROG zg
P 32768
SOLVENT CDCl3
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S 0
VH 8389.262 Hz
FIDRES 0.256020 Hz
P 1.9530228 sec
S 32
V 59.600 usec
S 6.50 usec
S 295.8 K
L 1.00000000 sec
CREST 0.00000000 sec
CWPRK 0.01500000 sec

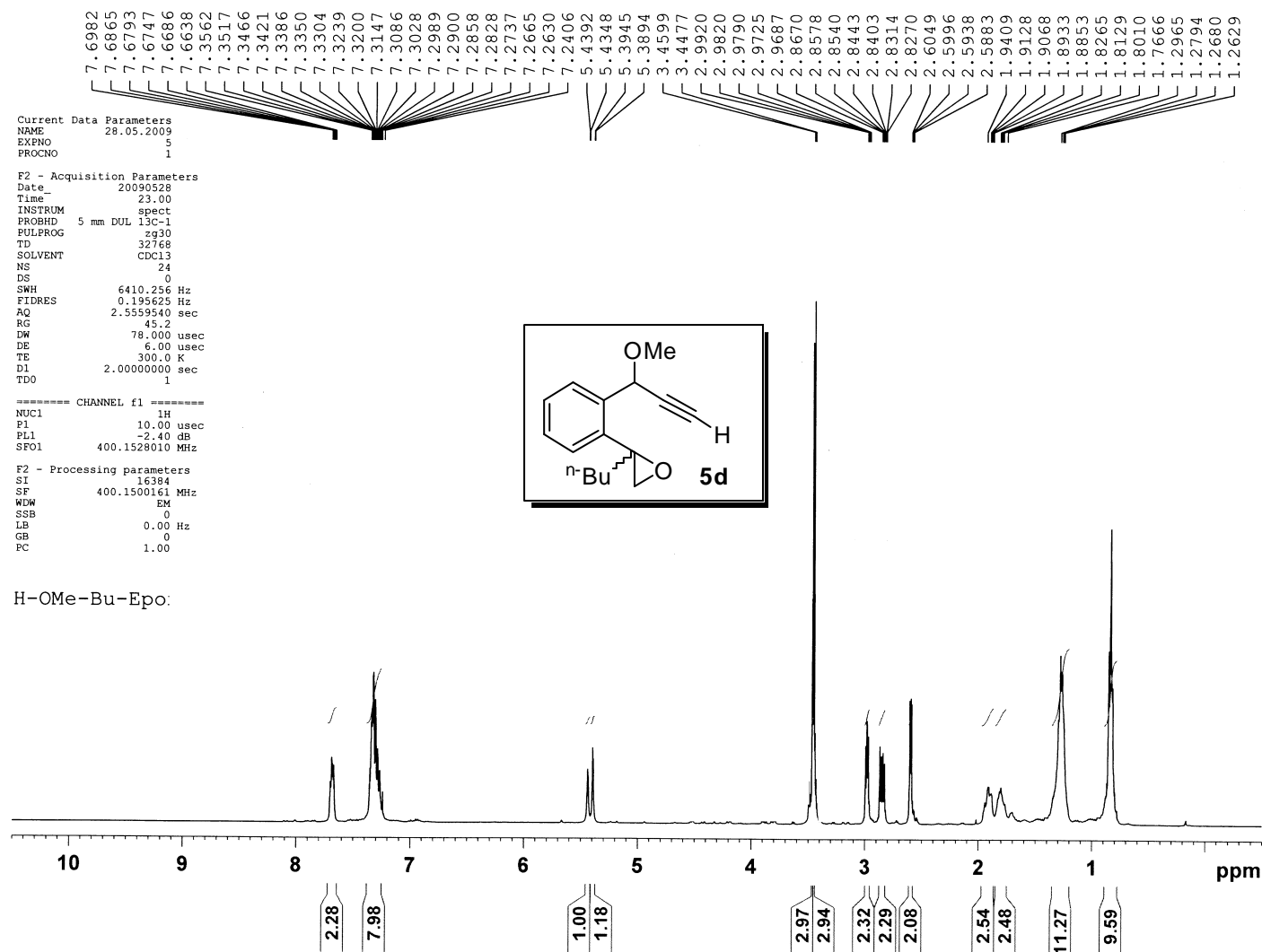
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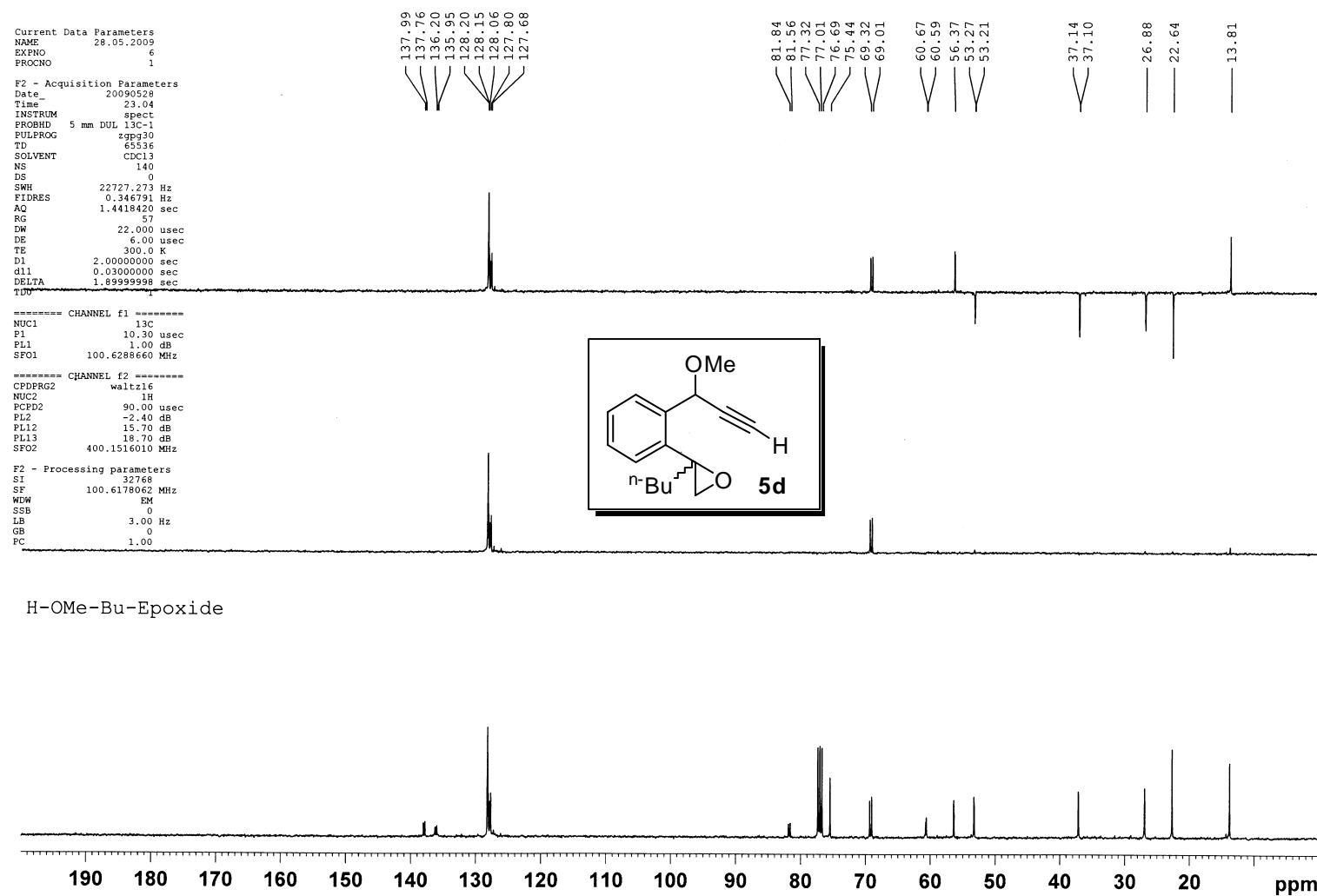
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S 1.00

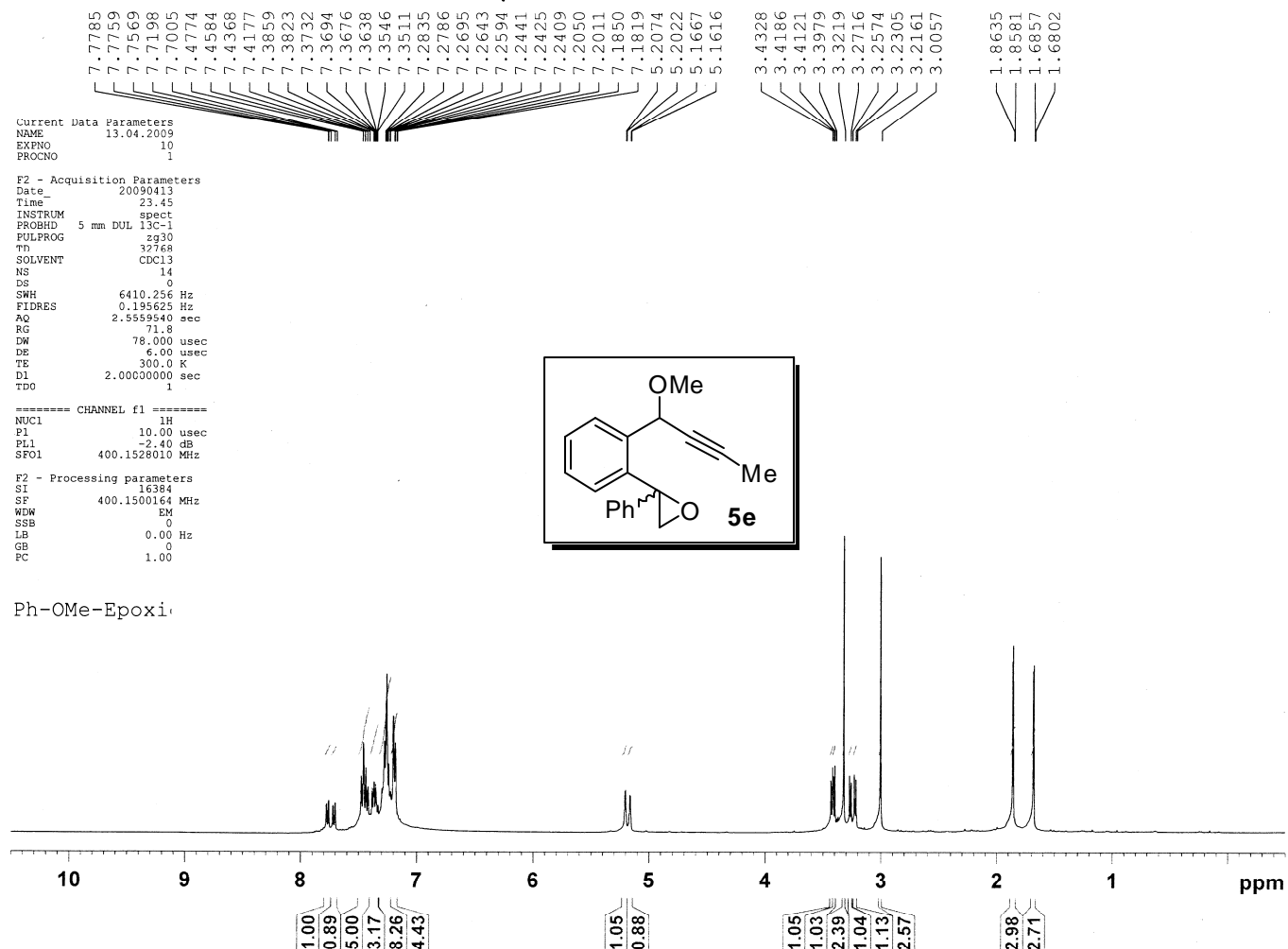
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S -299.60 Hz
PMCM 0.52500 ppm/cm
ZCM 314.58002 Hz/cm

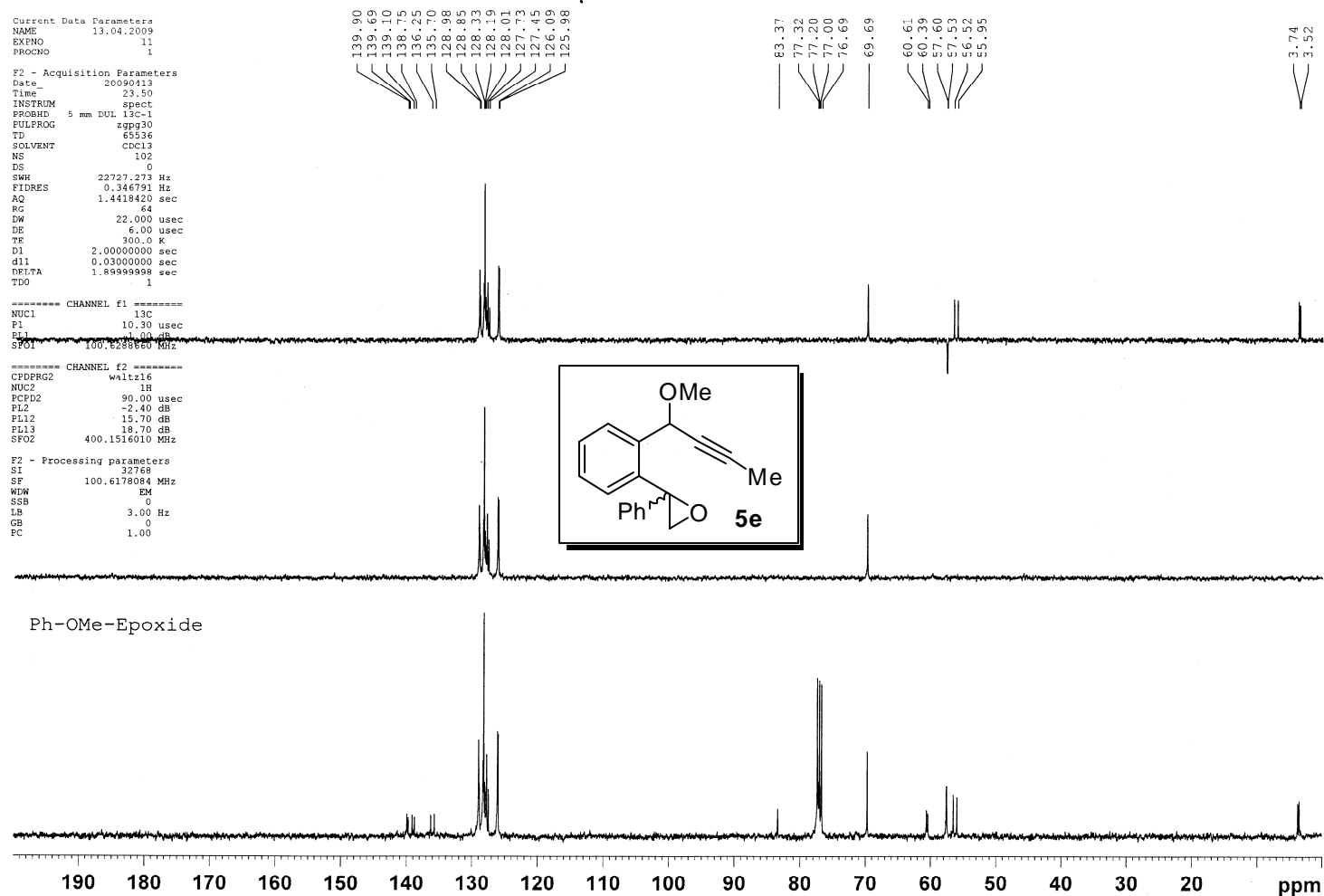


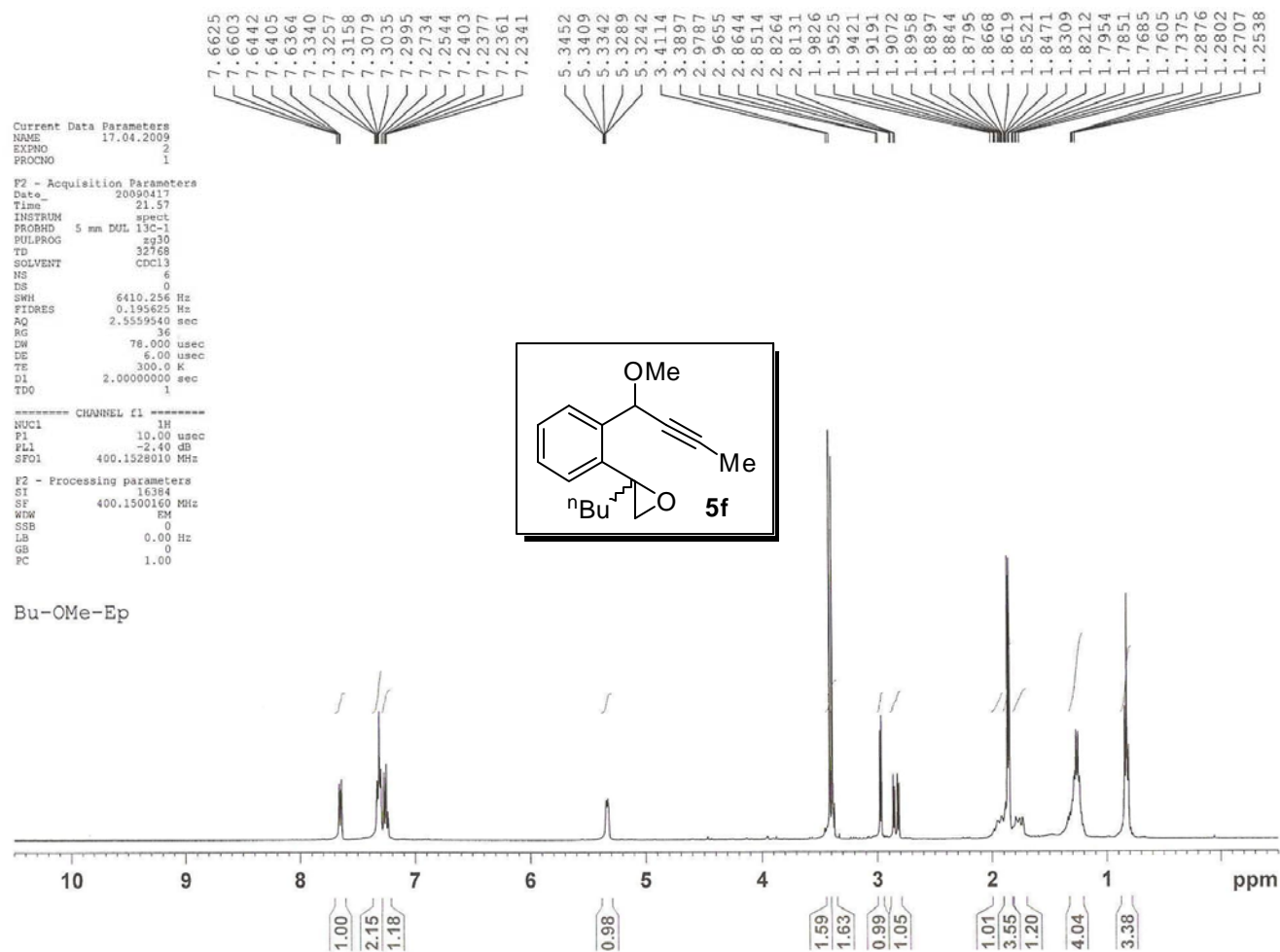


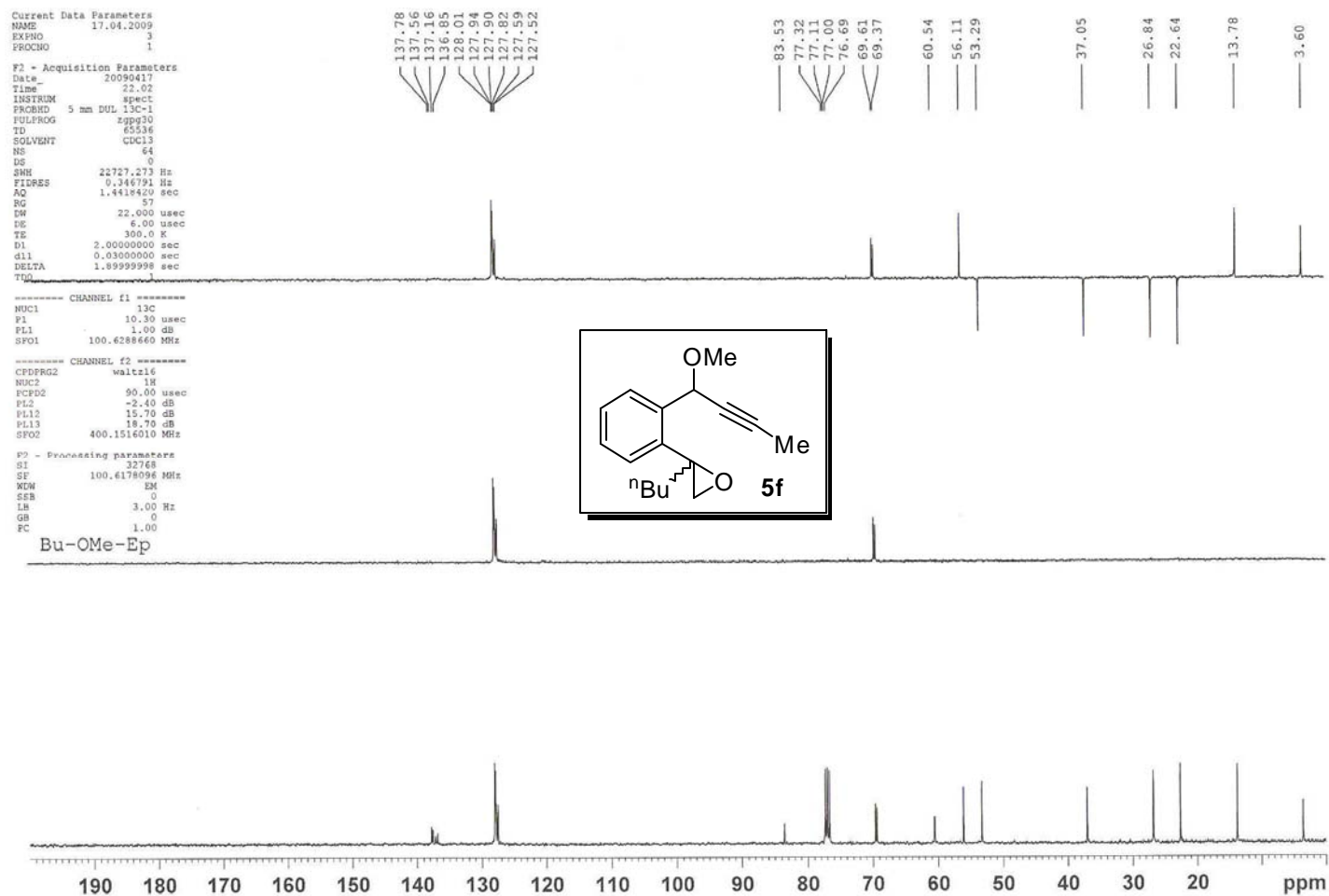


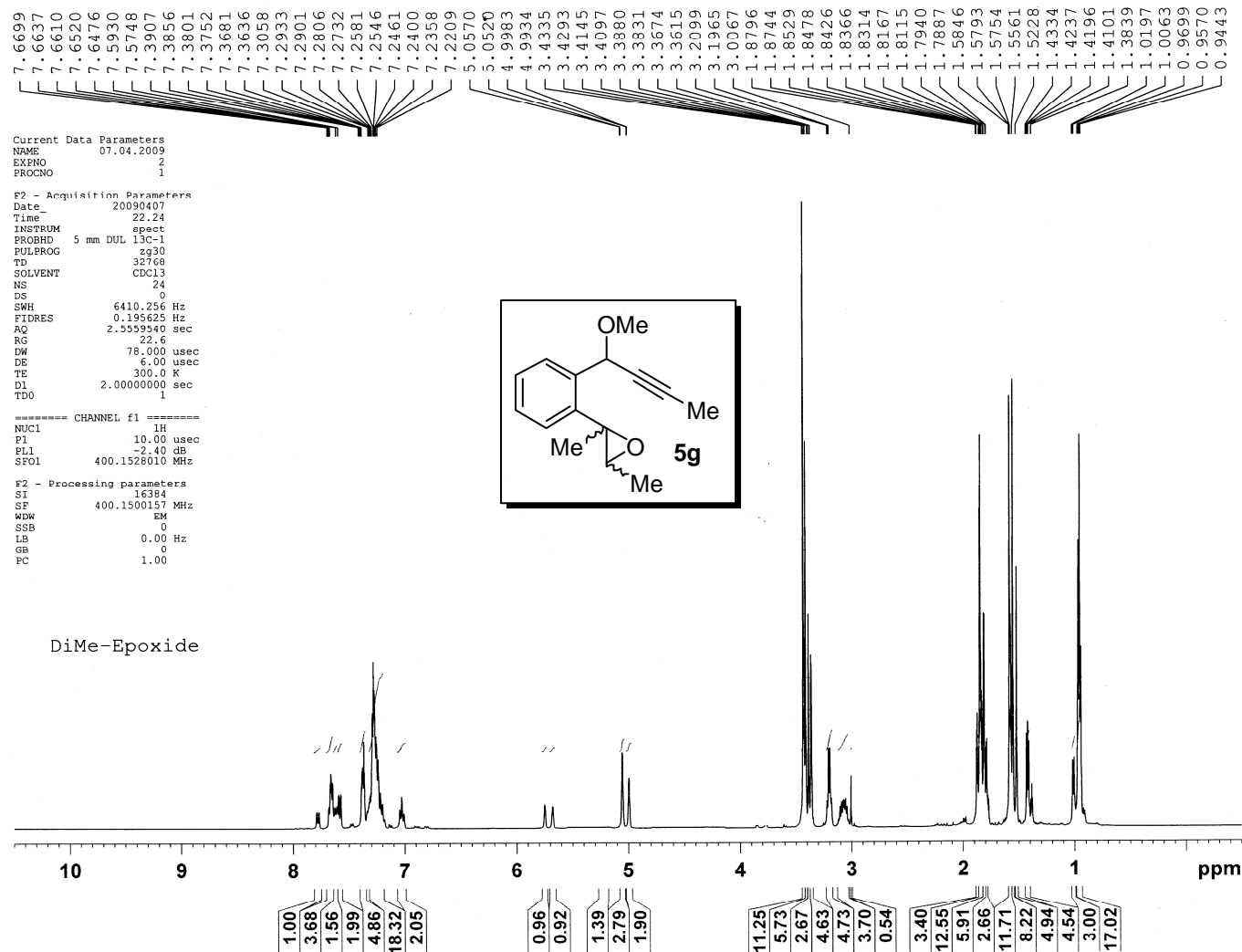


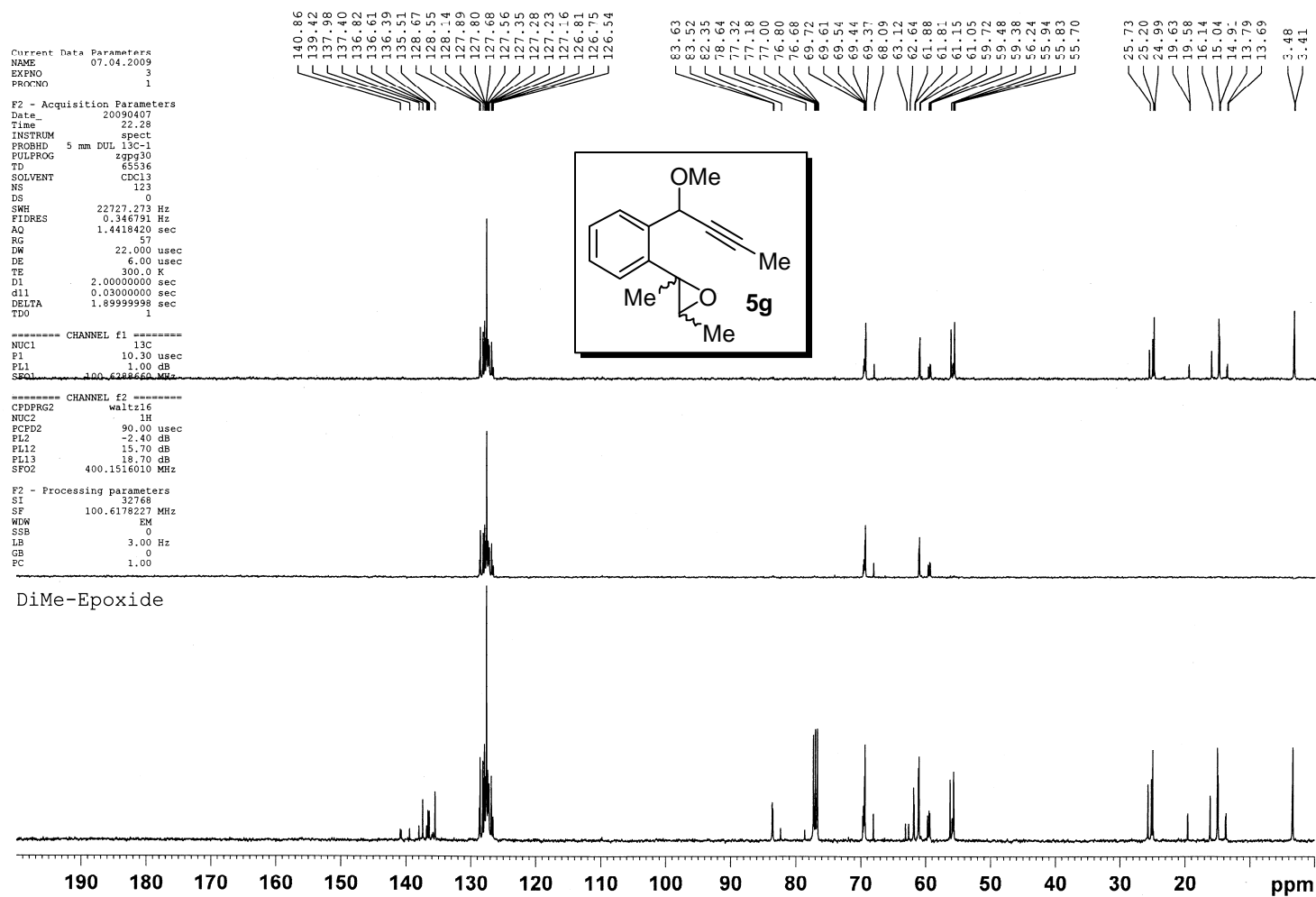


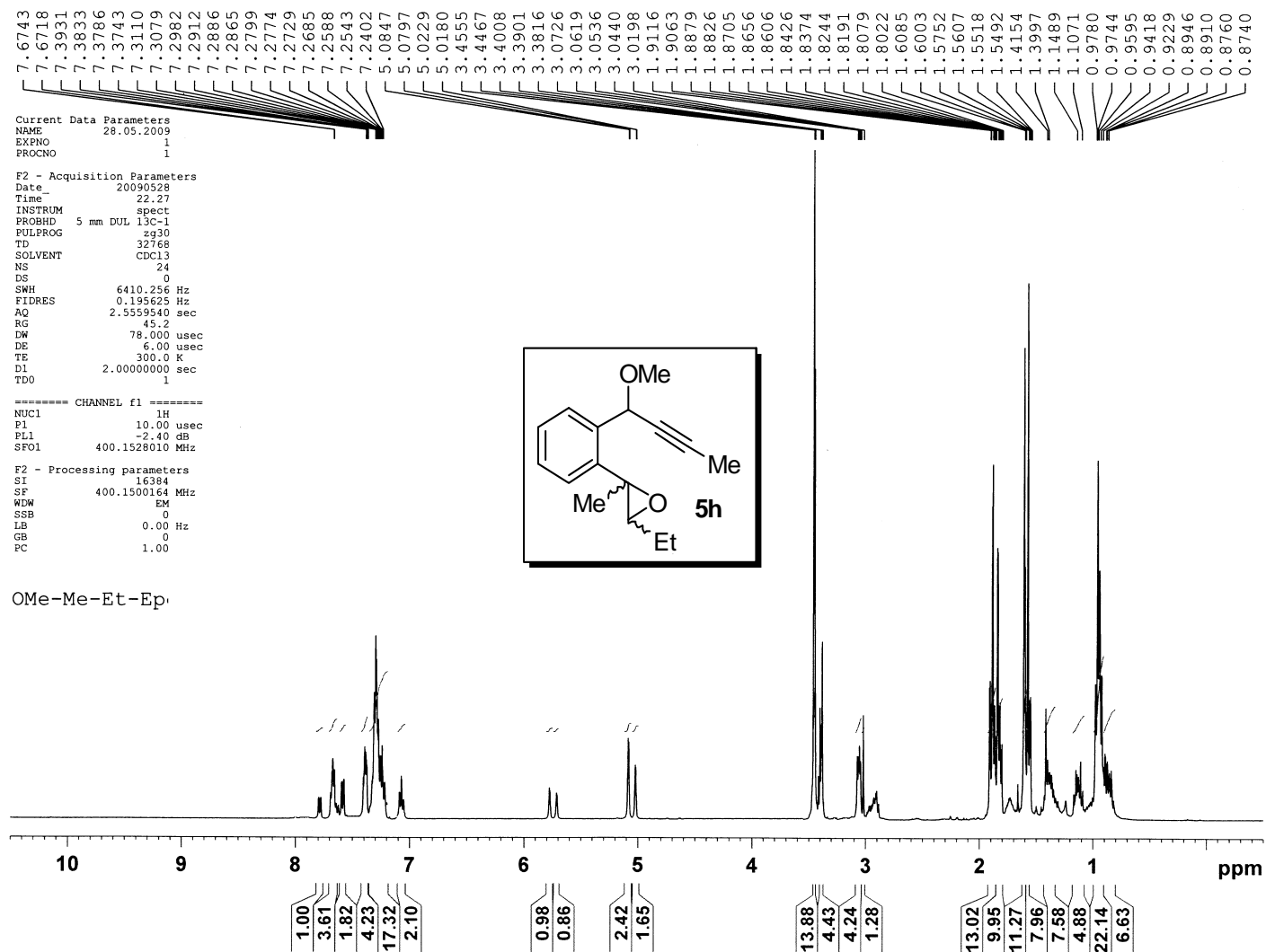


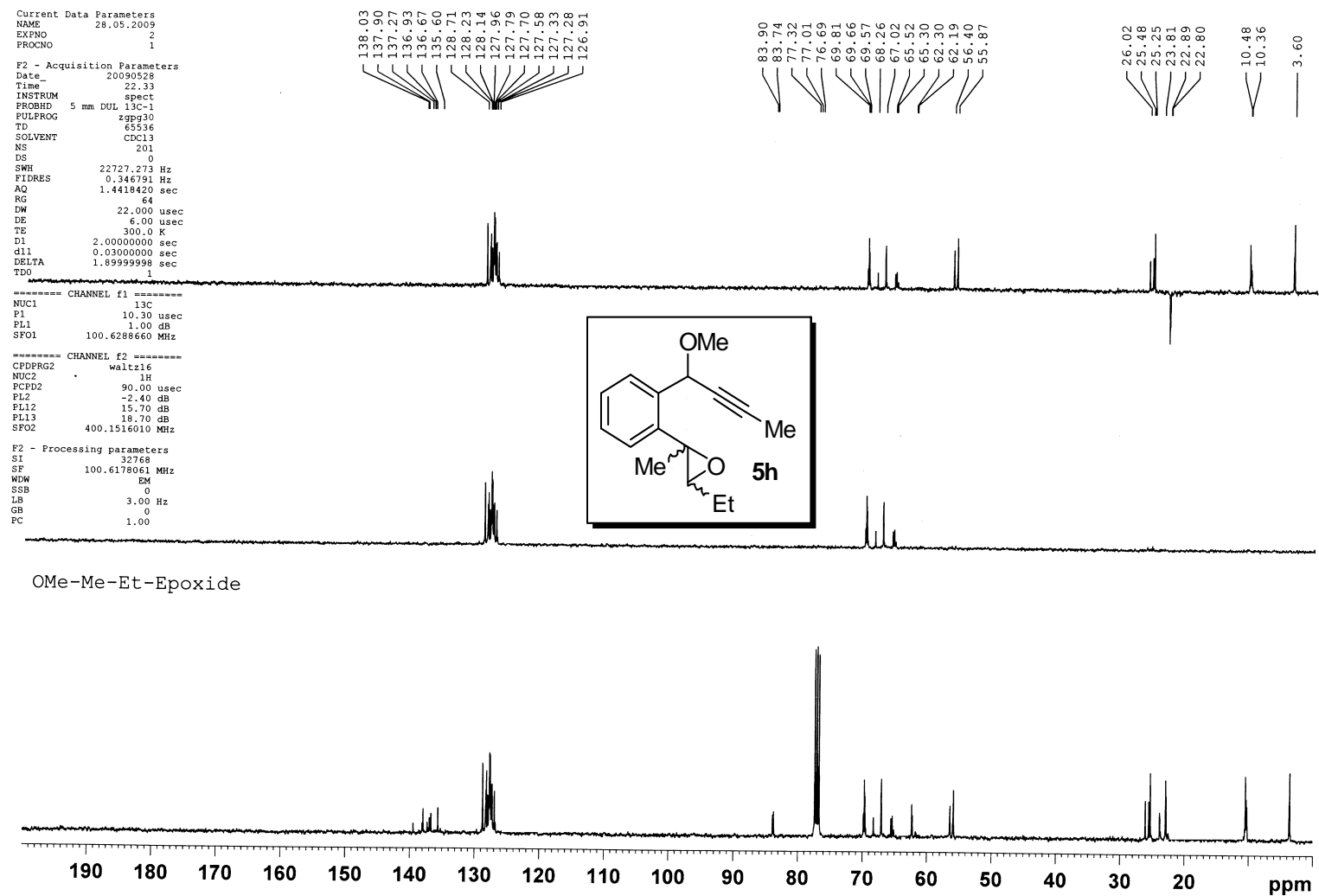


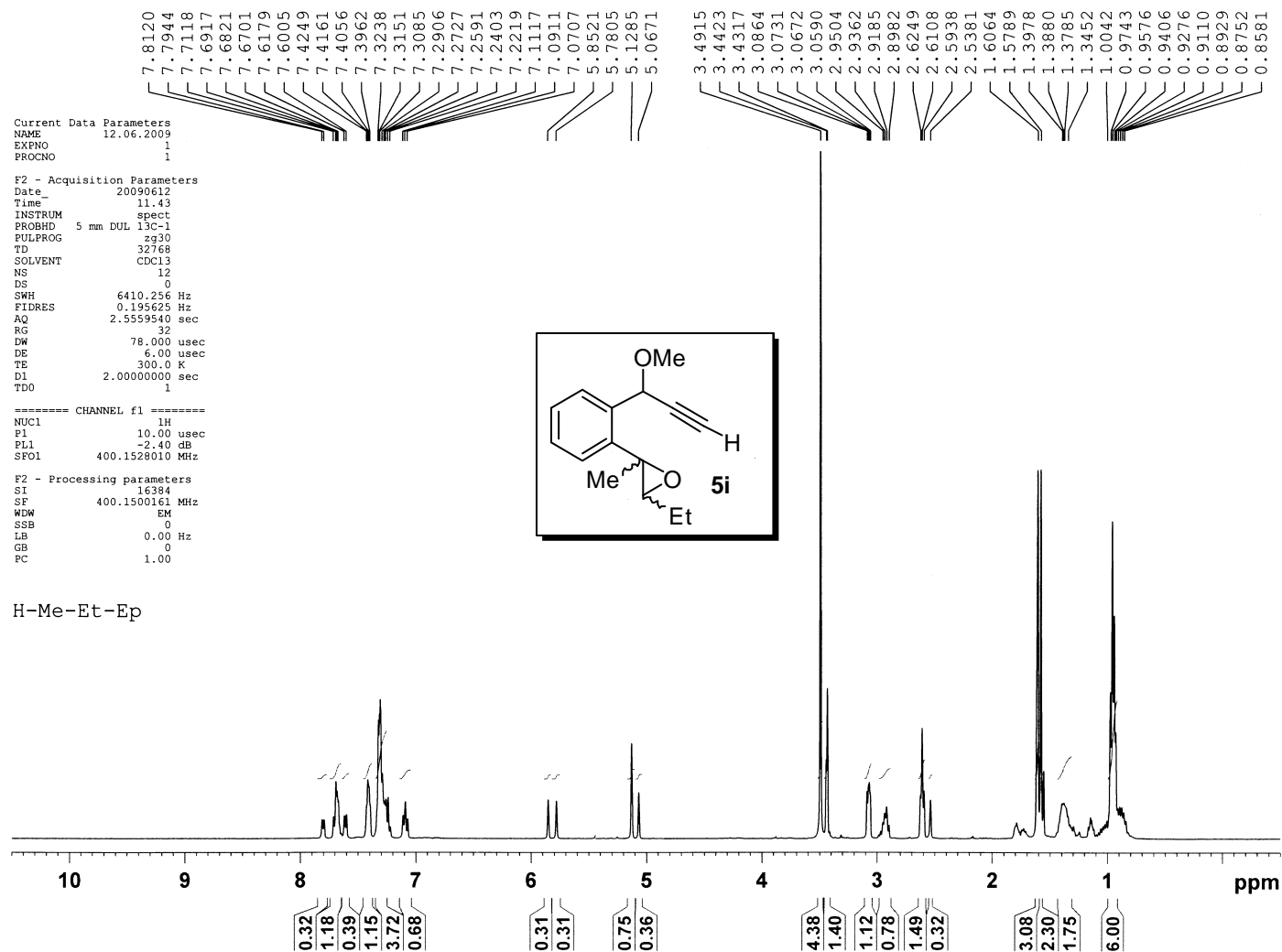


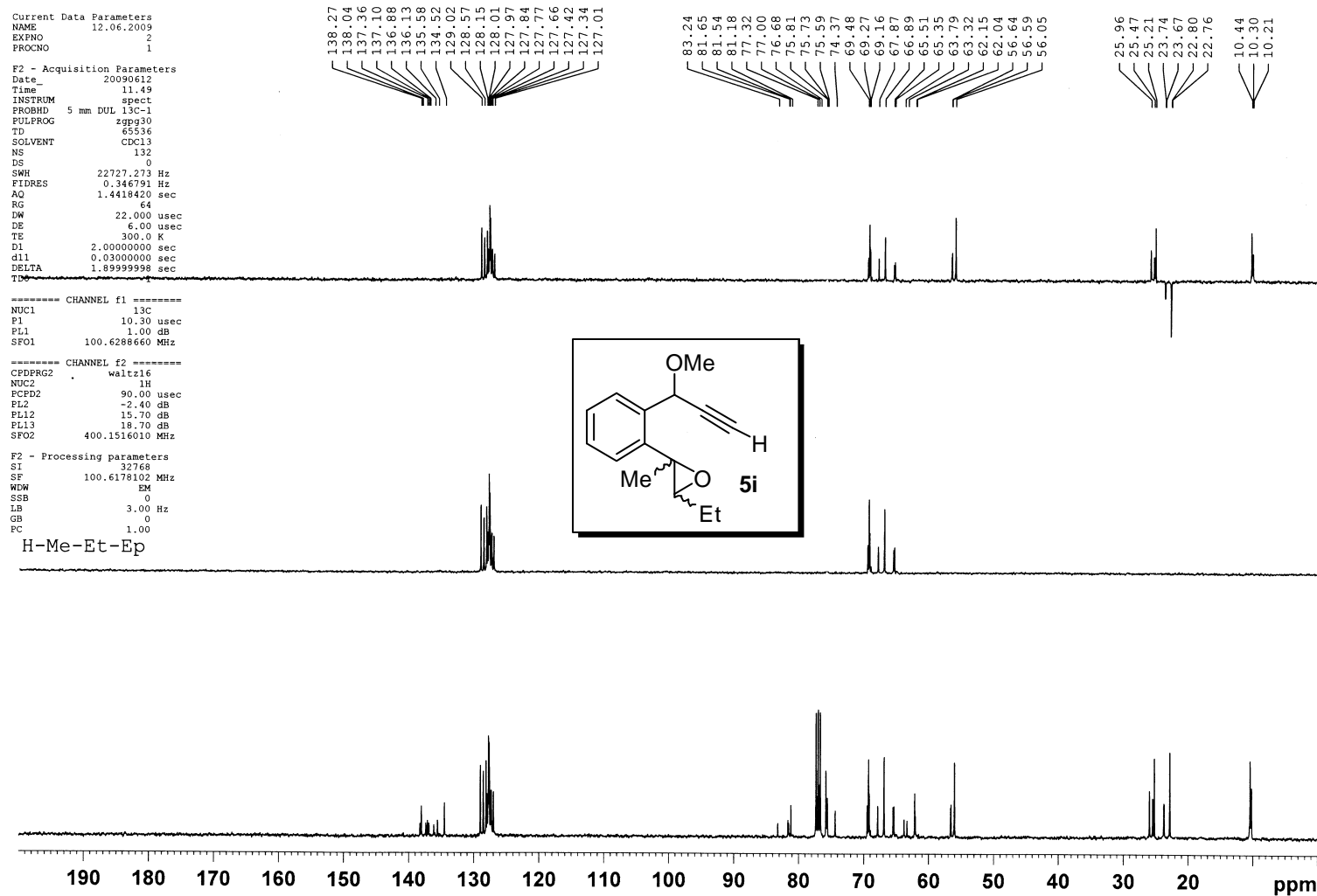


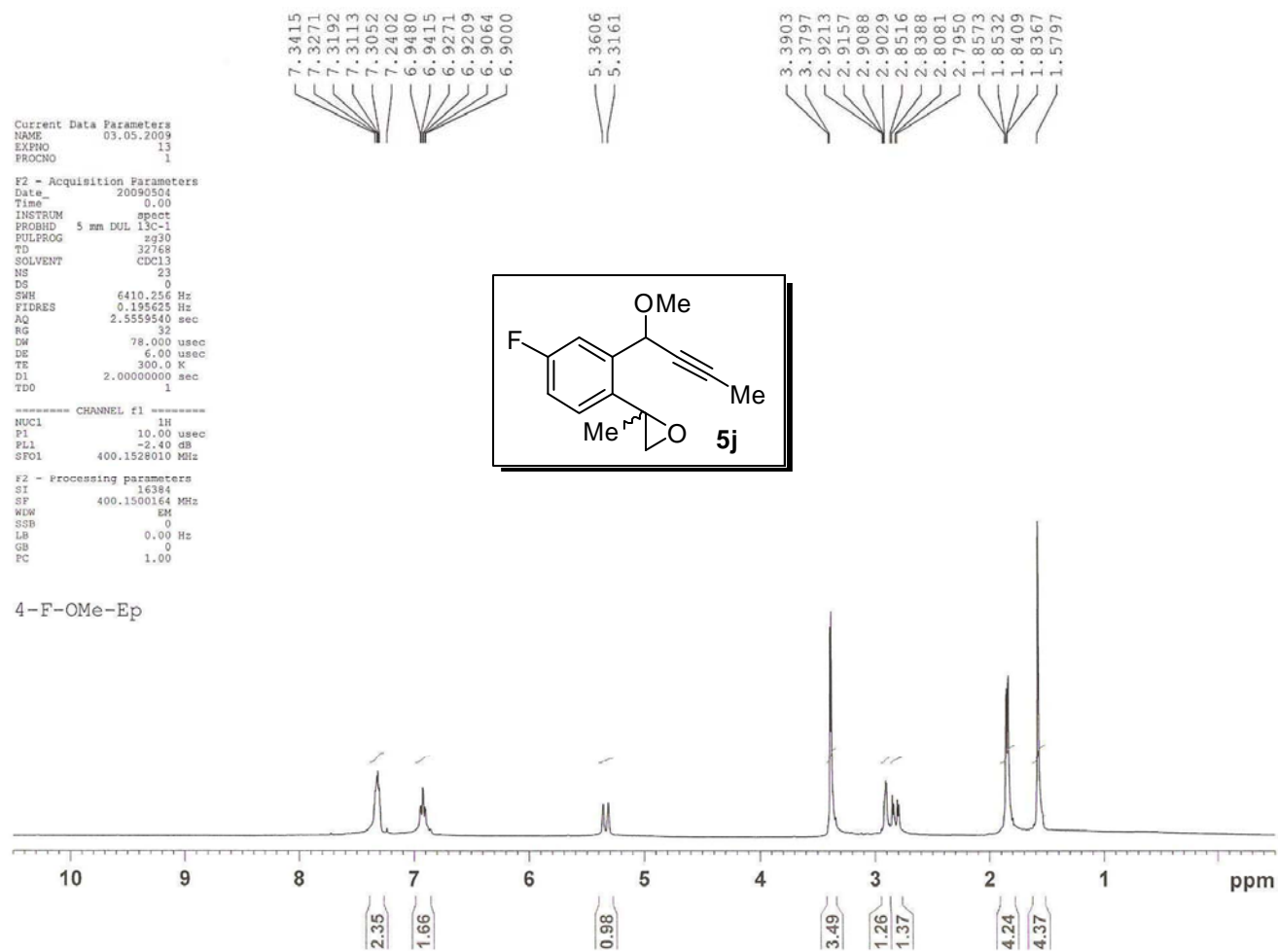


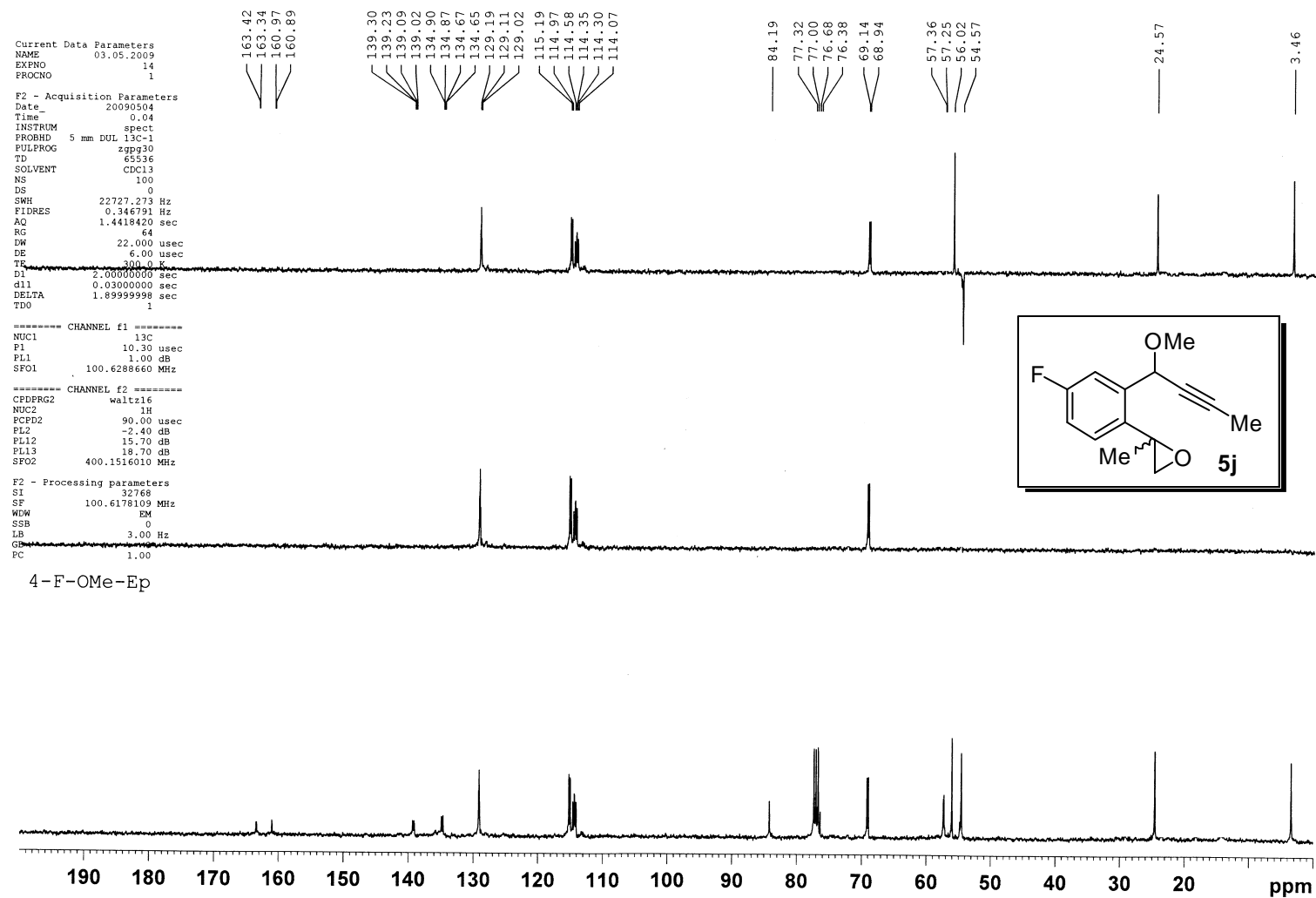


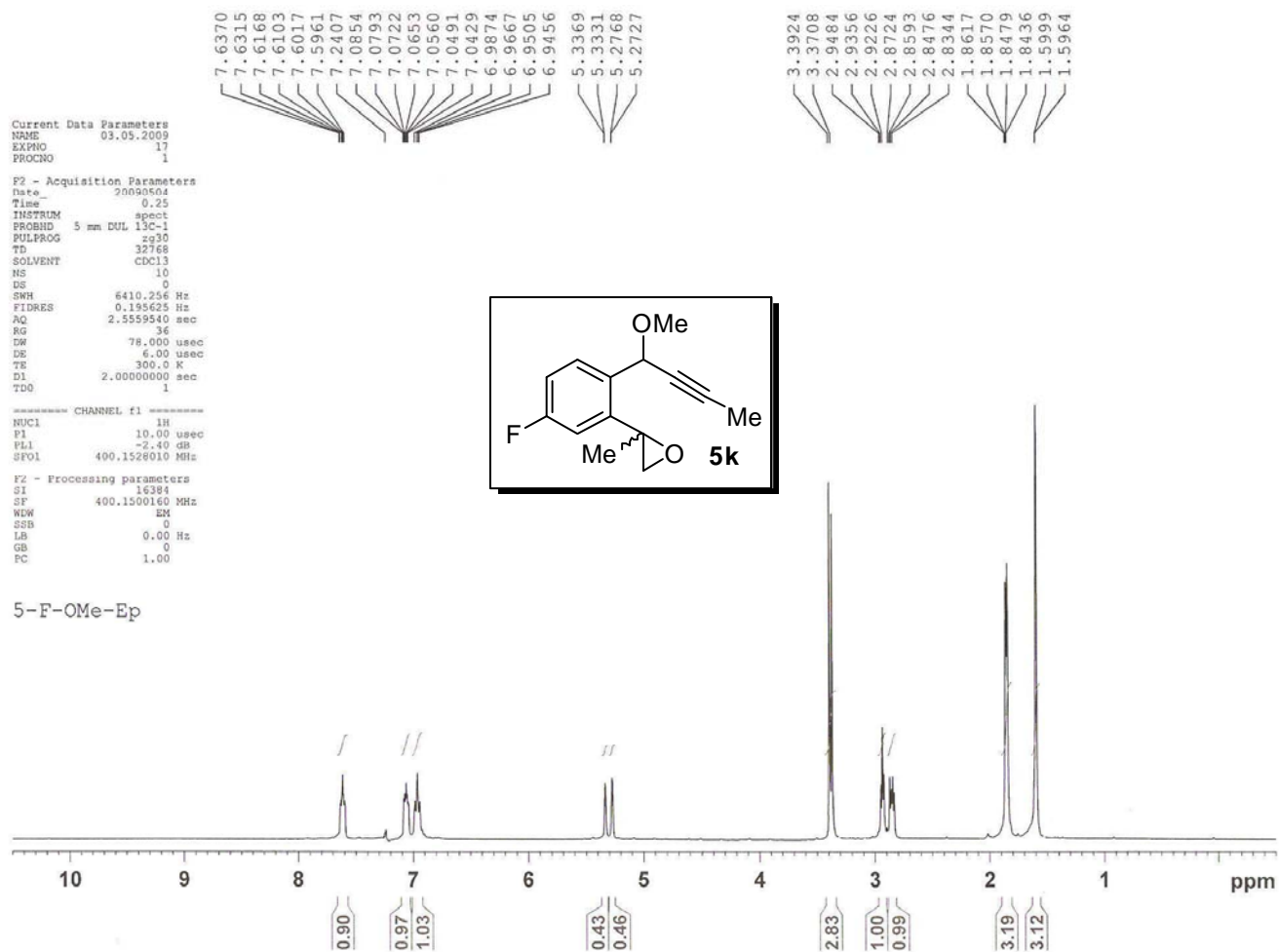


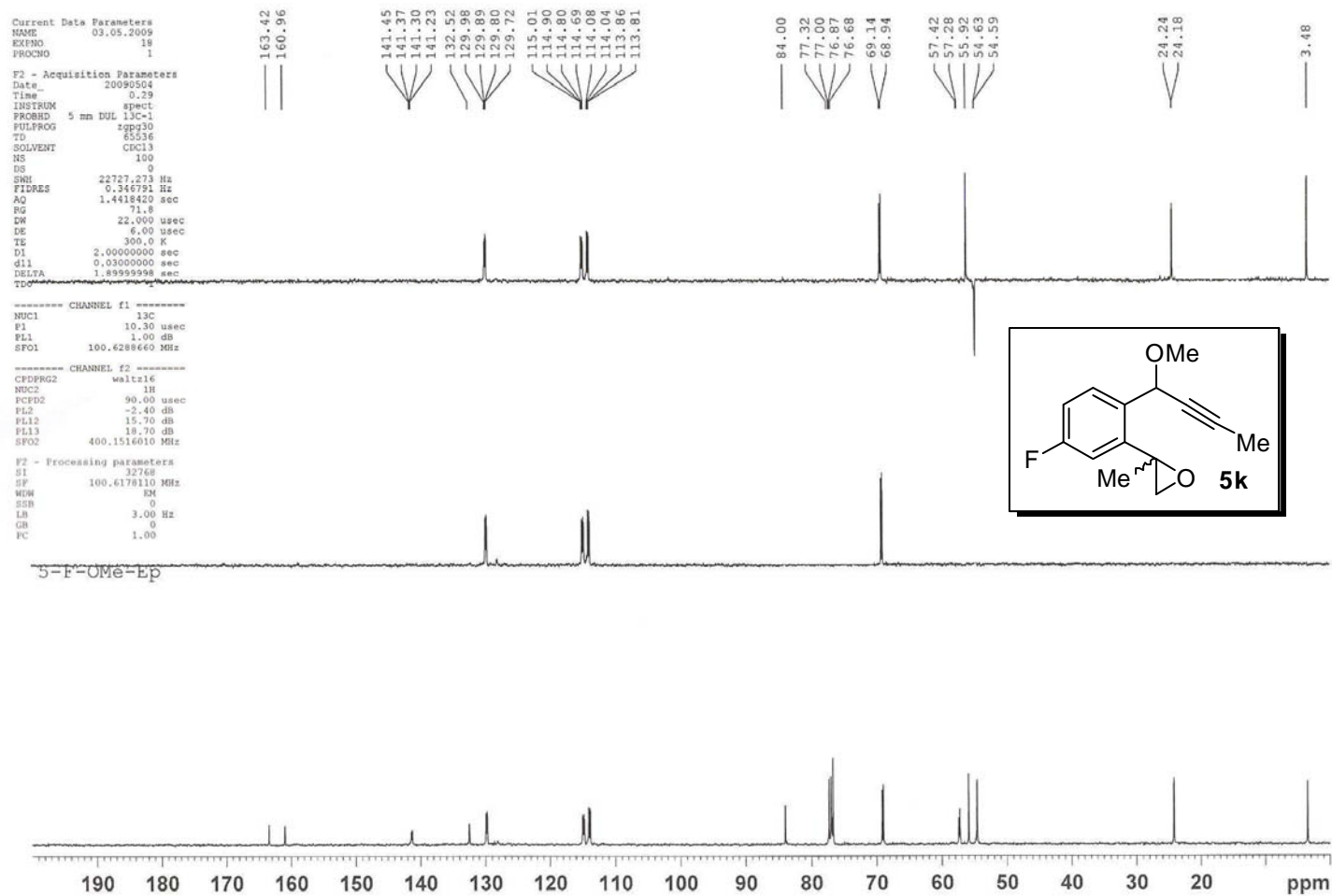


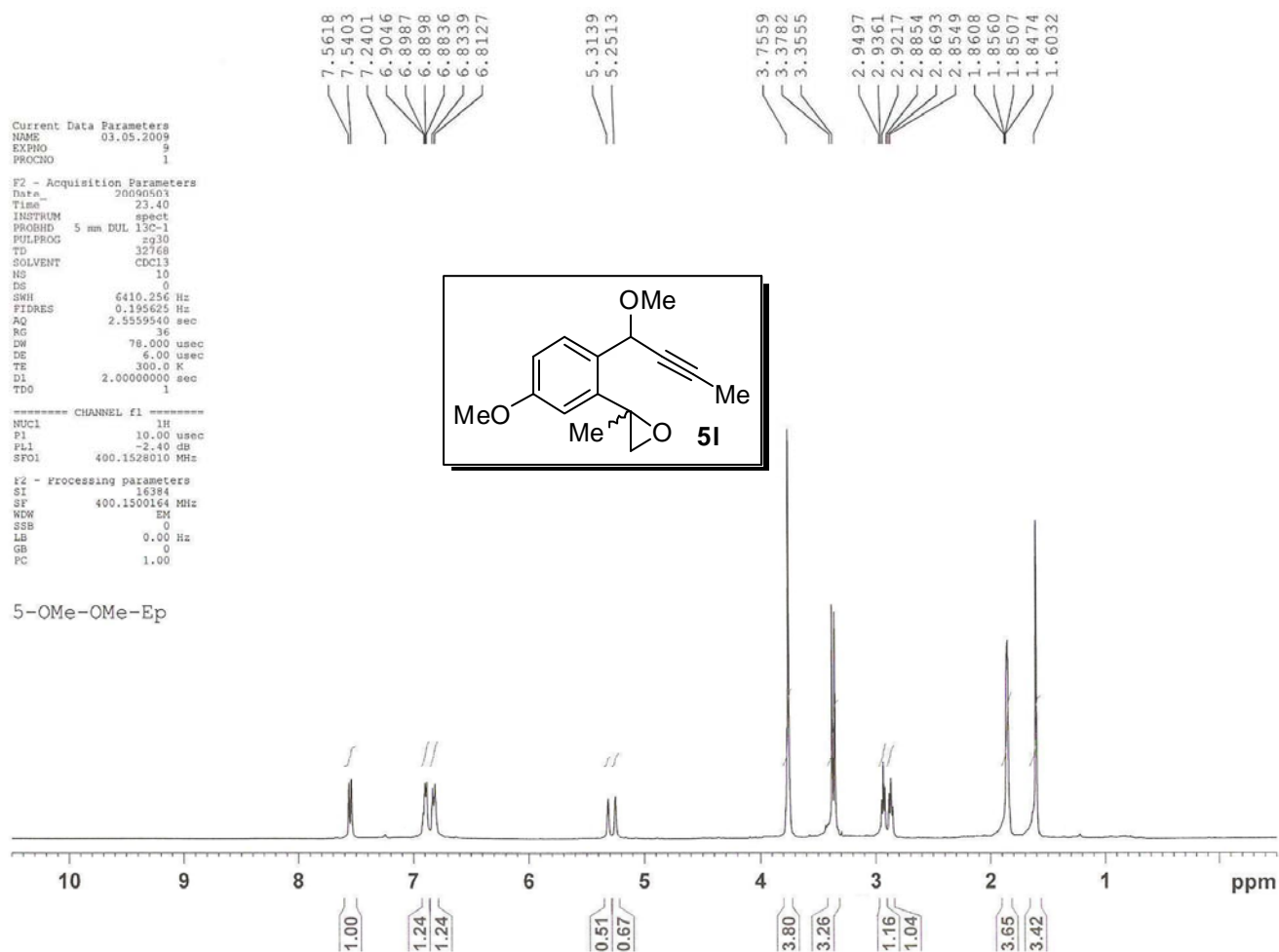


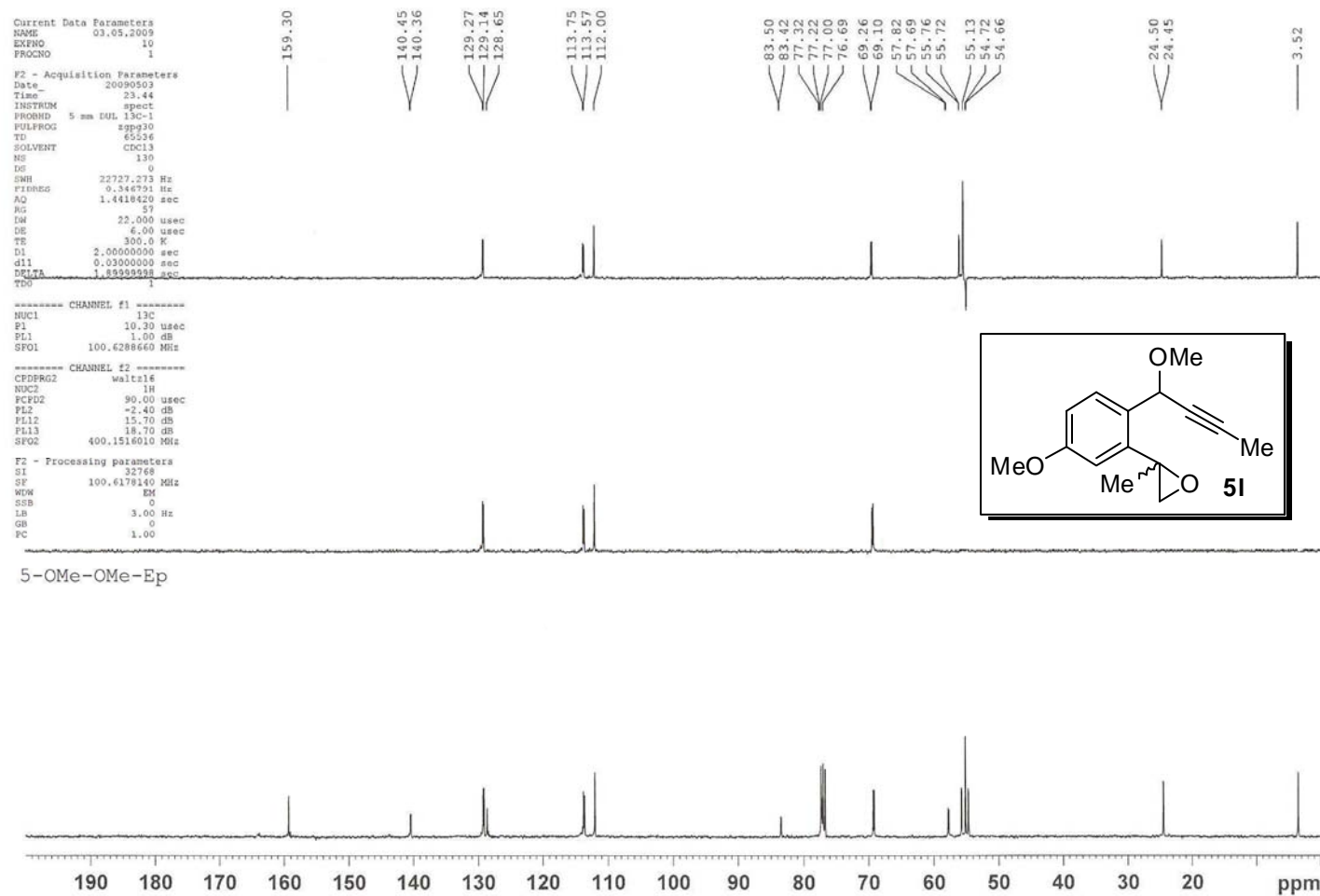


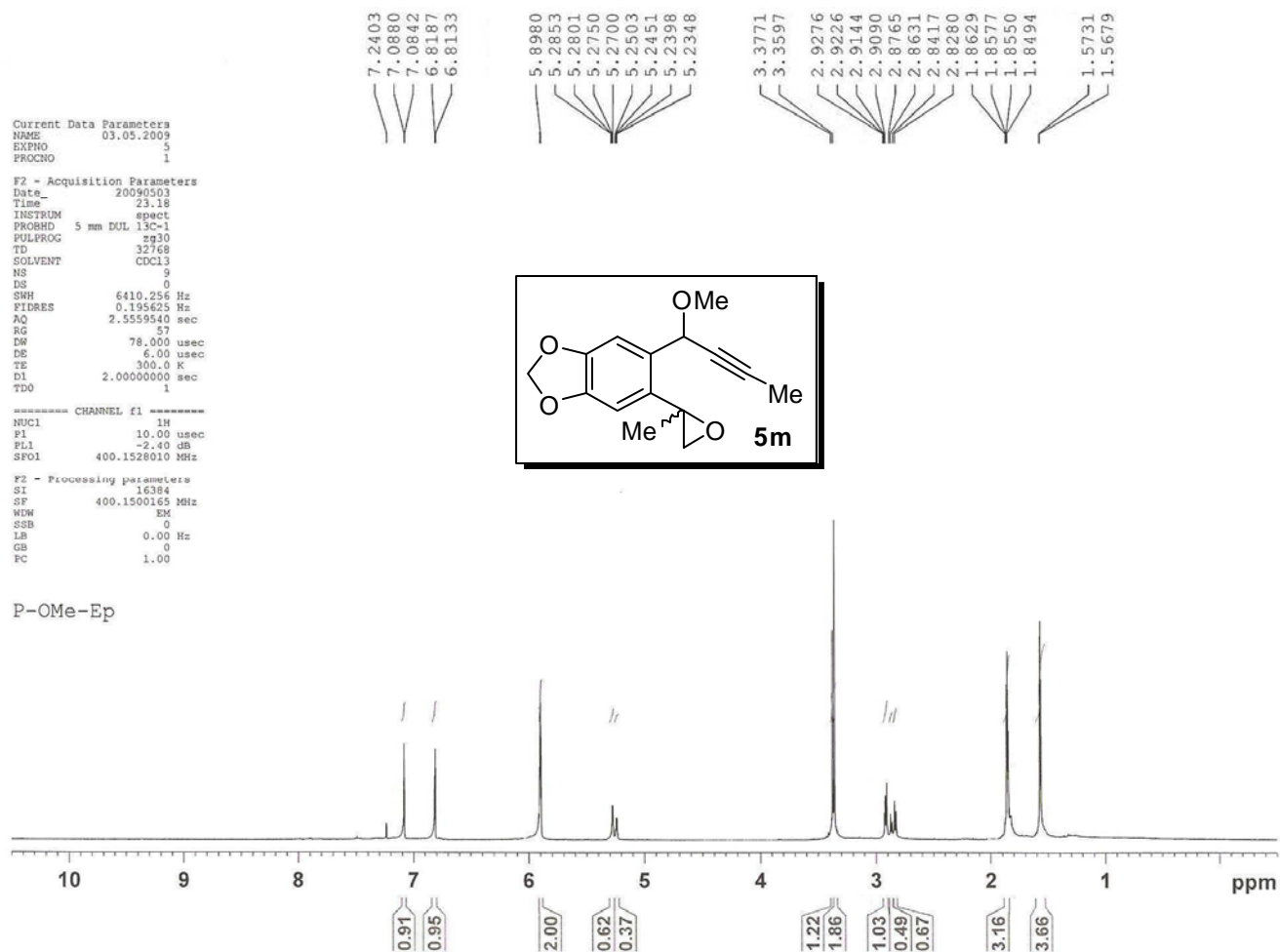


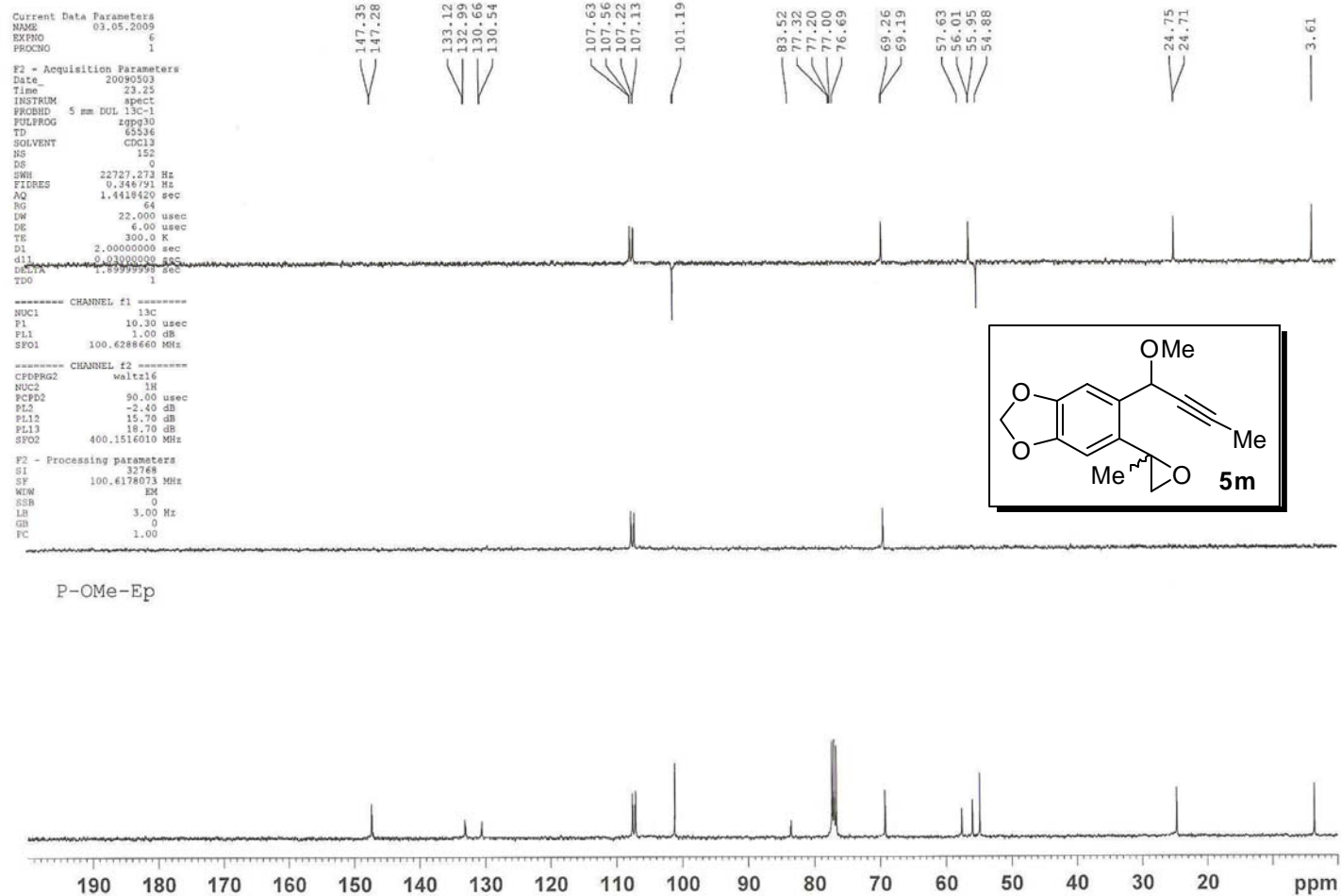


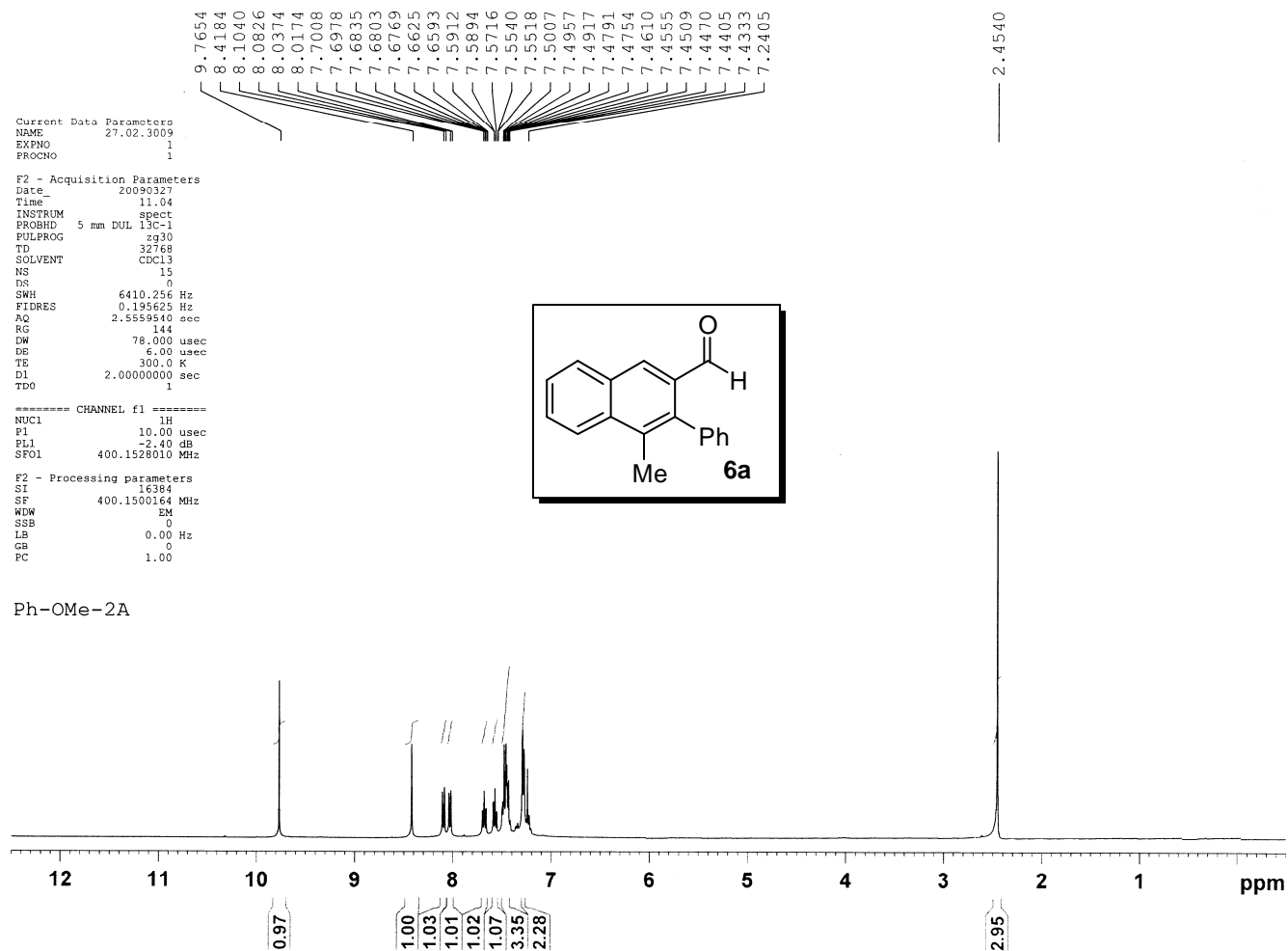


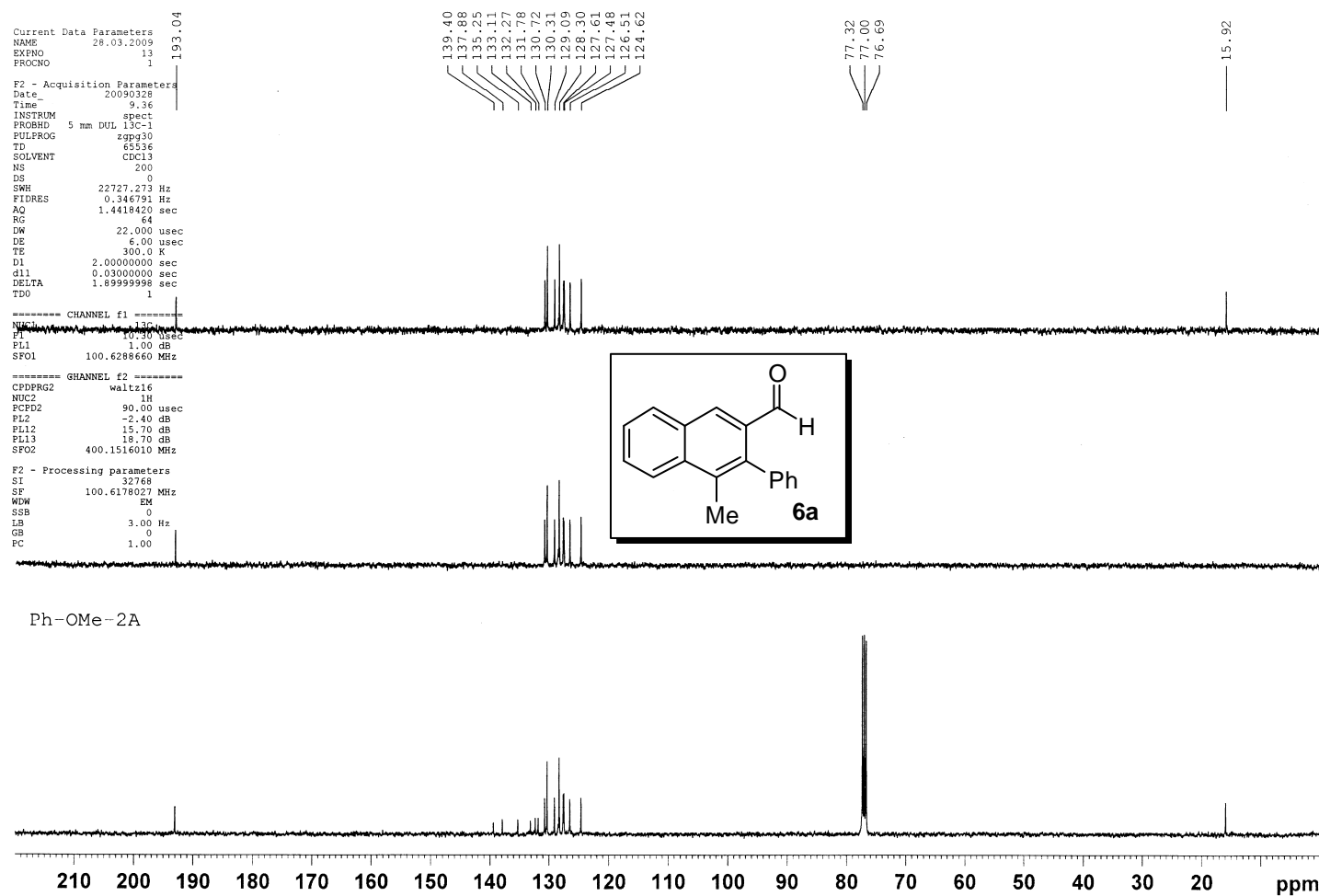


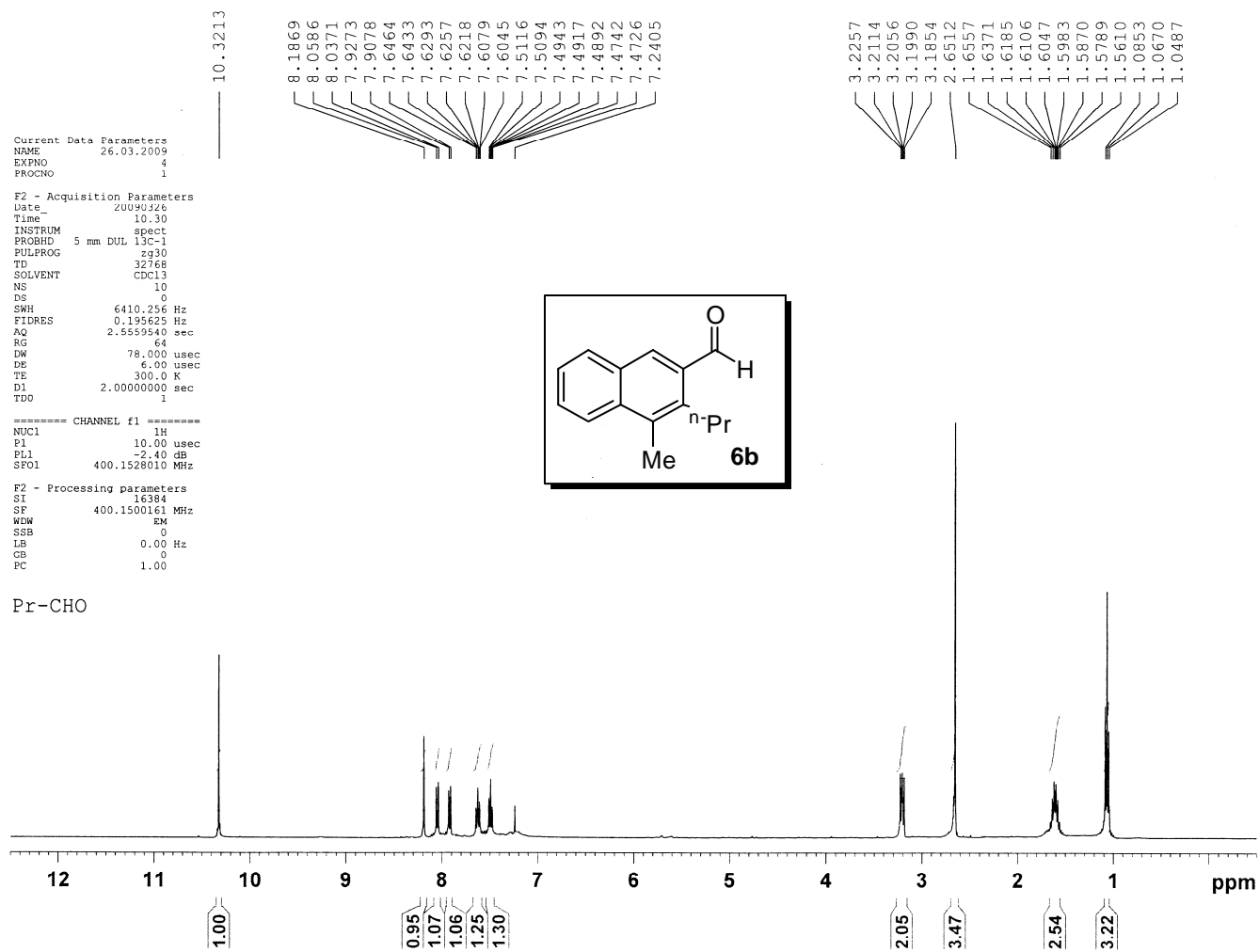


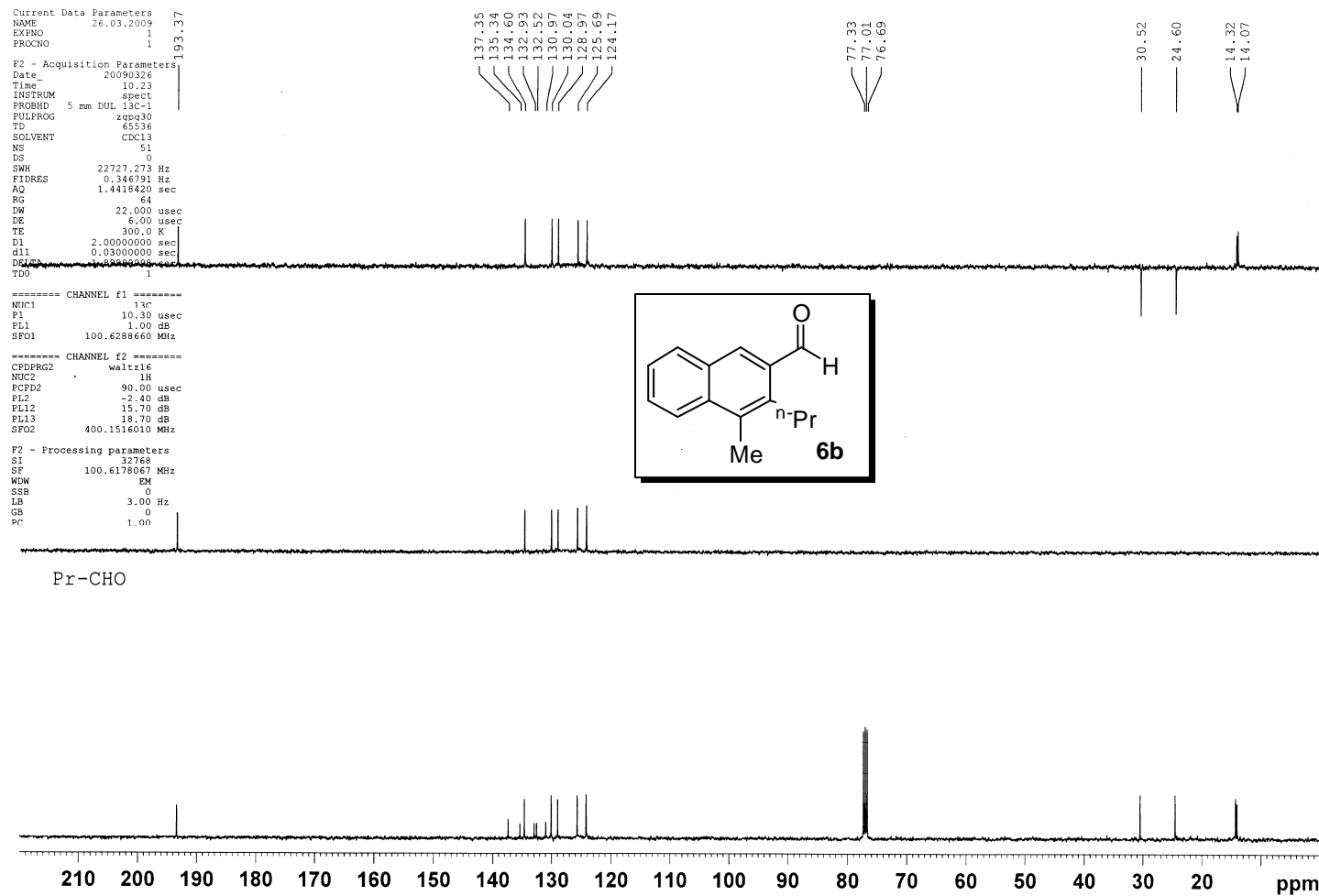


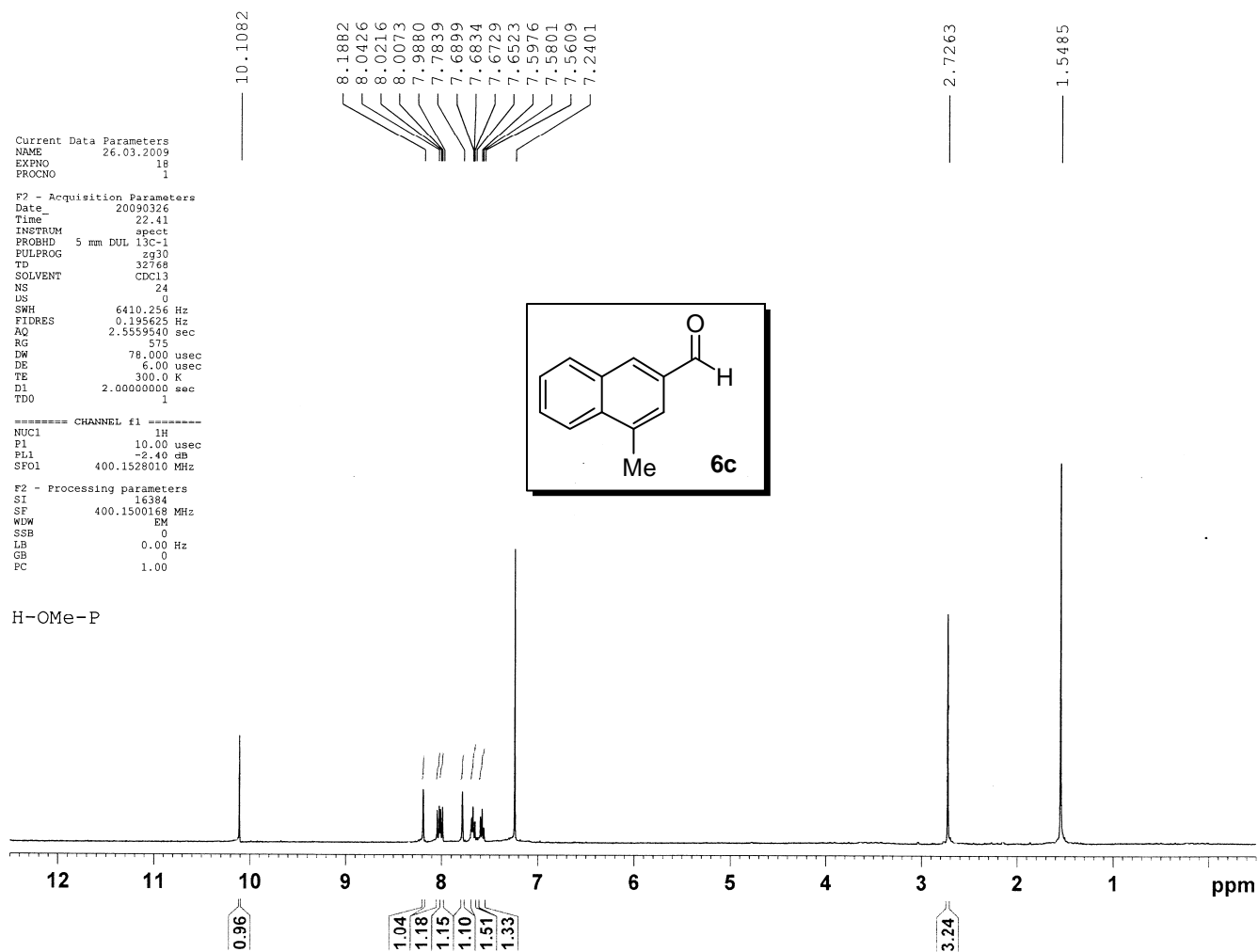


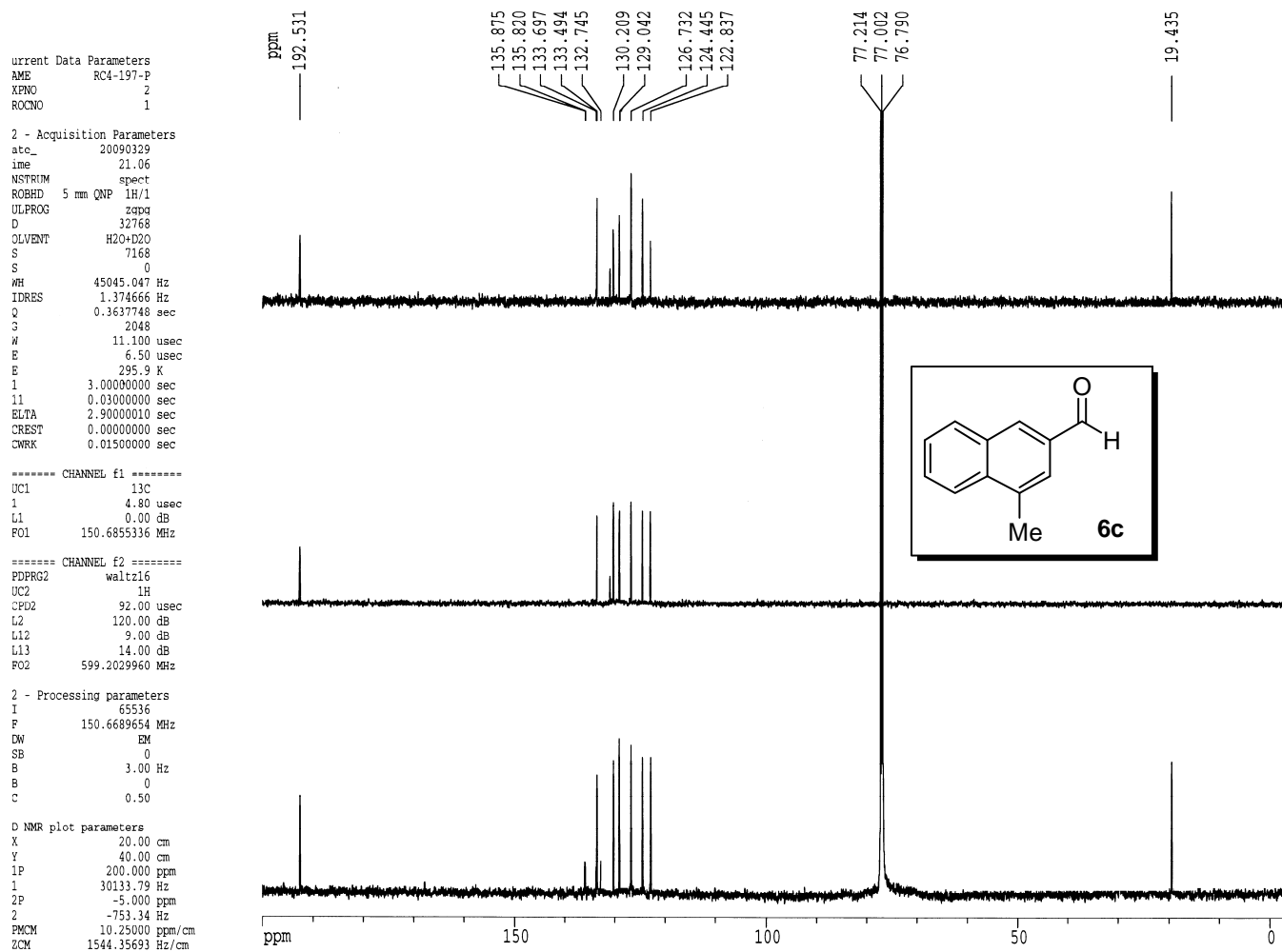




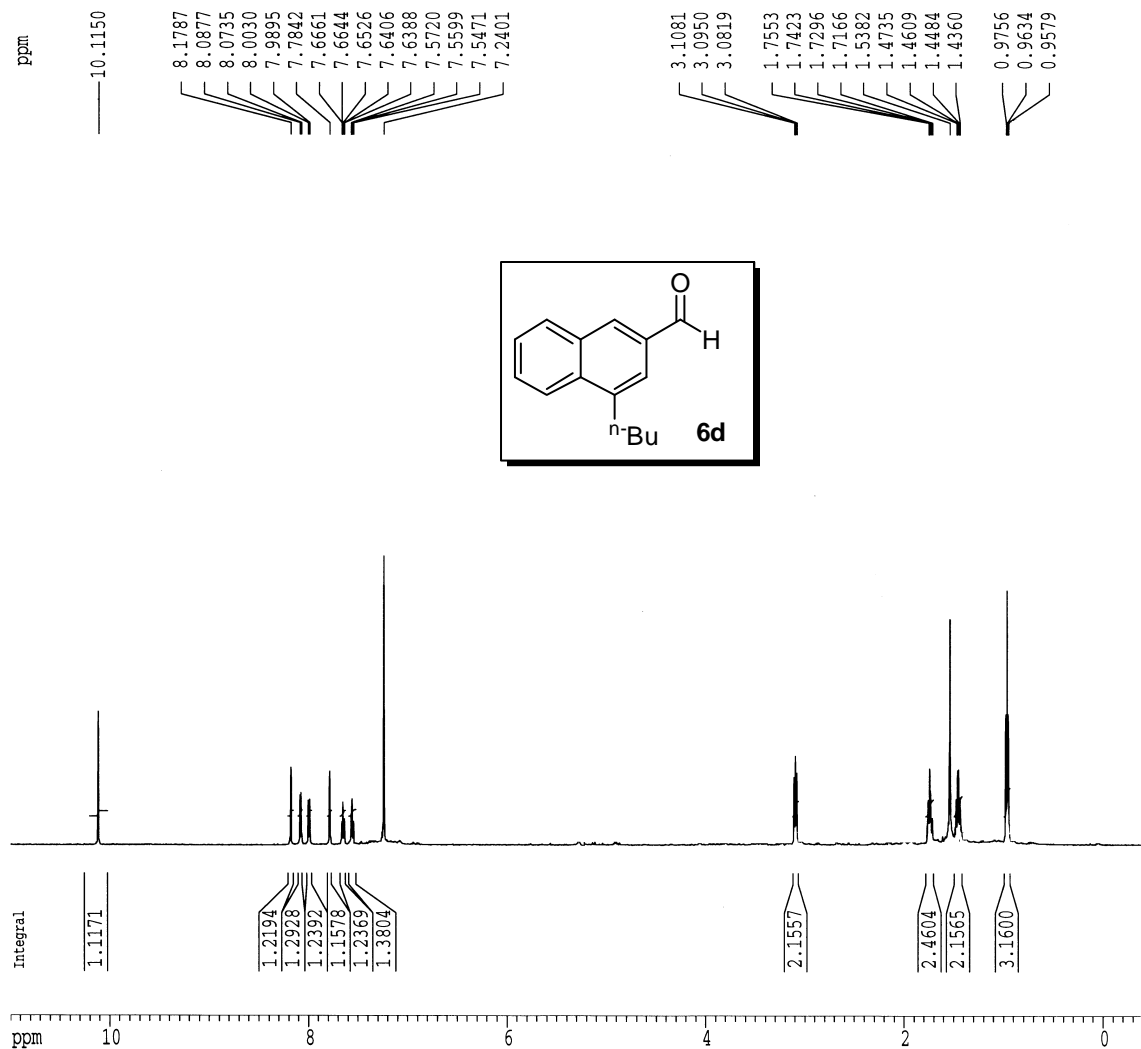








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R04-295P
1
1
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ID 5 mm QNP 1H/1
UDG 32768
DNT CXC13
16
0
9615.385 Hz
0.293438 Hz
1.7039860 sec
128
52.000 usec
6.50 usec
302.6 K
1.00000000 sec
0.00000000 sec
0.01500000 sec
*** CHANNEL f1 ***
1H
10.00 usec
3.00 dB
599.2031592 MHz
Processing parameters
32768
599.2000258 MHz
EM
0
1.00 Hz
0
1.00
R plot parameters
20.00 cm
12.00 cm
11.000 ppm
6591.20 Hz
-0.500 ppm
-299.40 Hz
0.57500 ppm/cm
344.54001 Hz/cm



```

ent Data Parameters
: RC4-295P
O 2
NO 1

Acquisition Parameters
: 20090604
: 22.45
RUN spect
HD 5 mm QNP 1H/1
ROG zgpg
32768
F2T1 CDC13
6144
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45045.047 Hz
ES 1.374666 Hz
0.3637748 sec
1024
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ST 0.00000000 sec
K 0.01500000 sec

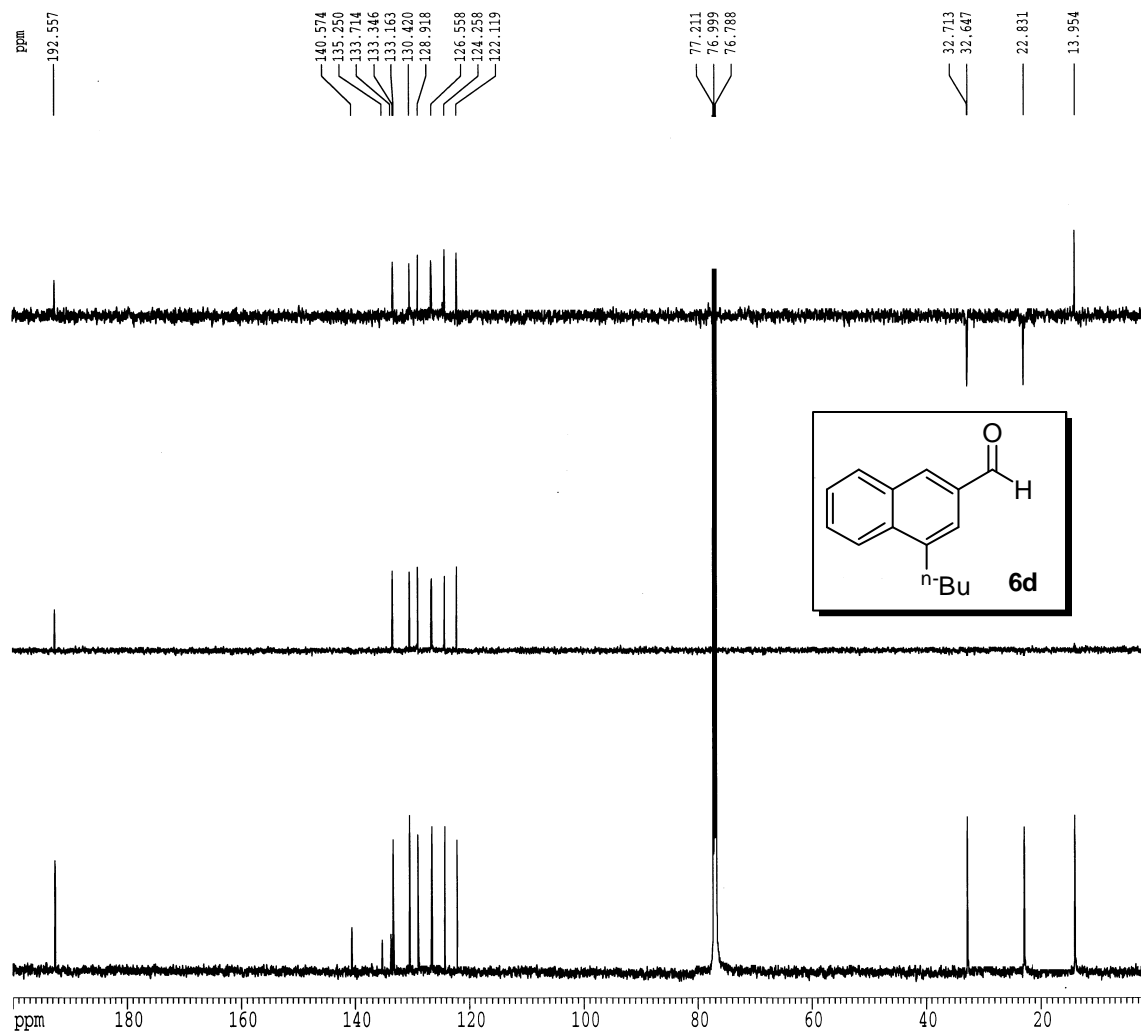
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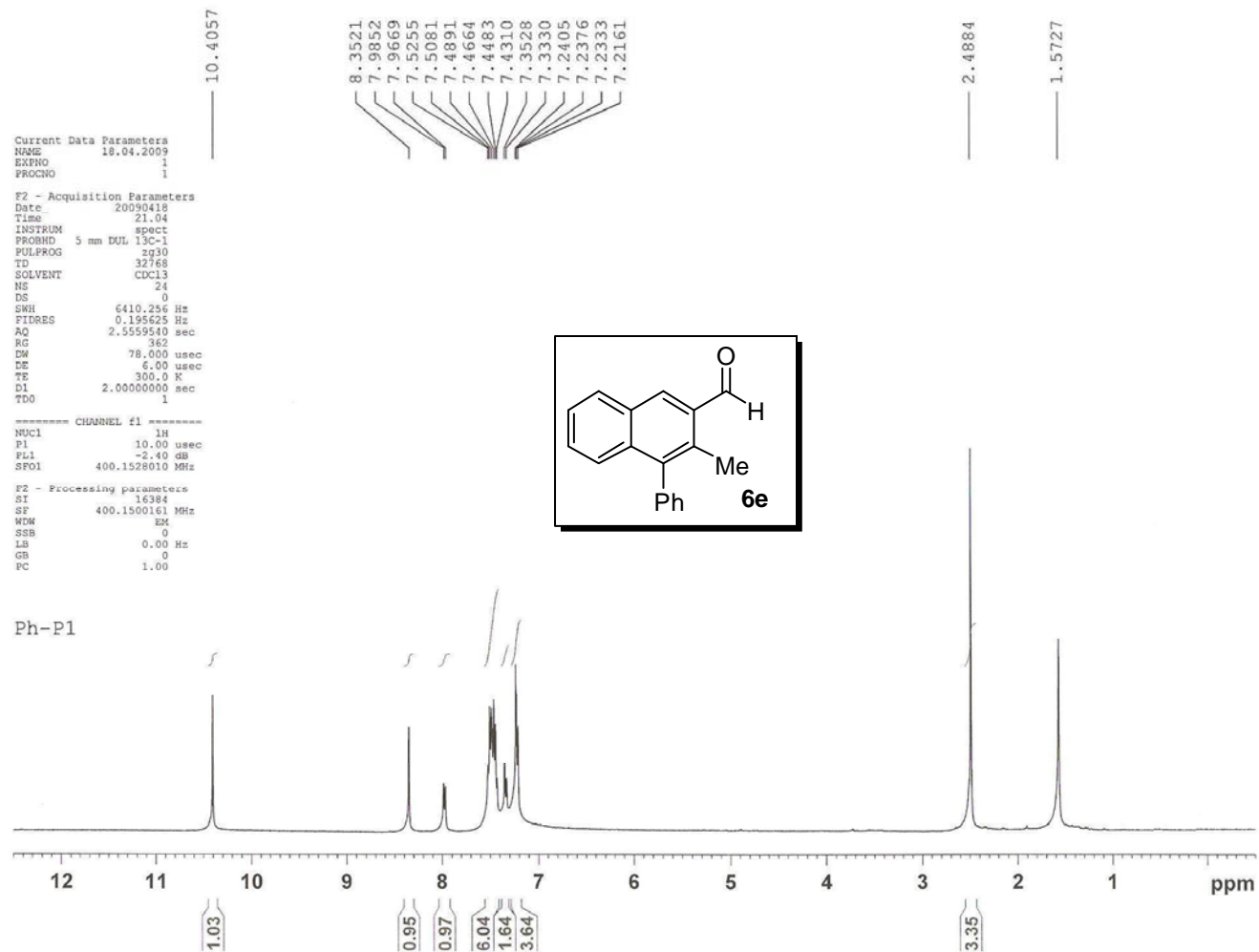
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11.30 dB
14.00 dB
599.2029960 MHz

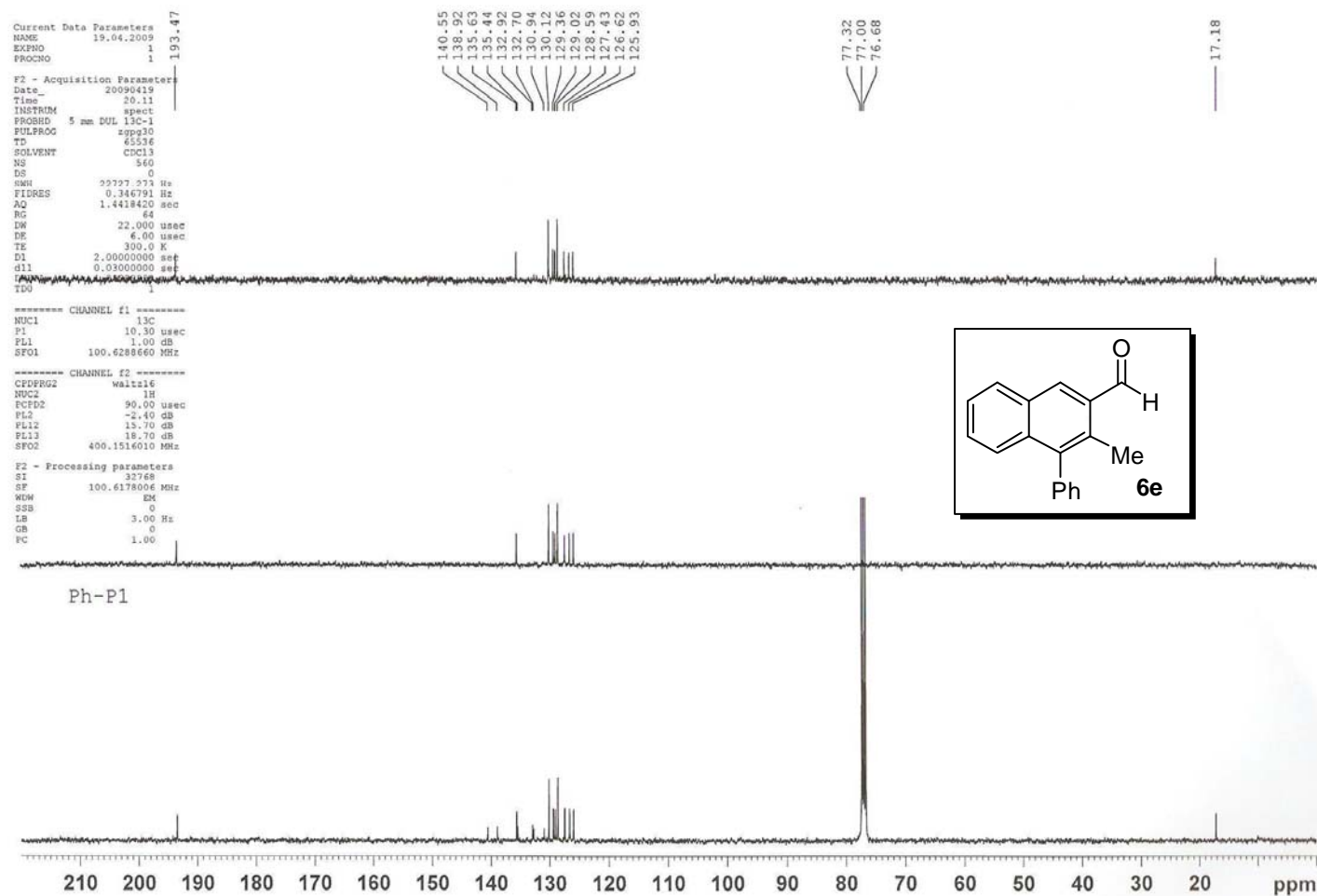
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EM
0
3.00 Hz
0
0.50

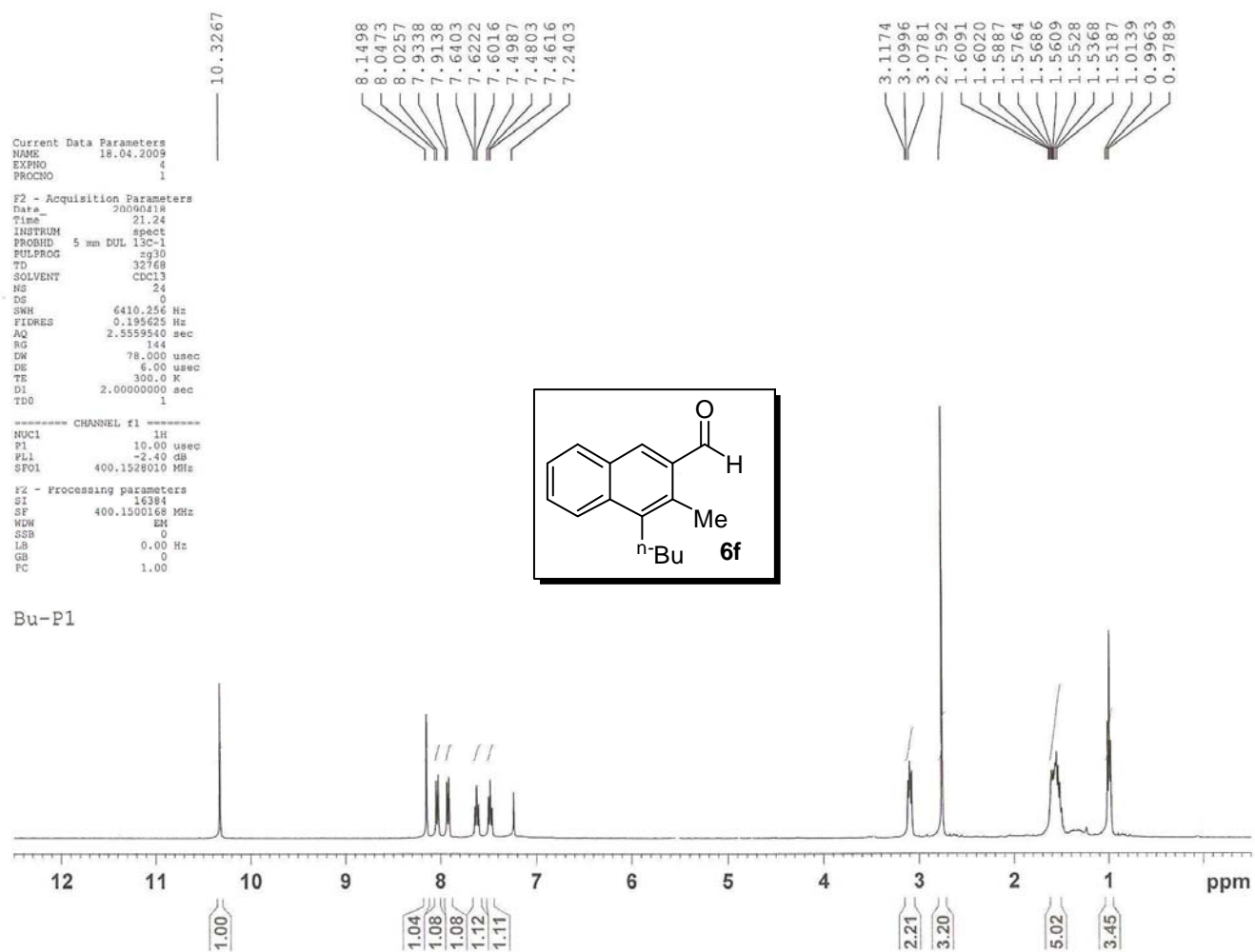
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30133.79 Hz
0.000 ppm
0.00 Hz
M 10.00000 ppm/cm
f 1506.68958 Hz/cm

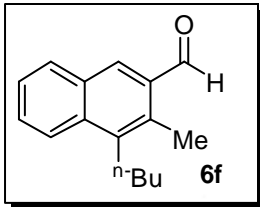
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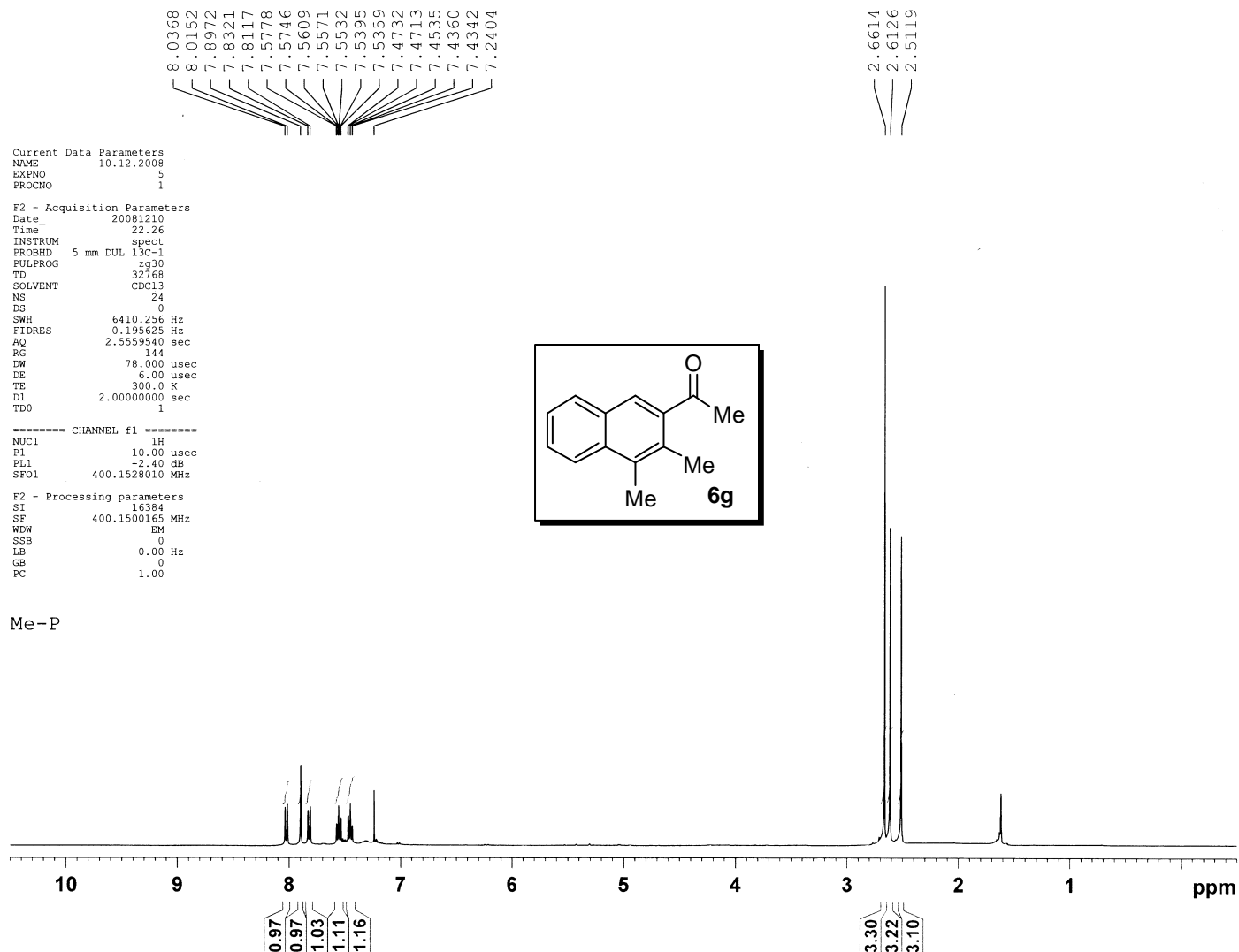


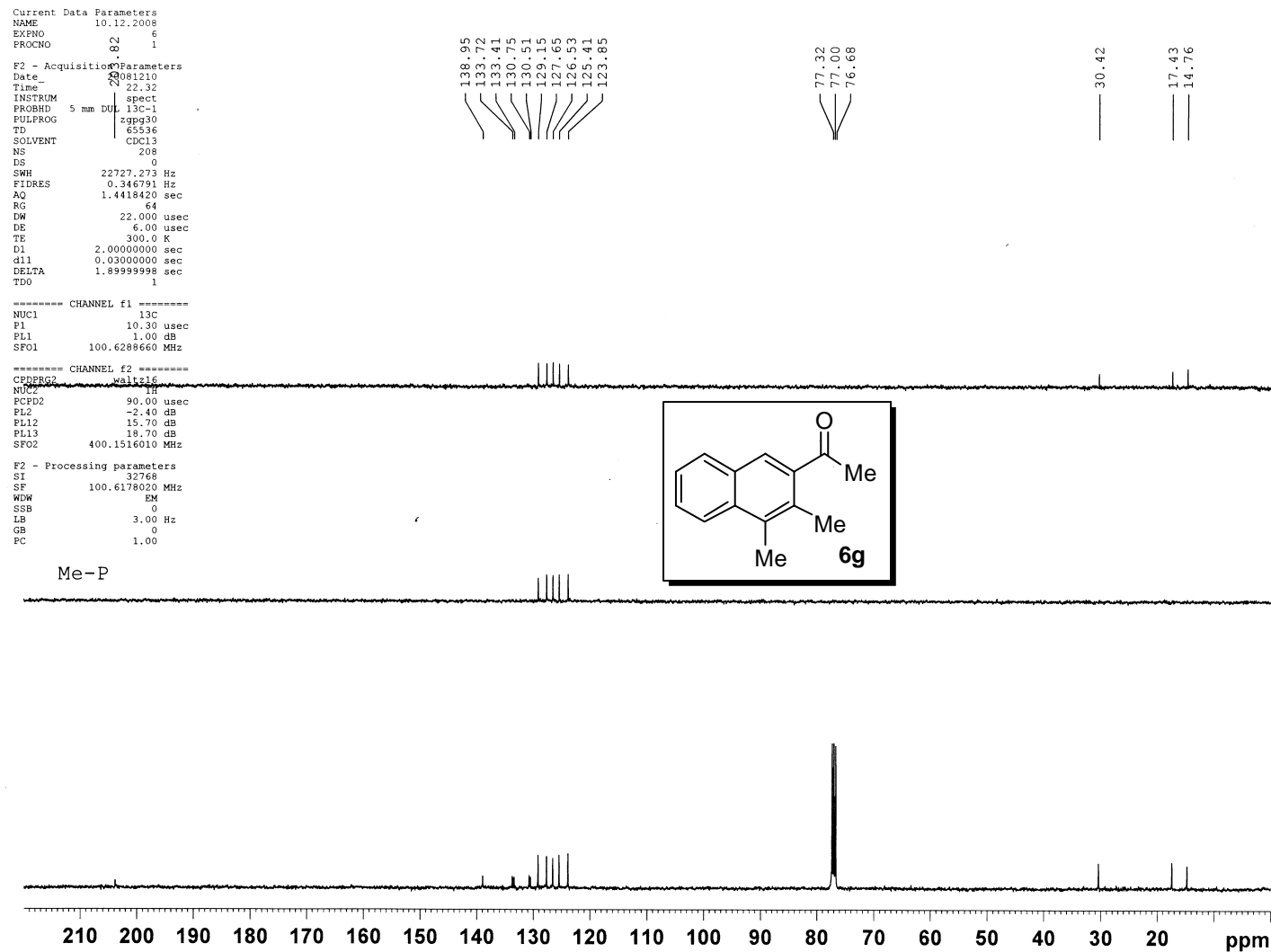


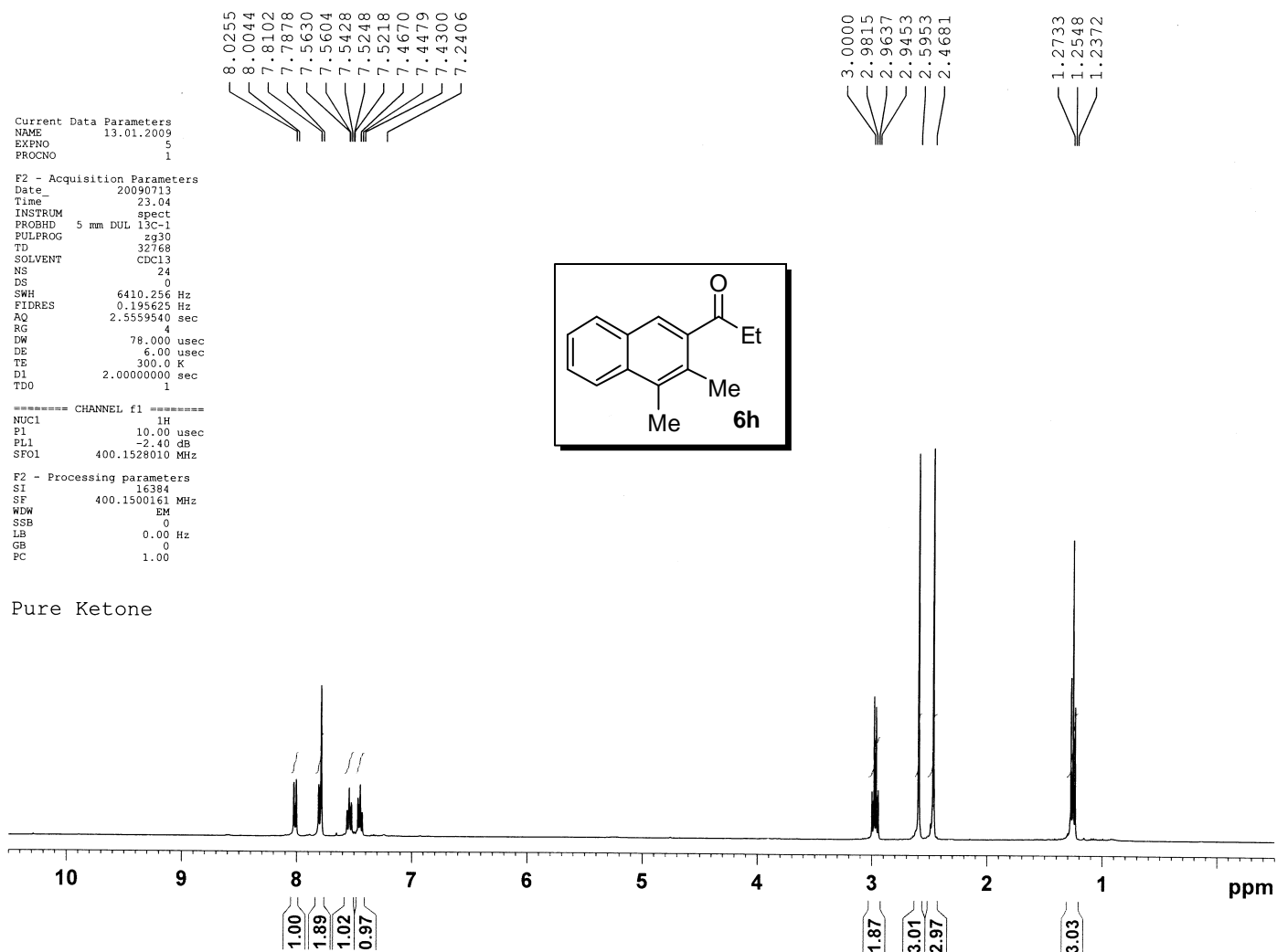


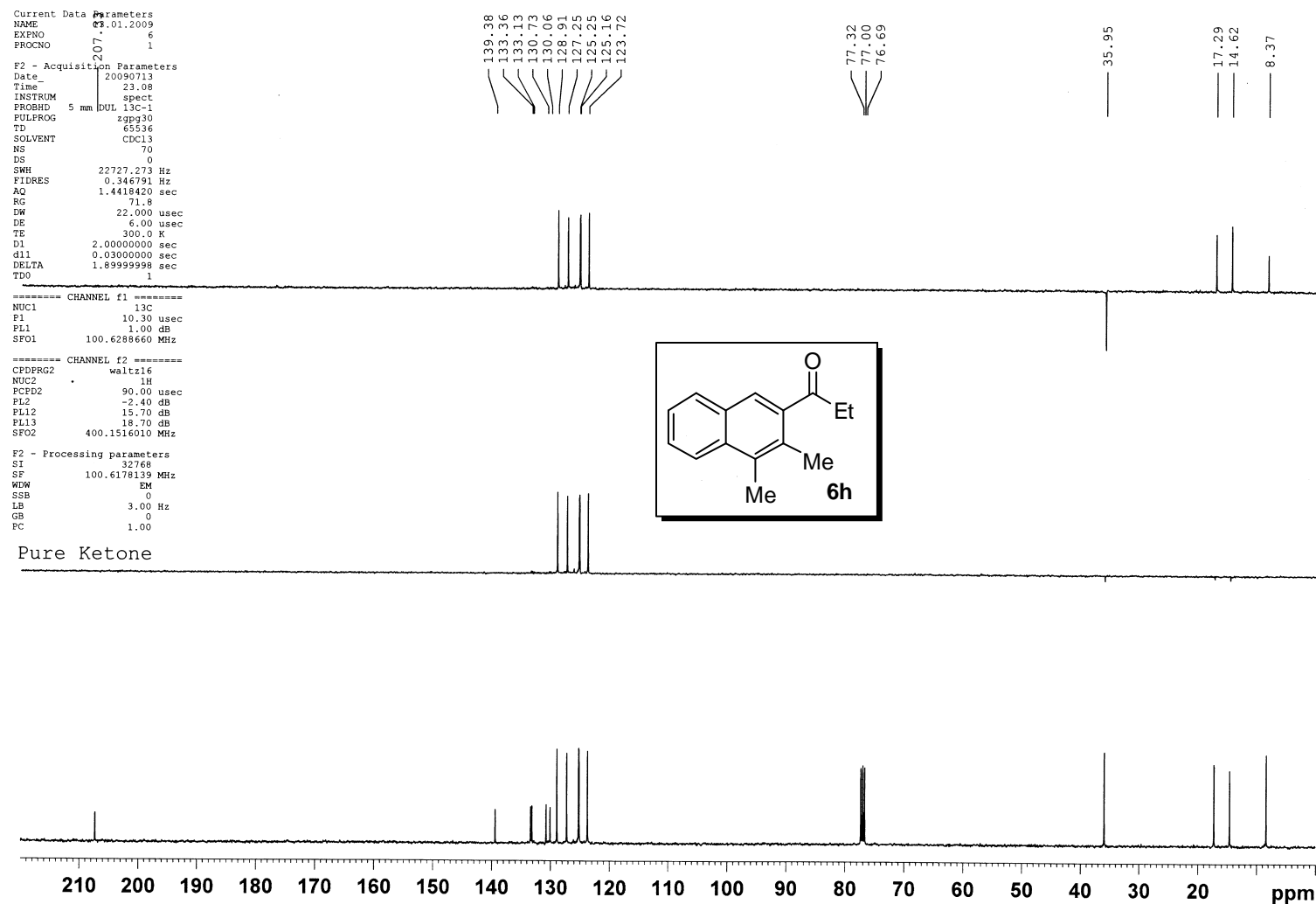












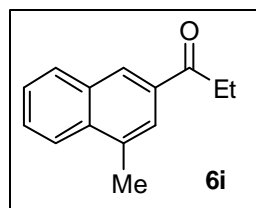
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7.6344
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7.6133
7.5995
7.5962
7.5563
7.5534
7.5391
7.5360
7.5332
7.5189
7.5161
7.2408

Current Data Parameters
NAME 16.06.2009
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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Time 8.14
INSTRUM spect
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
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RG 362
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

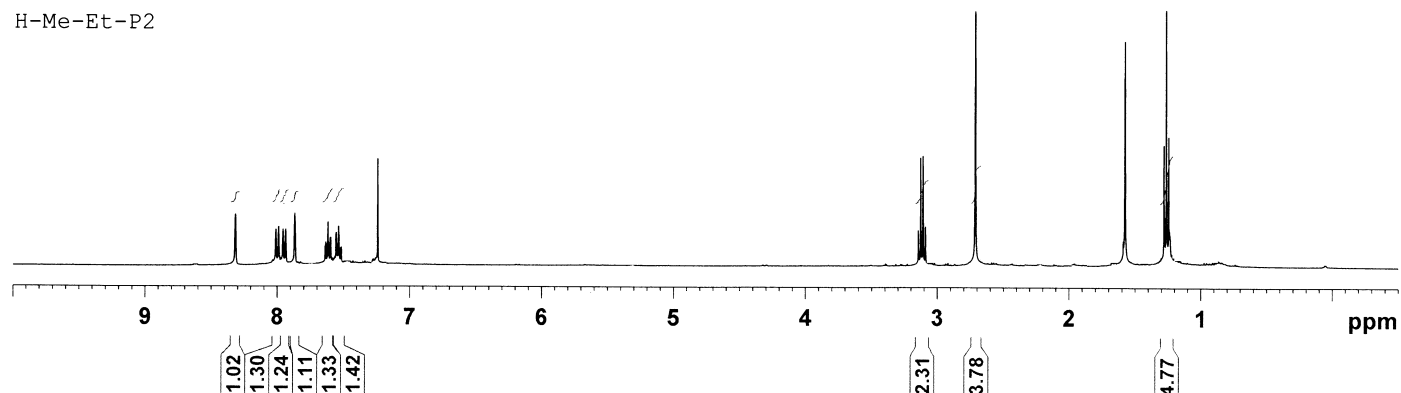
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PL1 -2.40 dB
SFO1 400.1528010 MHz

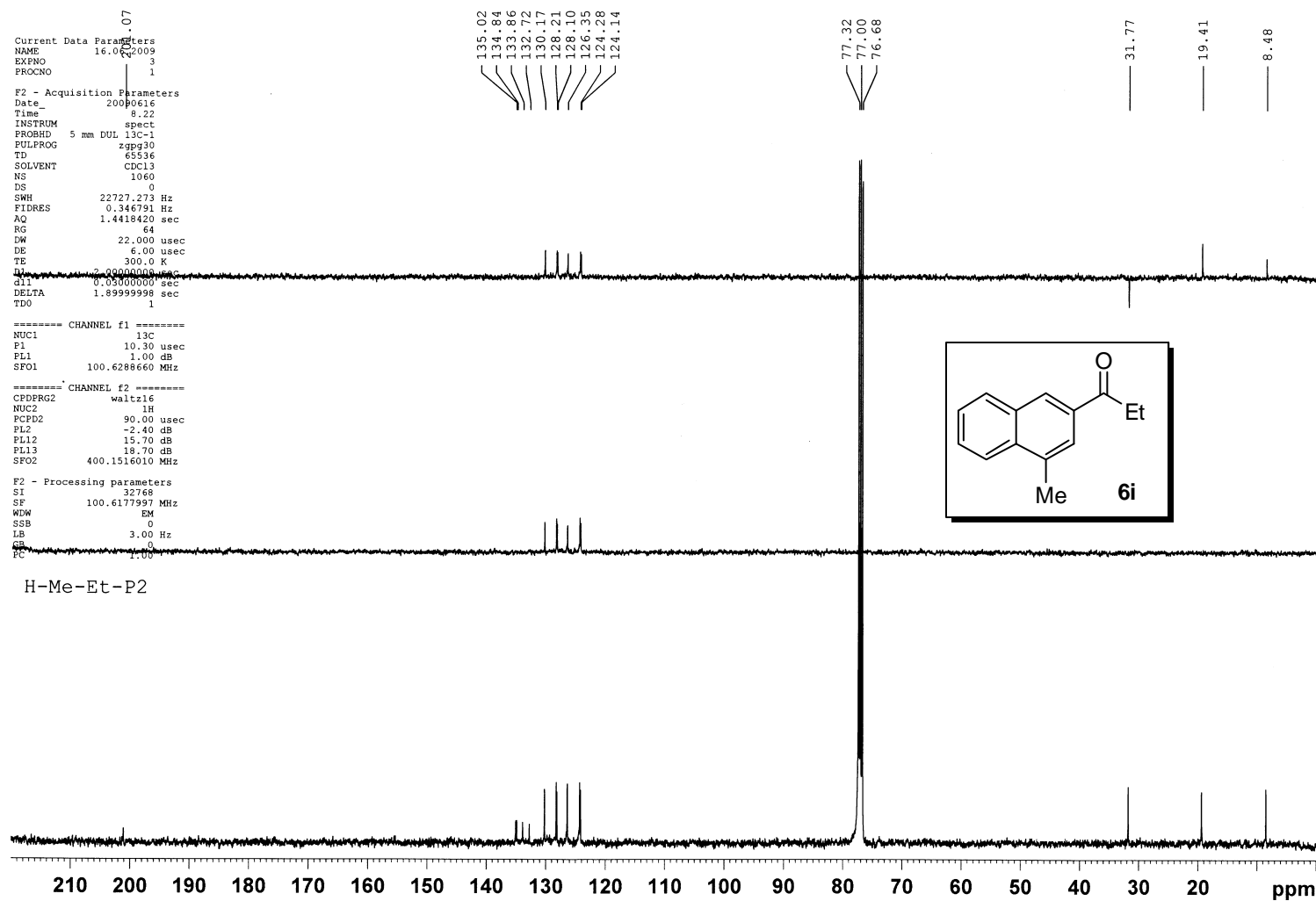
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SF 400.1500164 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



3.1454
3.1271
3.1092
3.0909
2.7130

1.5770
1.2820
1.2642
1.2458





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Current Data Parameters
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OCNO    1

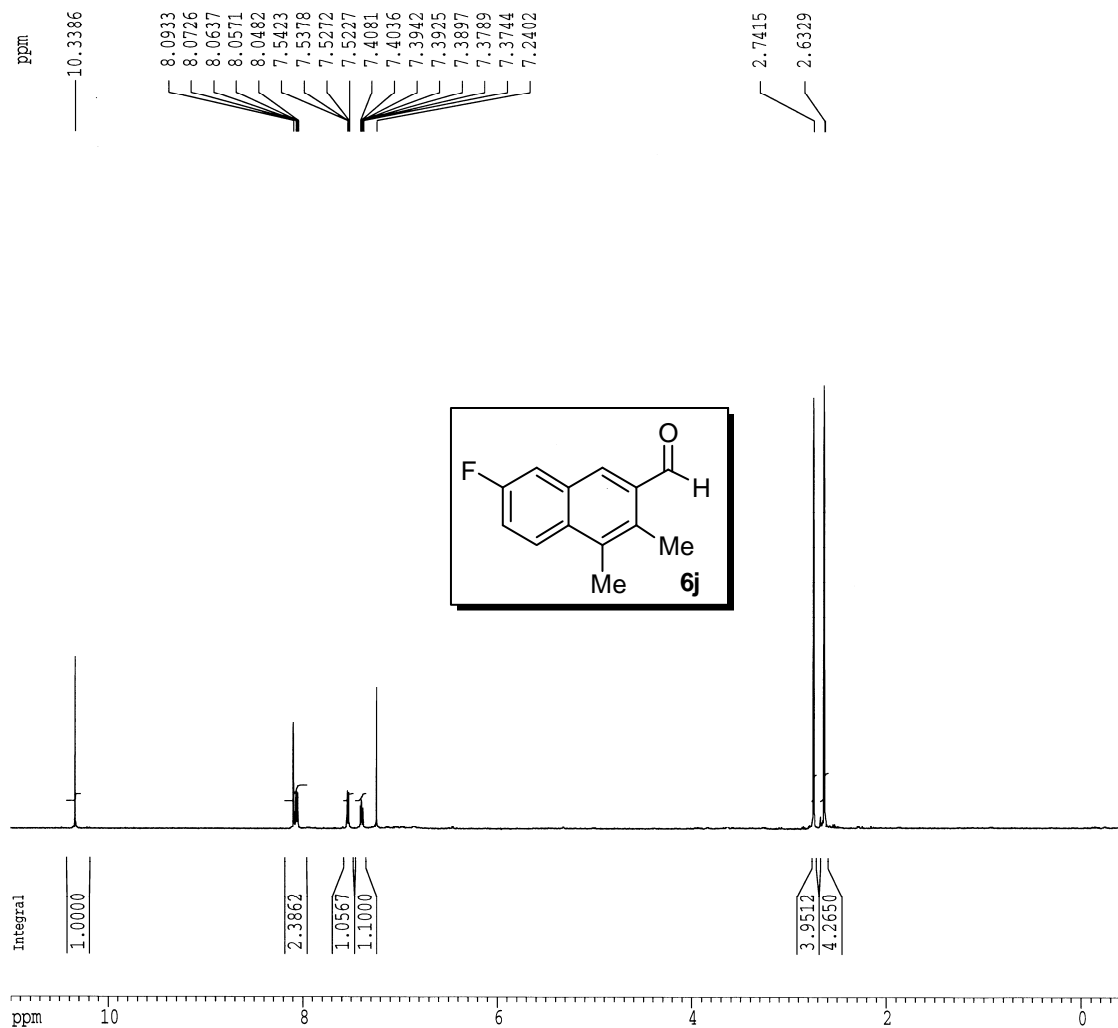
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me      22.33
STRUM    spect
OBHD     5 mm QNP 1H/1
LPROG    zg
         32768
LVENT    CDC13
         16
         0
H        9615.385 Hz
DRES     0.293438 Hz
         1.7039860 sec
         256
         52.000 usec
         6.50 usec
         299.9 K
         1.00000000 sec
REST     0.00000000 sec
WRK      0.01500000 sec

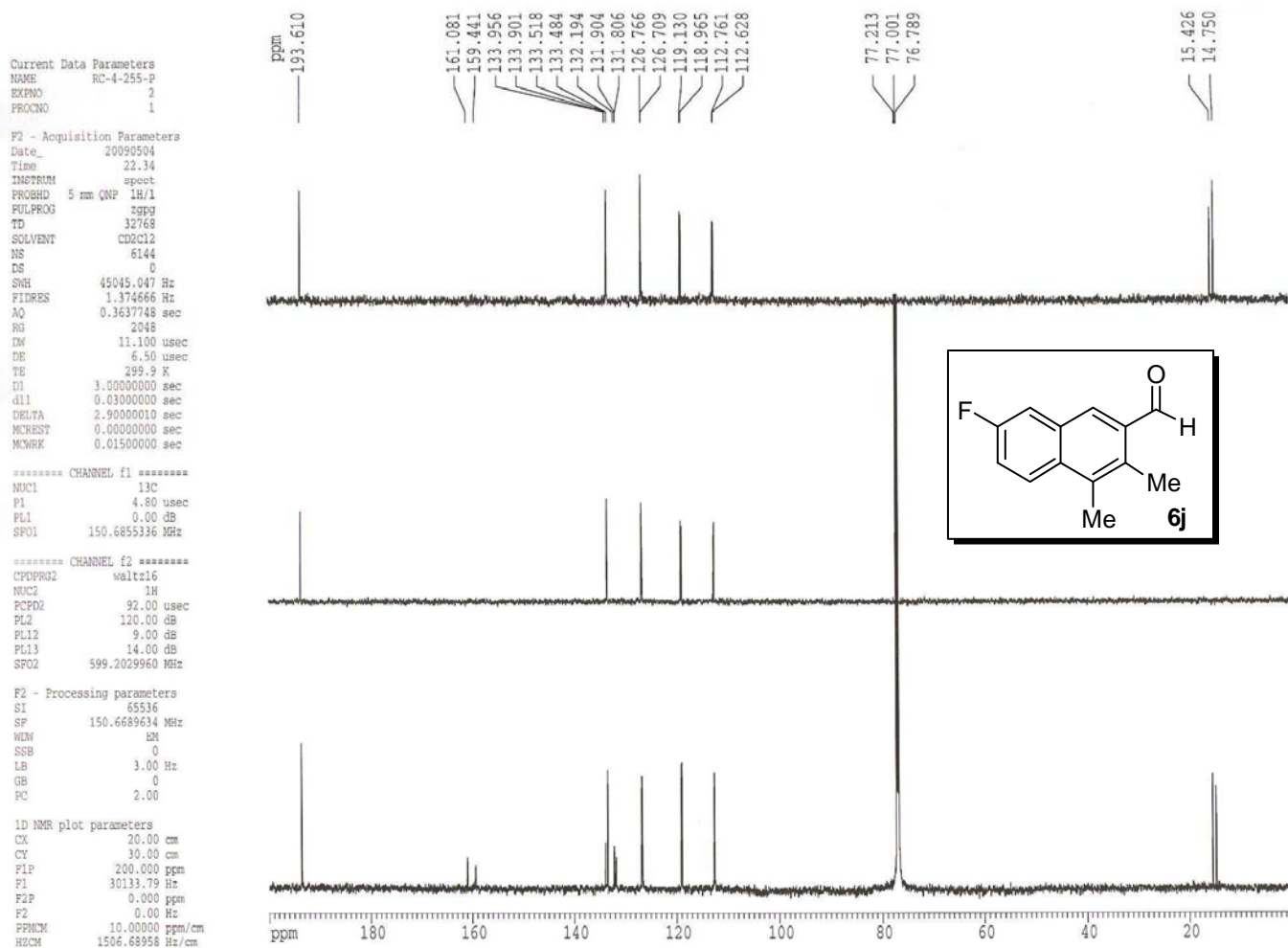
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1        -5.00 dB
O1       599.2035952 MHz

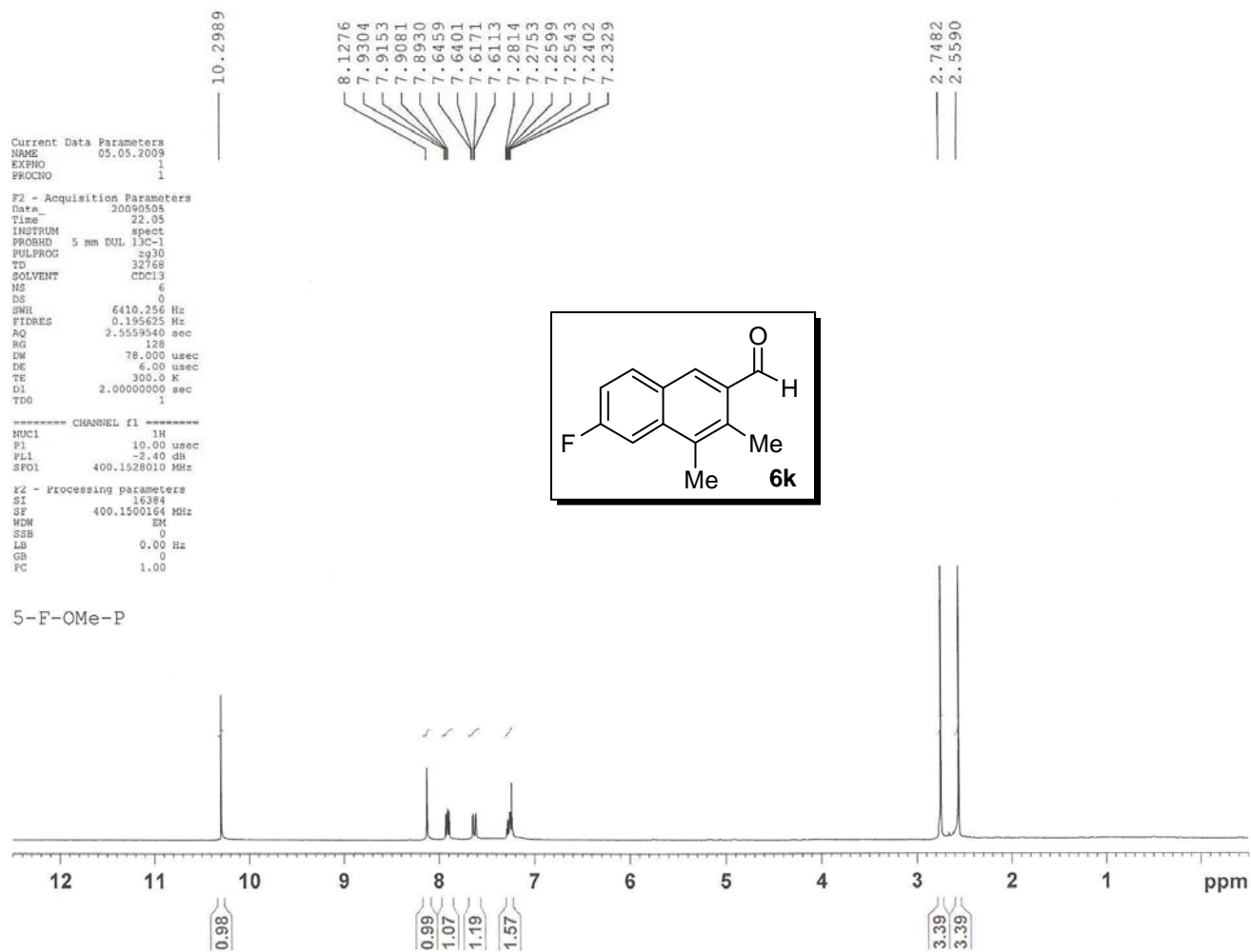
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W        no
B        0
         0.00 Hz
         0
         1.00

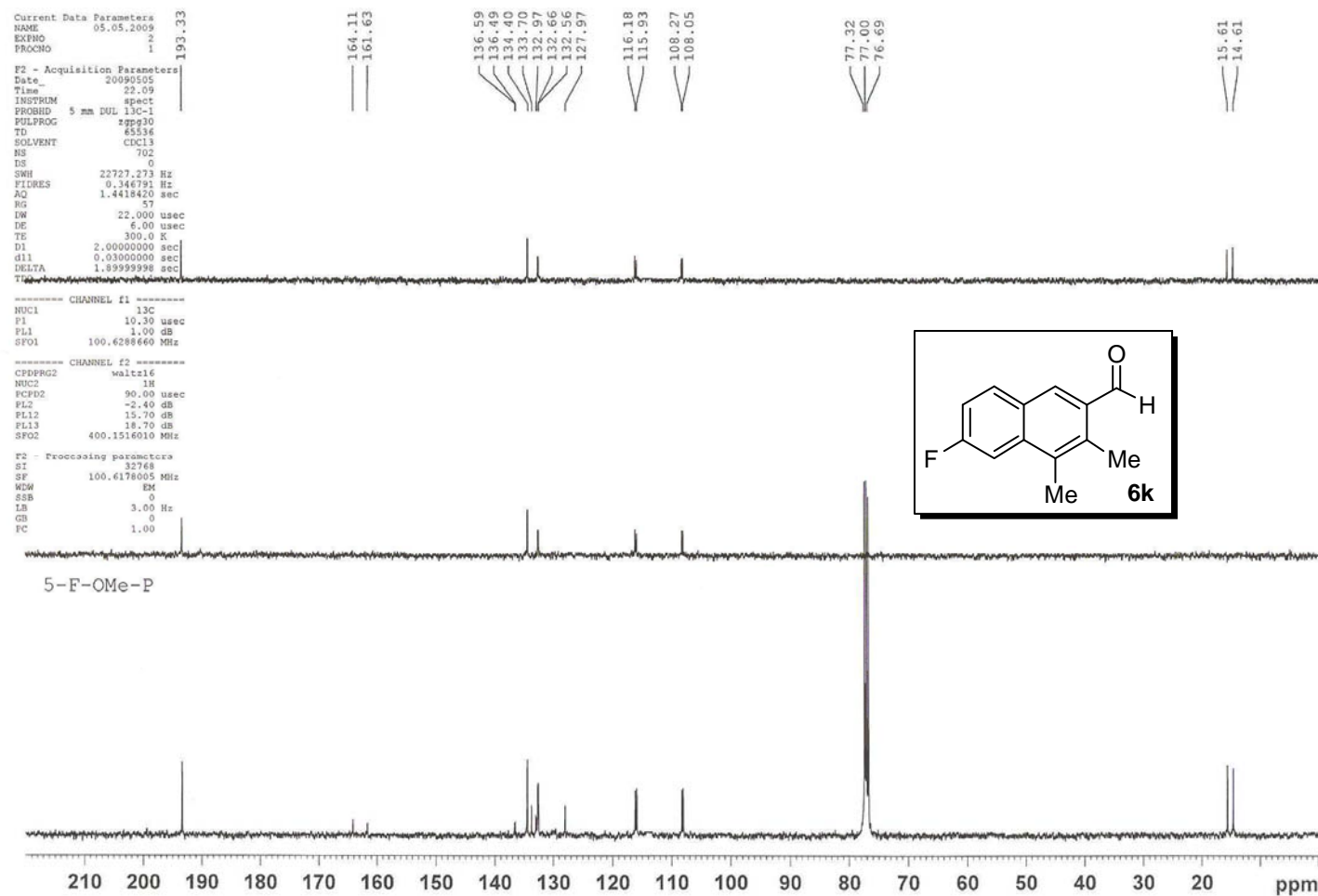
NMR plot parameters
         20.00 cm
         8.00 cm
P        11.000 ppm
         6591.20 Hz
P        -0.500 ppm
         -299.60 Hz
MCM      0.57500 ppm/cm
CM       344.54001 Hz/cm

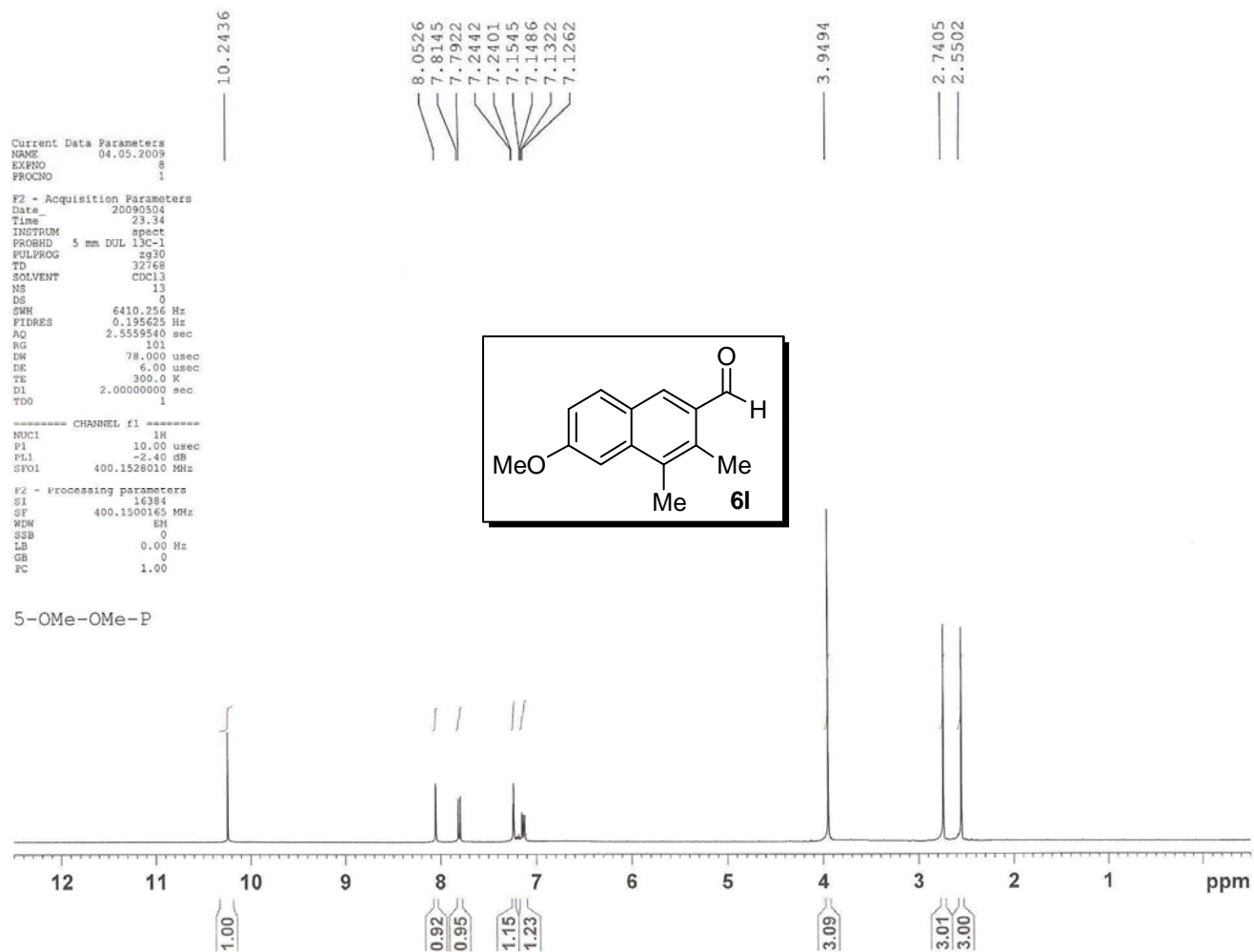
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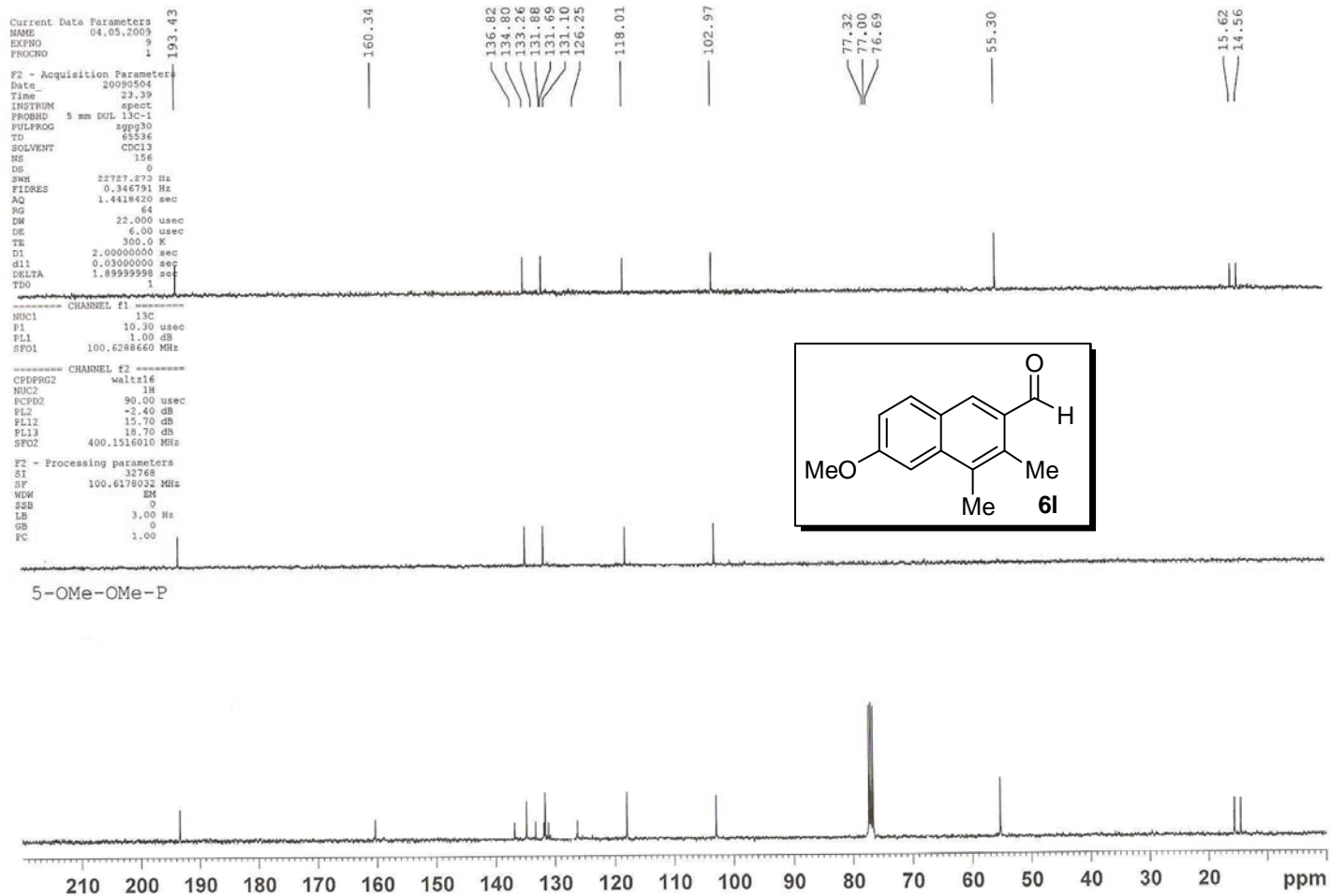


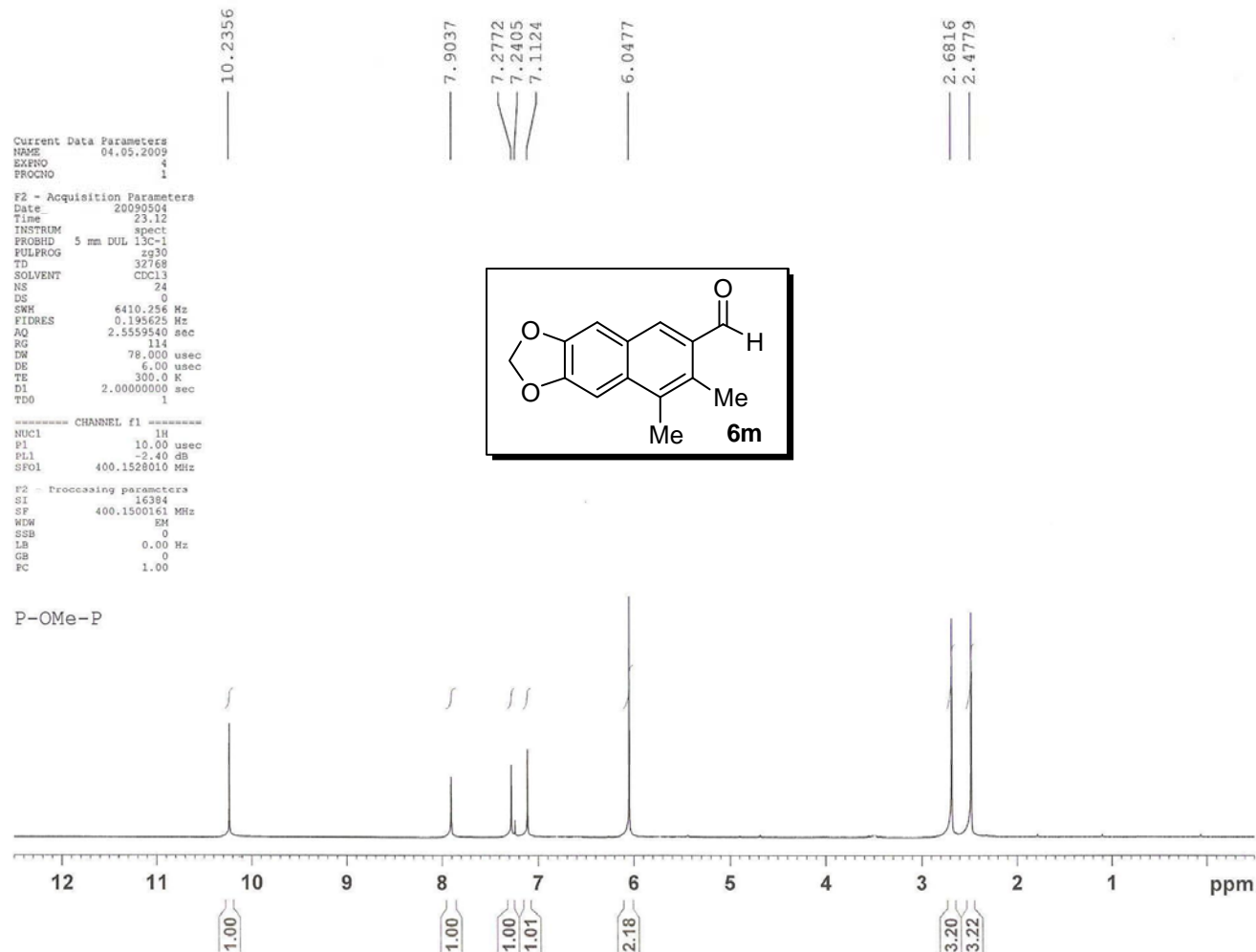


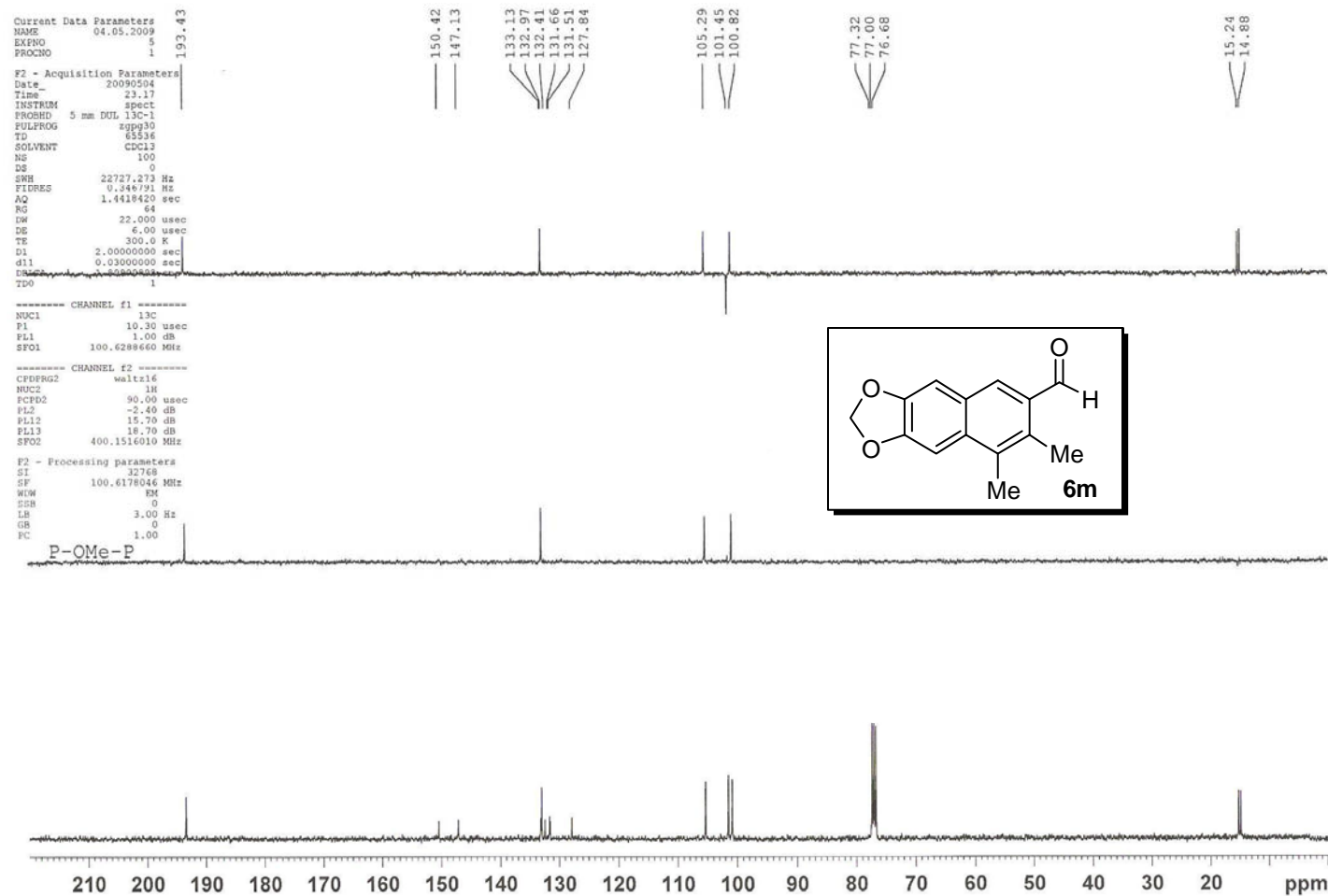


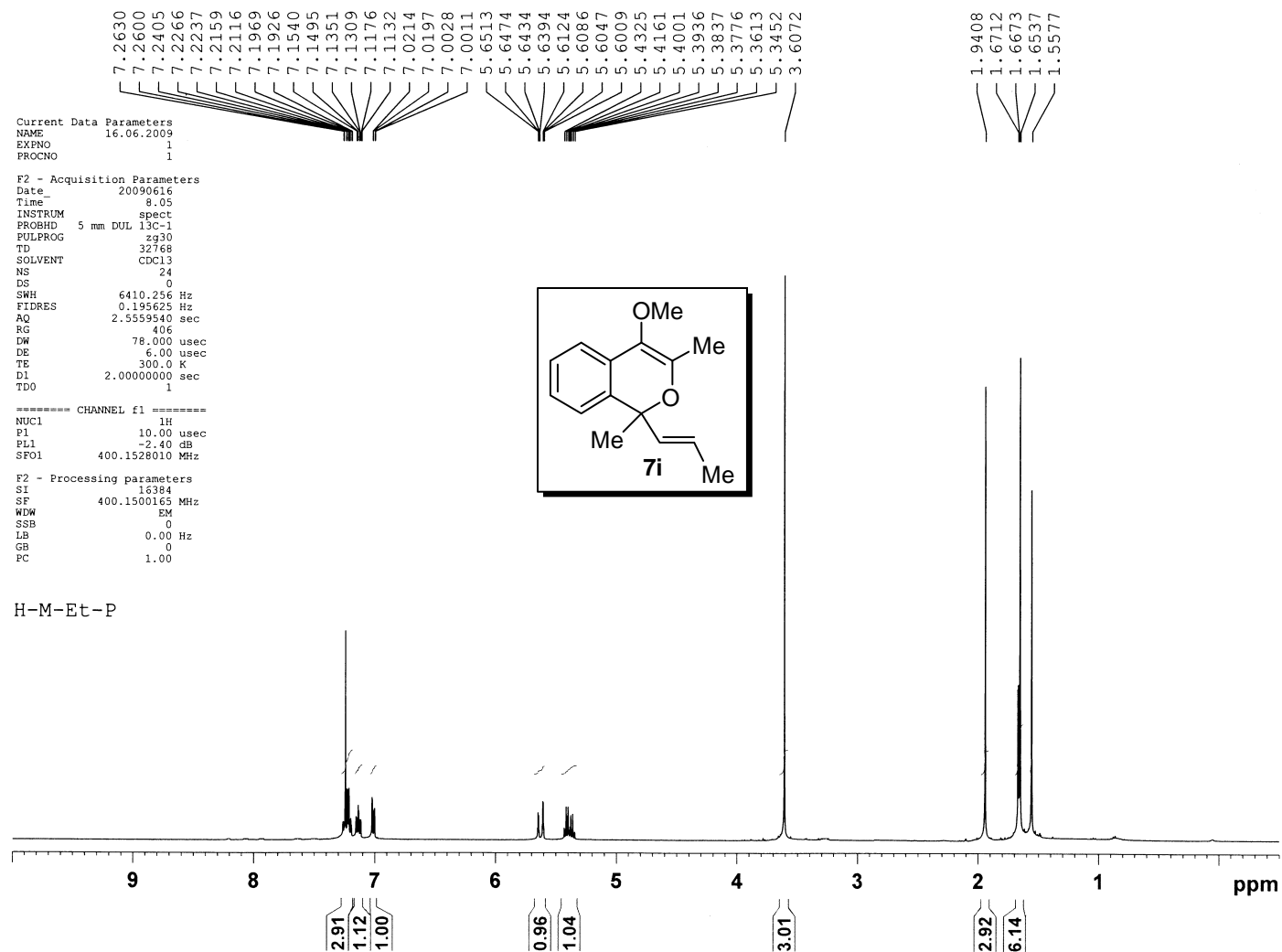


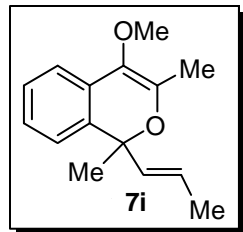


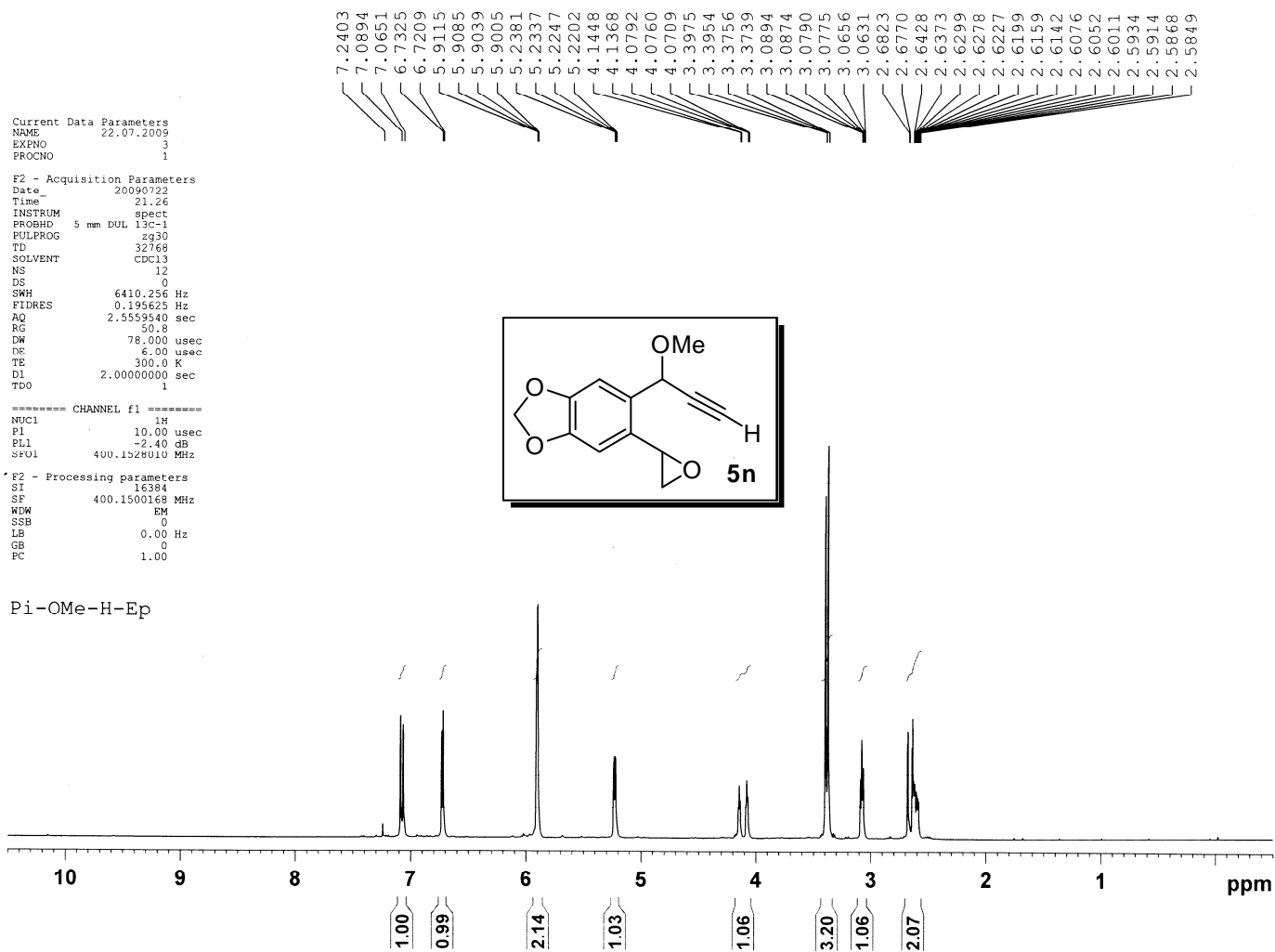












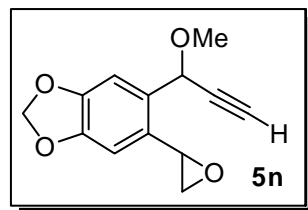
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EXPNO 2
PROCNO 1

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NS 200
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

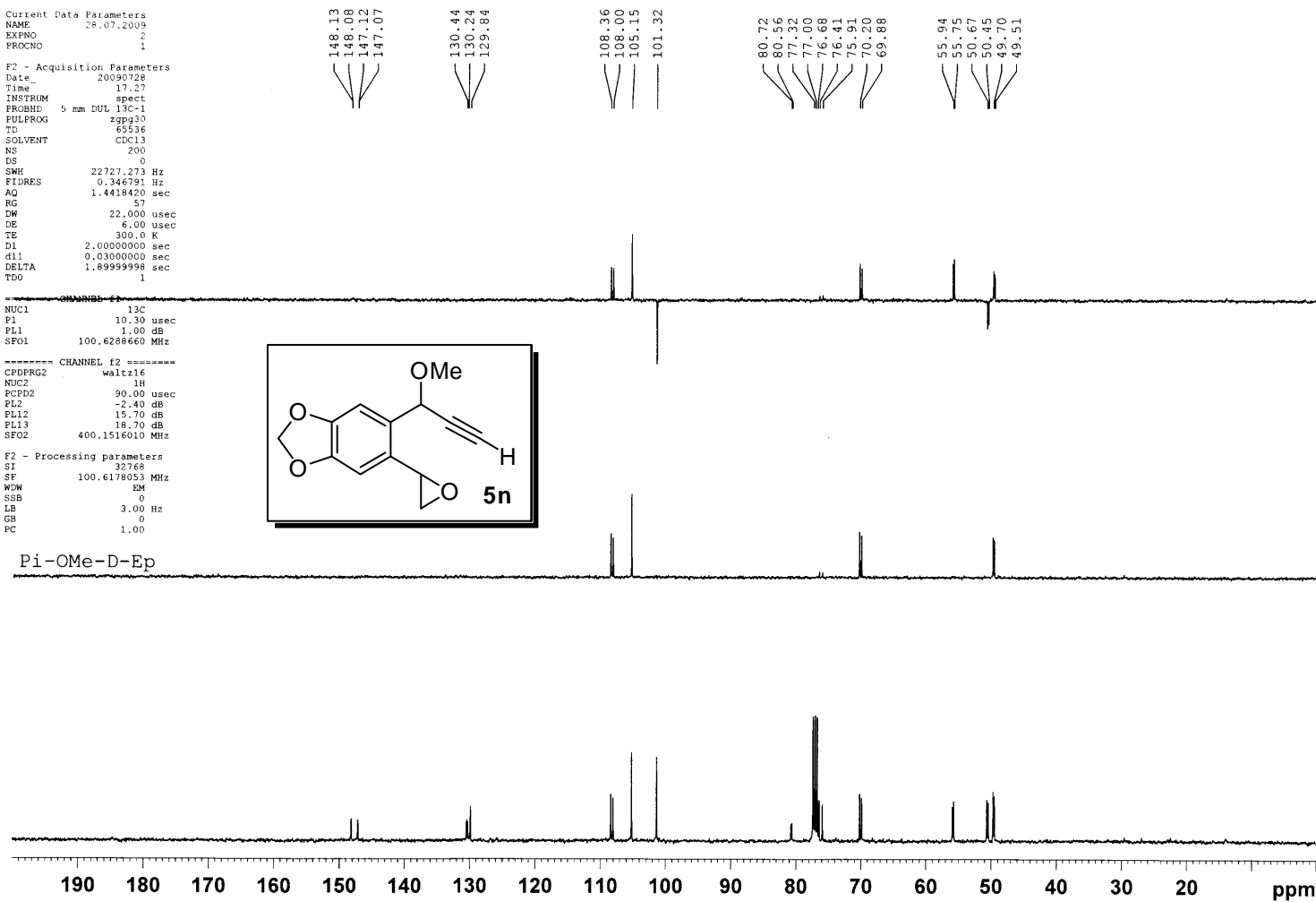
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PL1 1.00 dB
SFO1 100.6288660 MHz

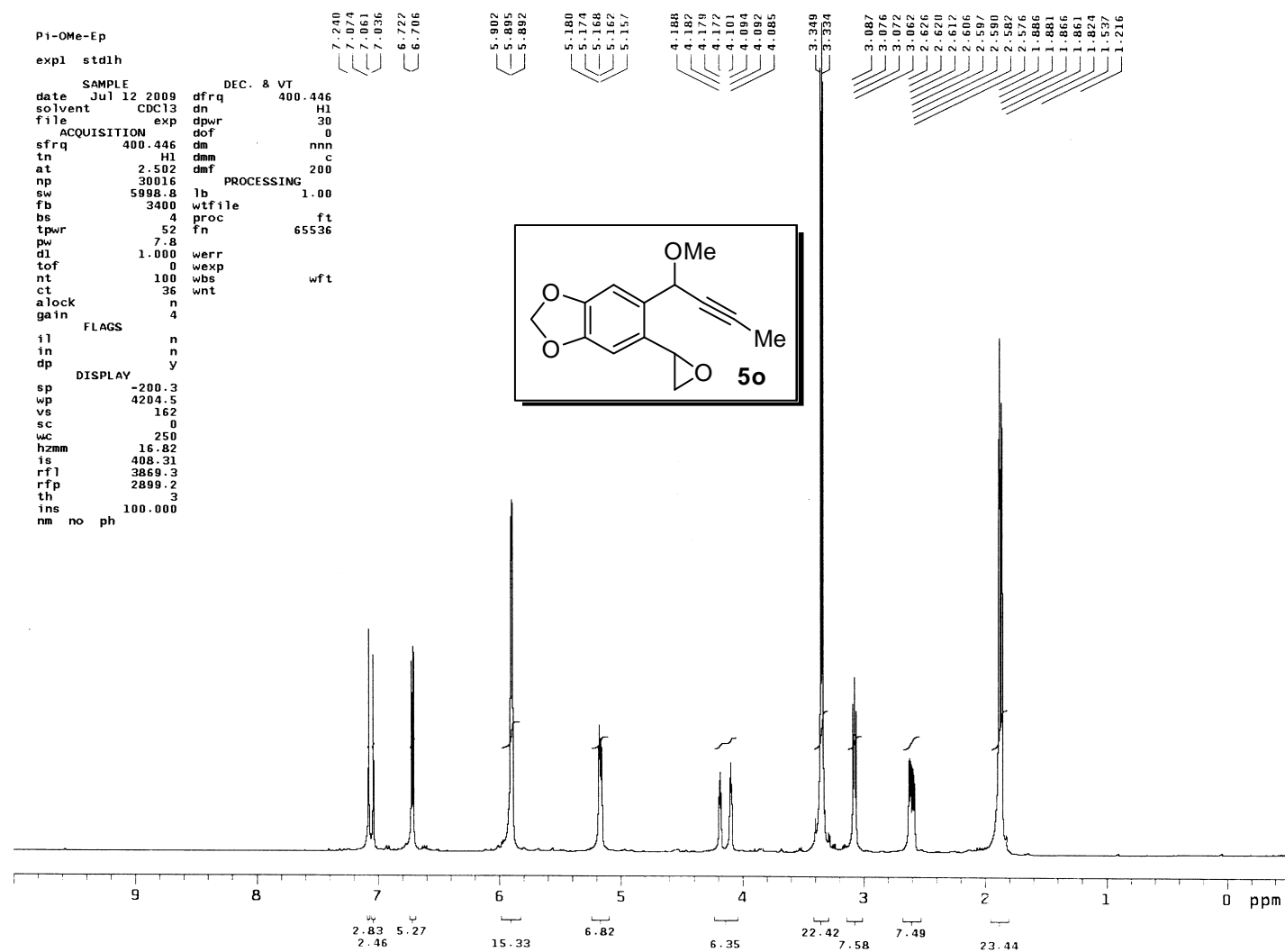
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CPDPRG2 waltz16
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PCPD2 30.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

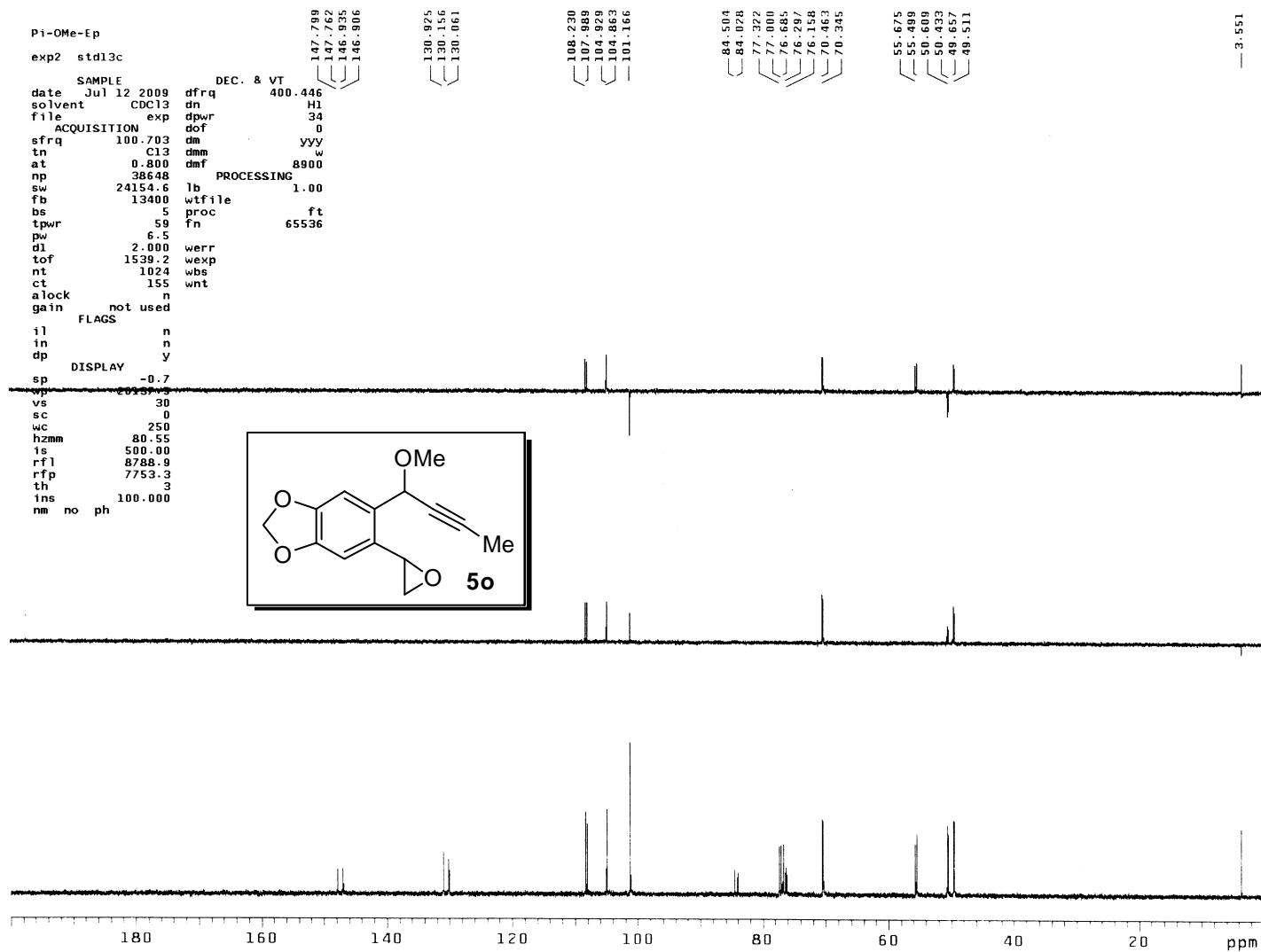
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WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

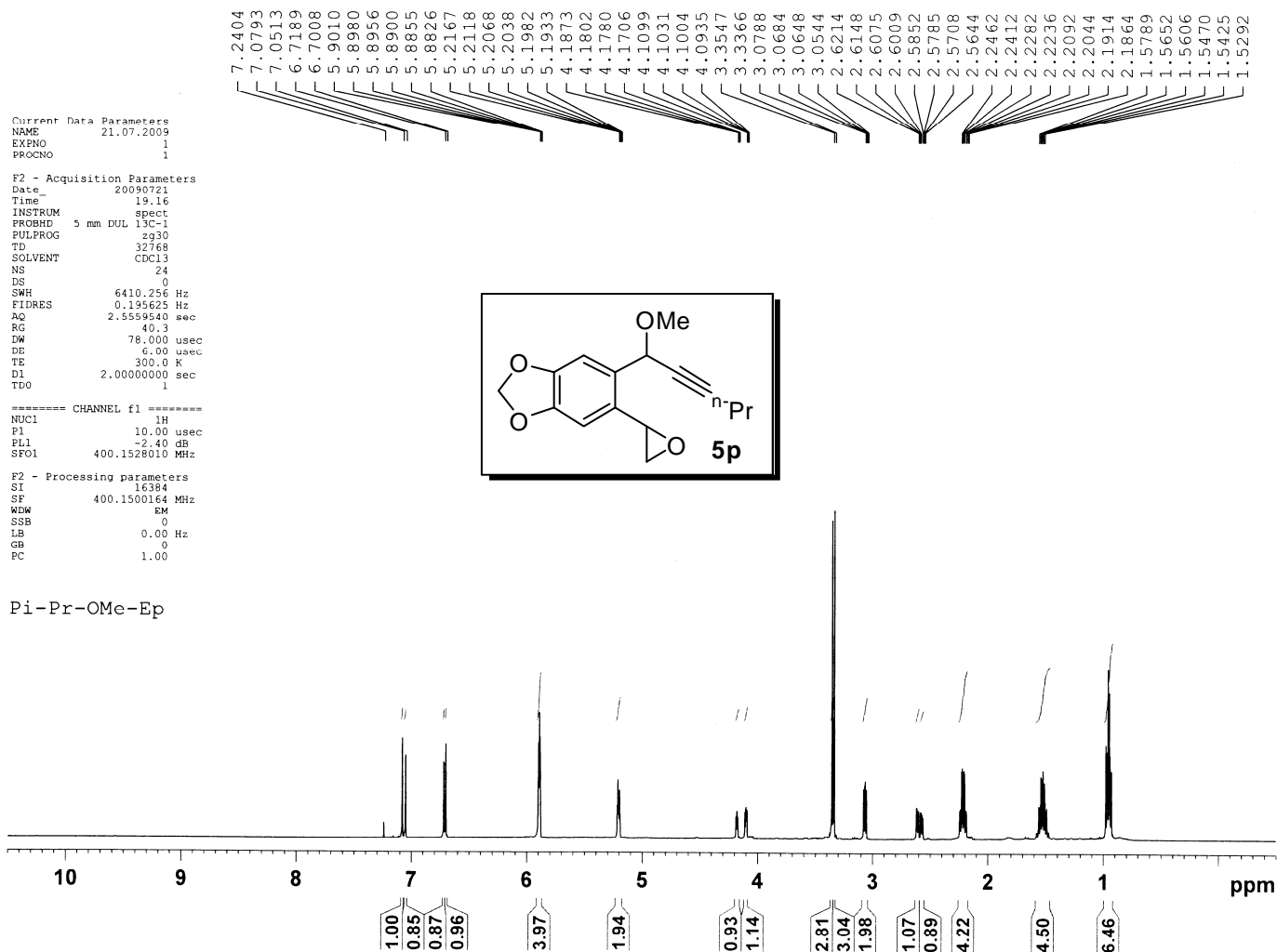


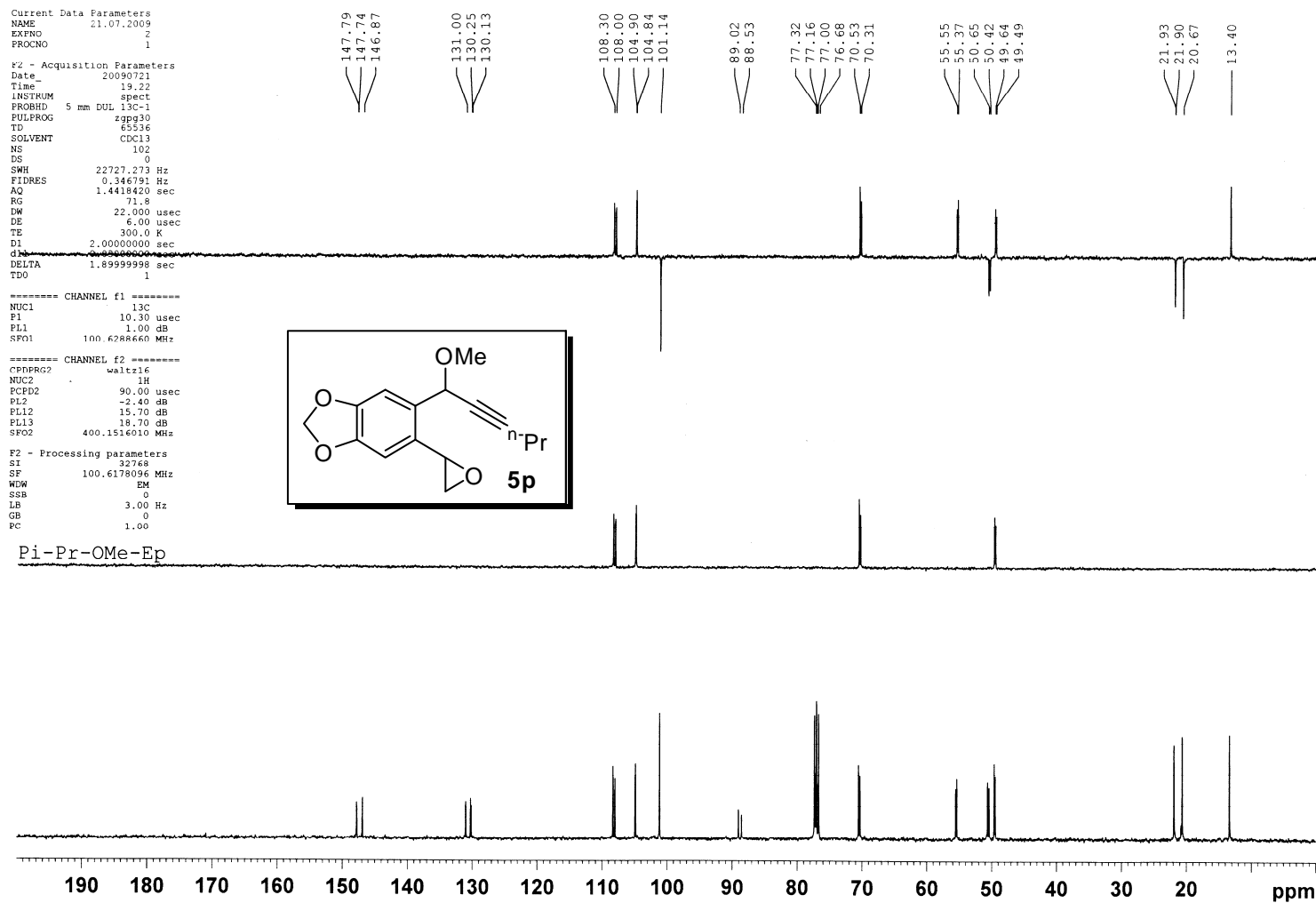
Pi-OMe-D-Ep

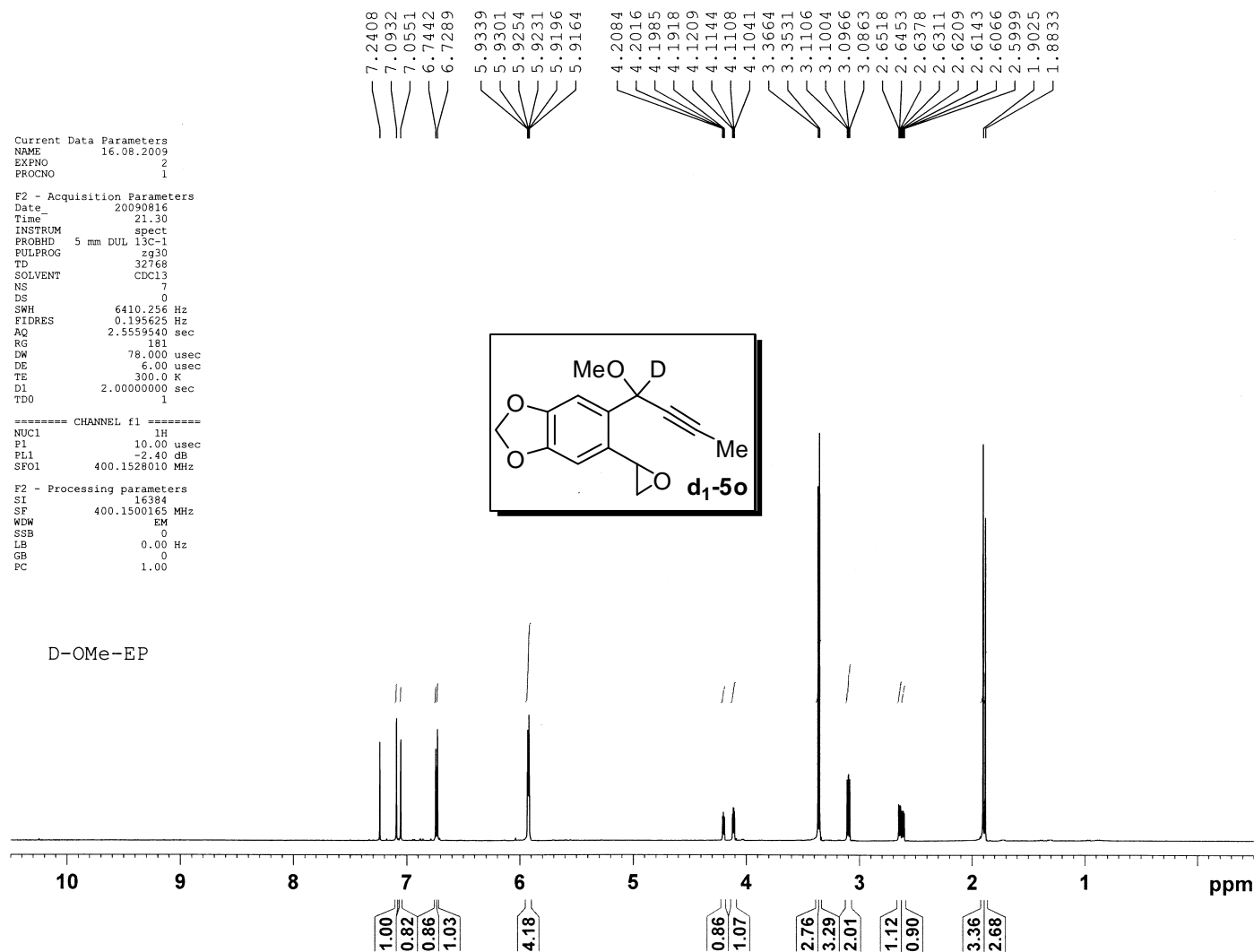


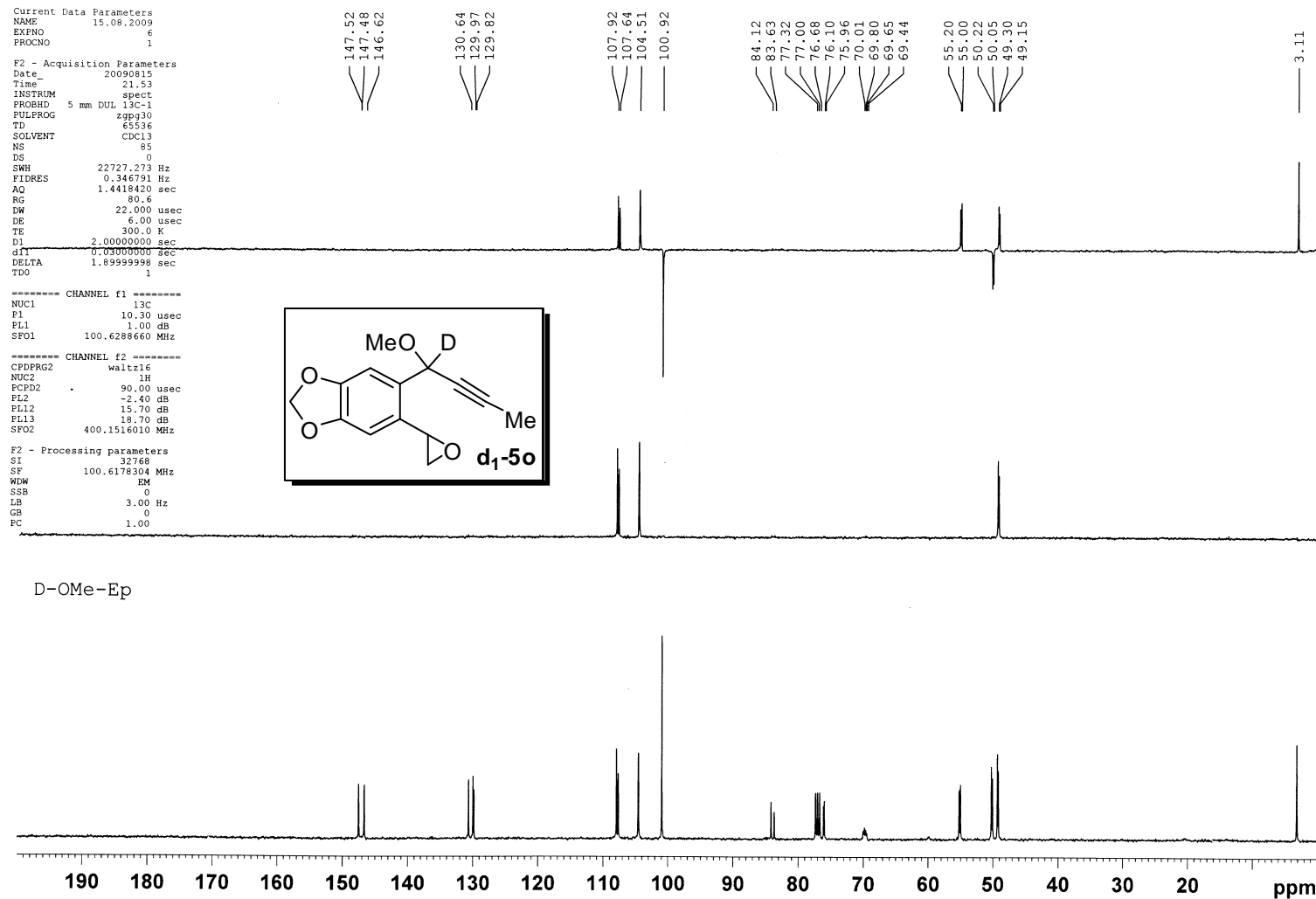


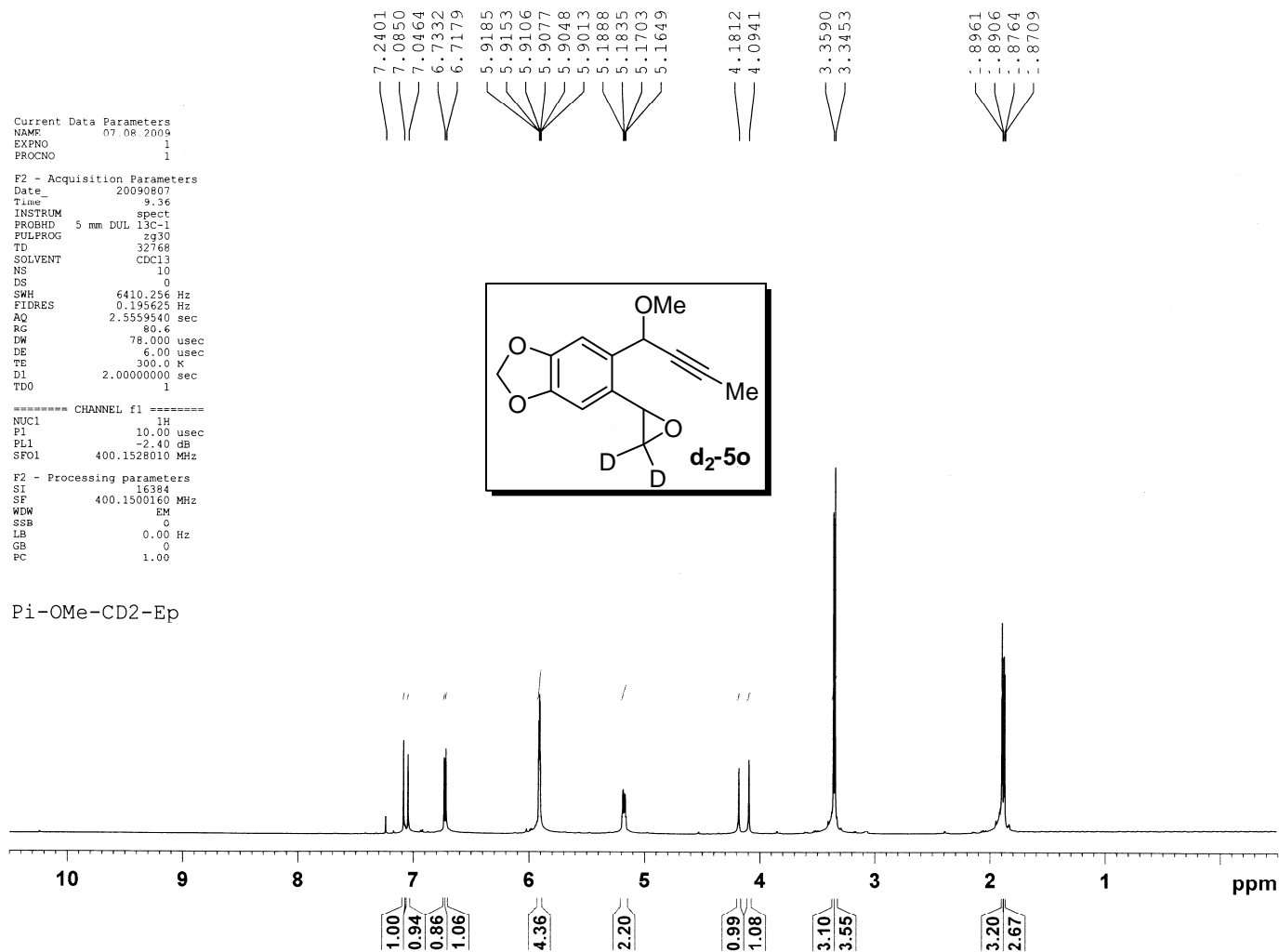


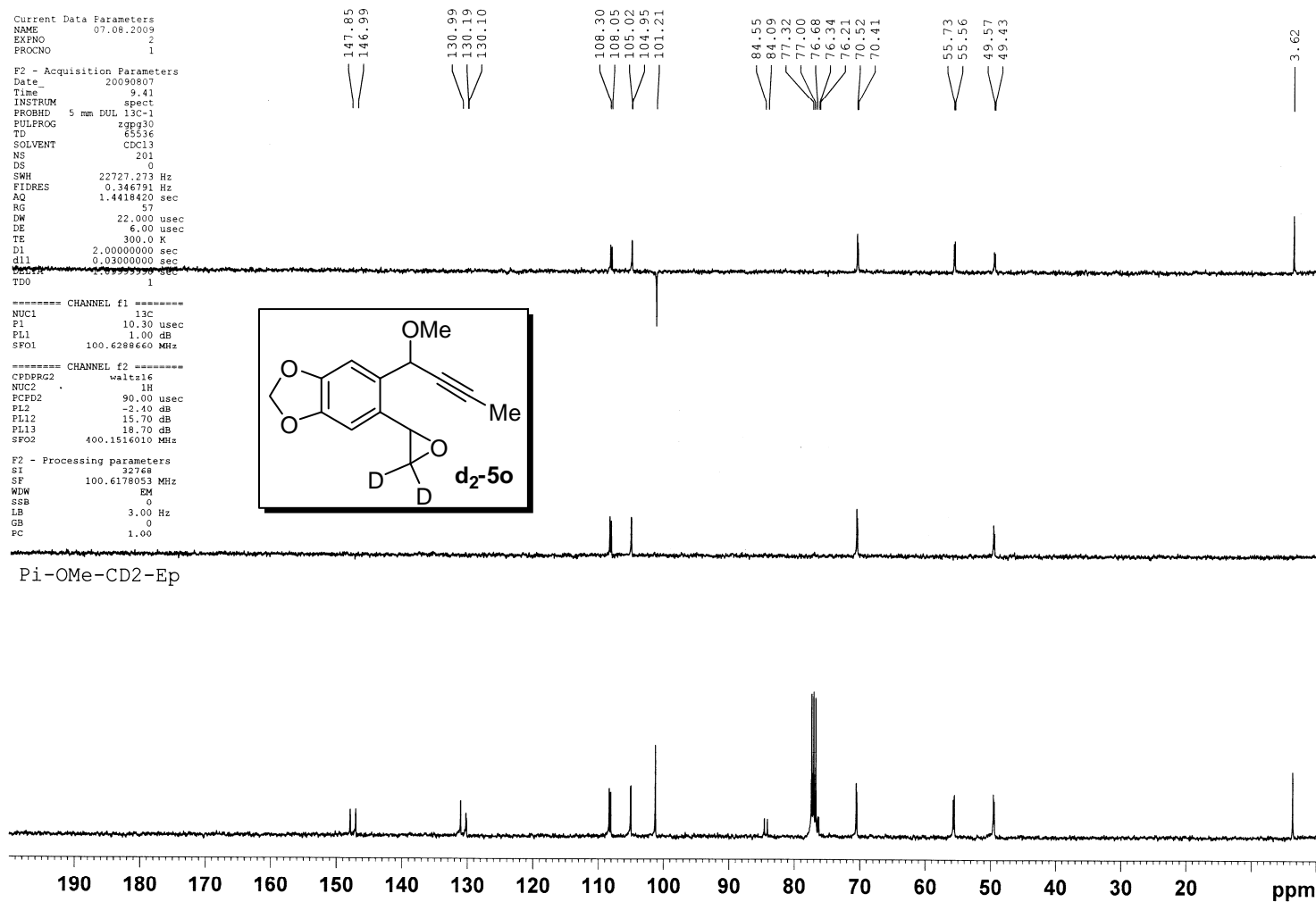


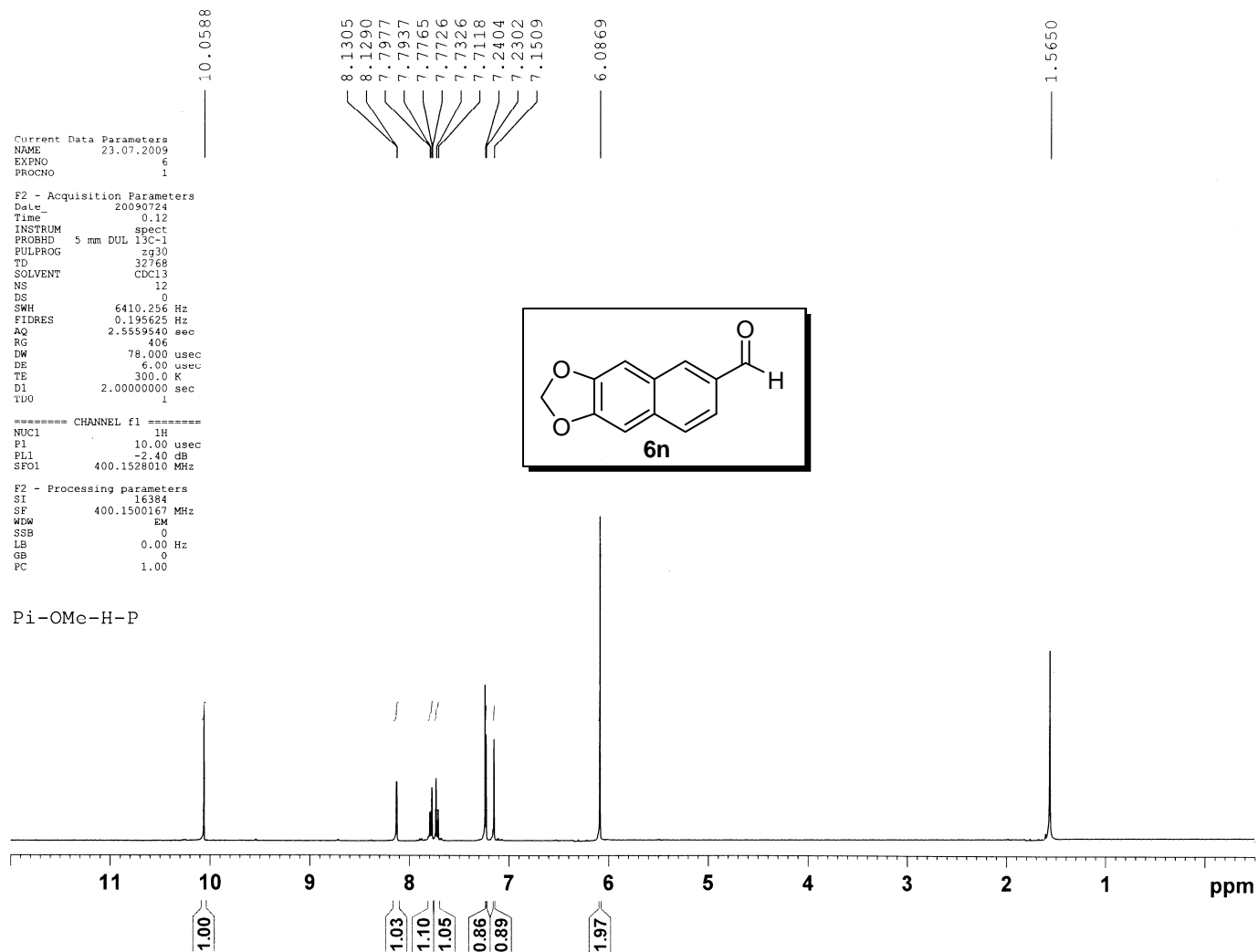


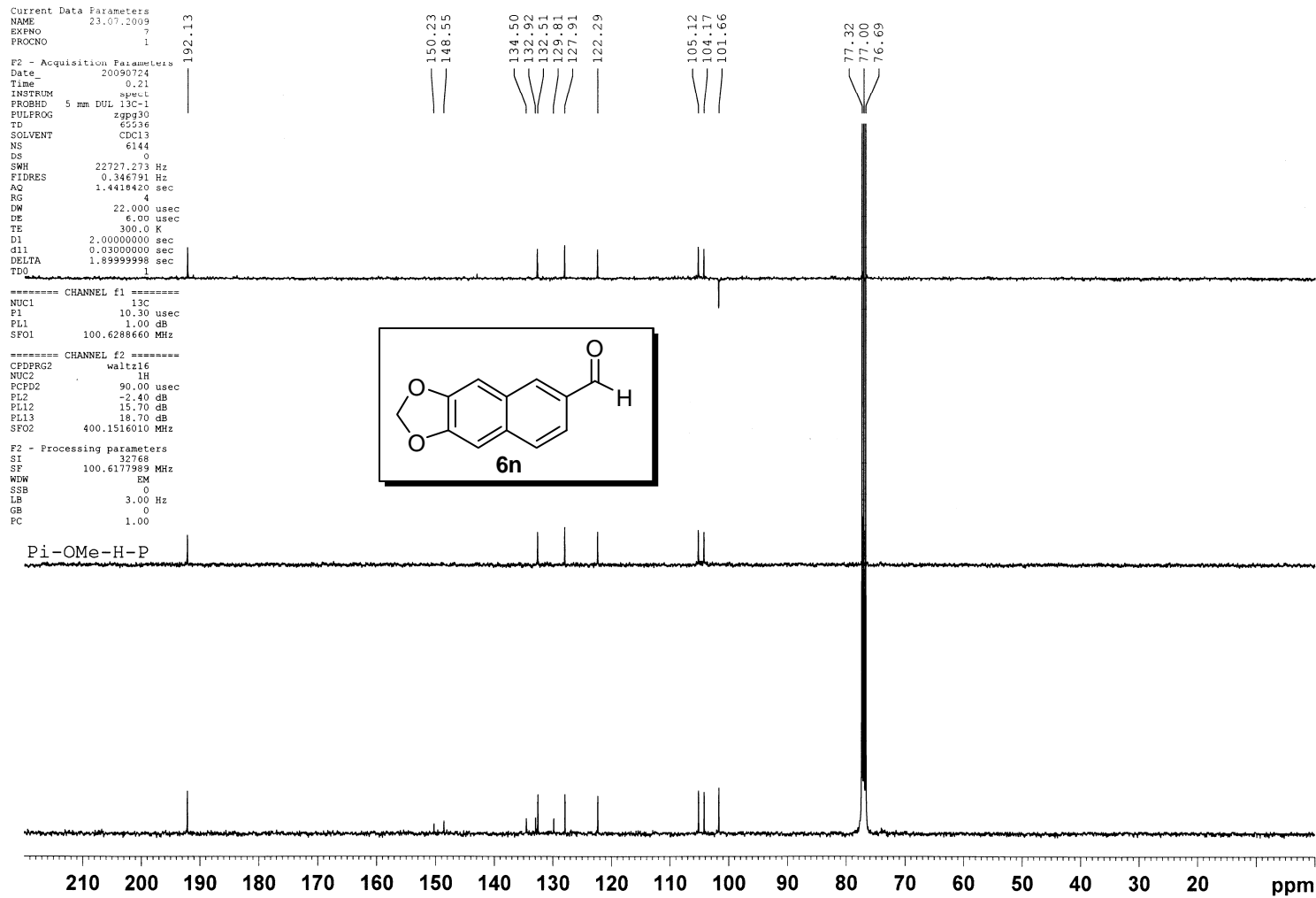


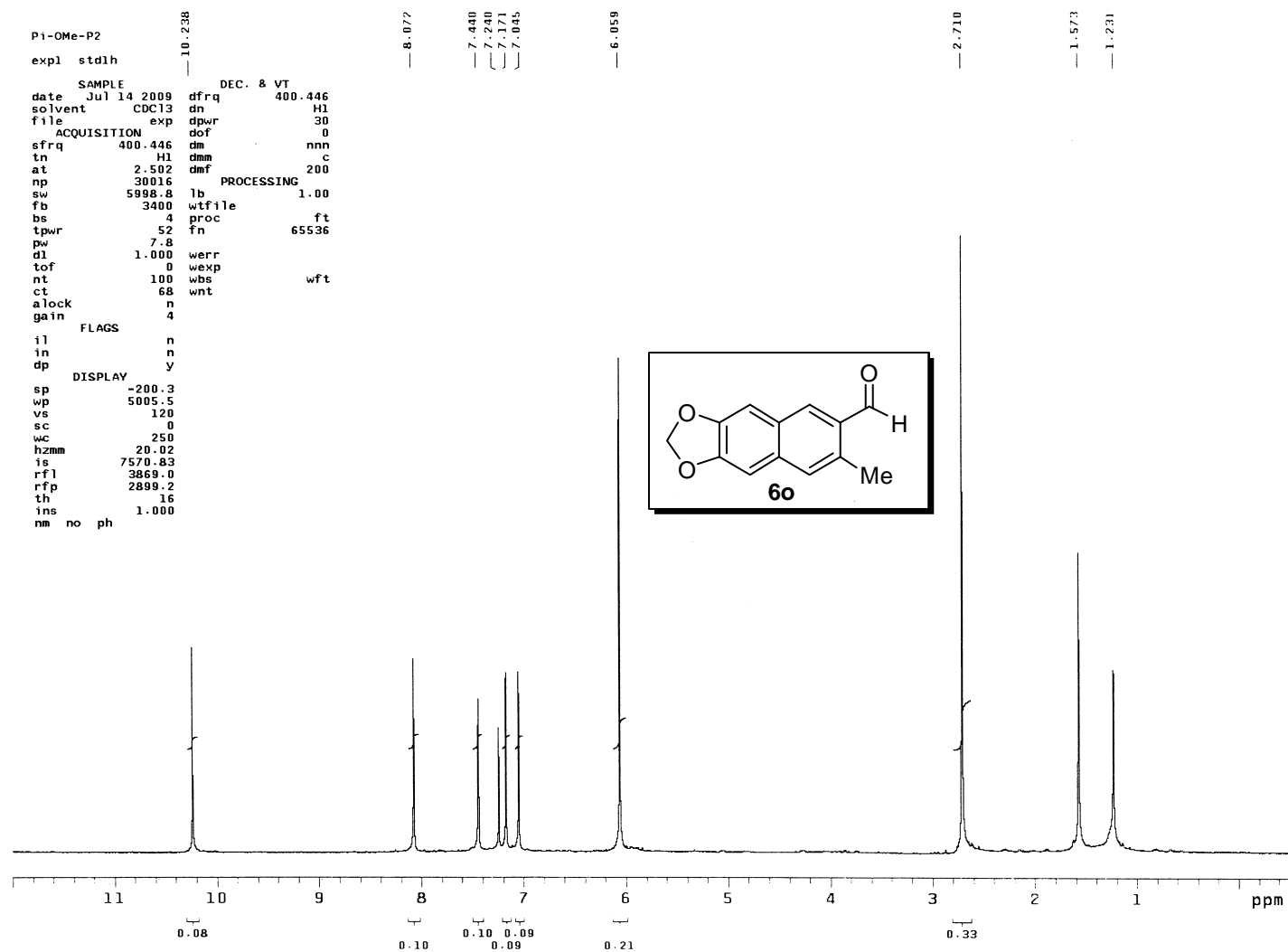
















```

Current Data Parameters
ME RC-5-42-P
FWD 1
OCND 1

- Acquisition Parameters
fe_ 20090723
me 12.20
STRUM spec
OBHD 5 mm QNP 1H/1
ILPROG zgpg
32768
NUC1 13C
F1 101.25
F2 101.25
M 45045.047 Hz
DRES 1.374666 Hz
1 0.3637748 sec
1 1024
1 11.100 usec
1 6.50 usec
1 302.7 K
1 3.50000000 sec
1 0.03000000 sec
1 3.40000010 sec
REST 0.00000000 sec
WRK 0.01500000 sec

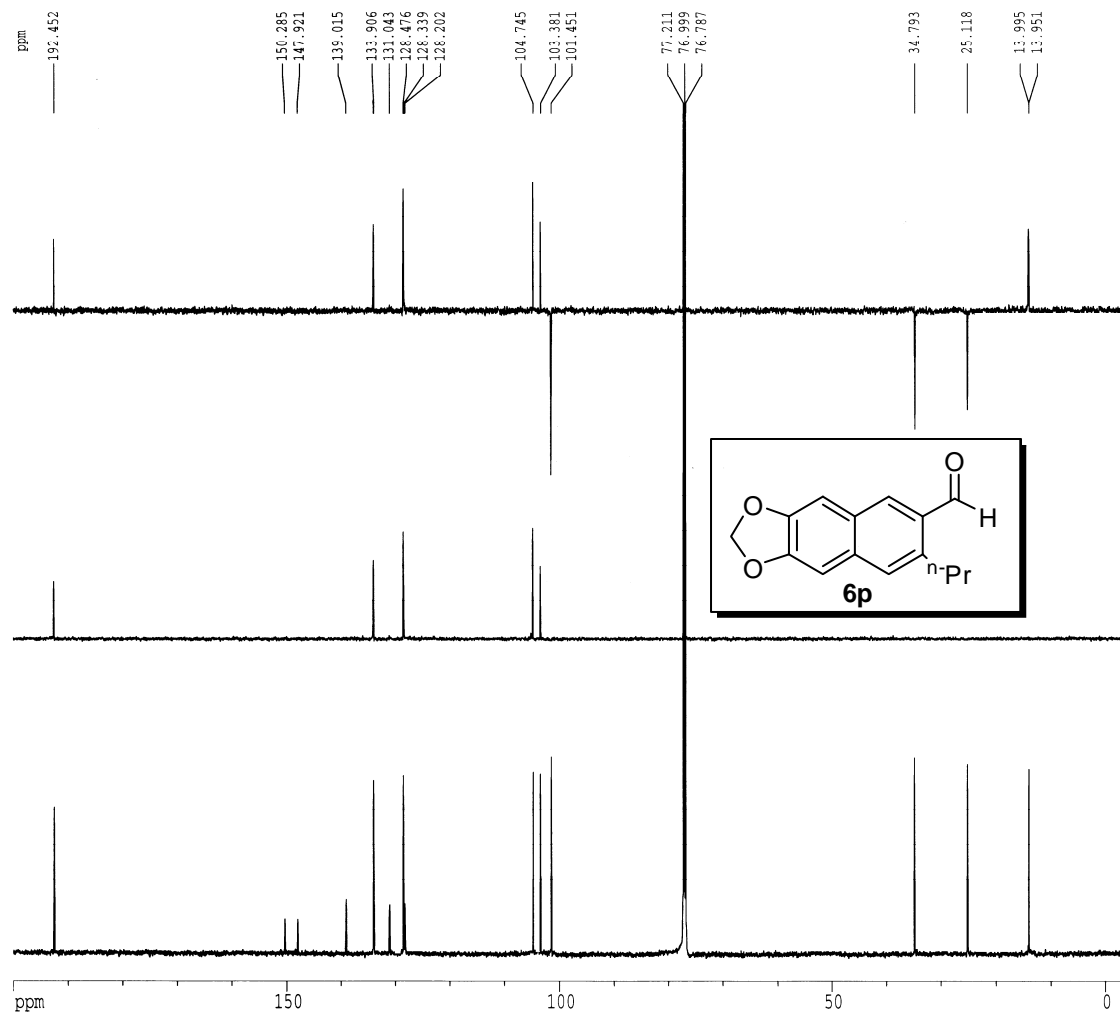
===== CHANNEL f1 =====
IC1 13C
1 4.50 usec
1 0.00 dB
V1 150.6855336 MHz

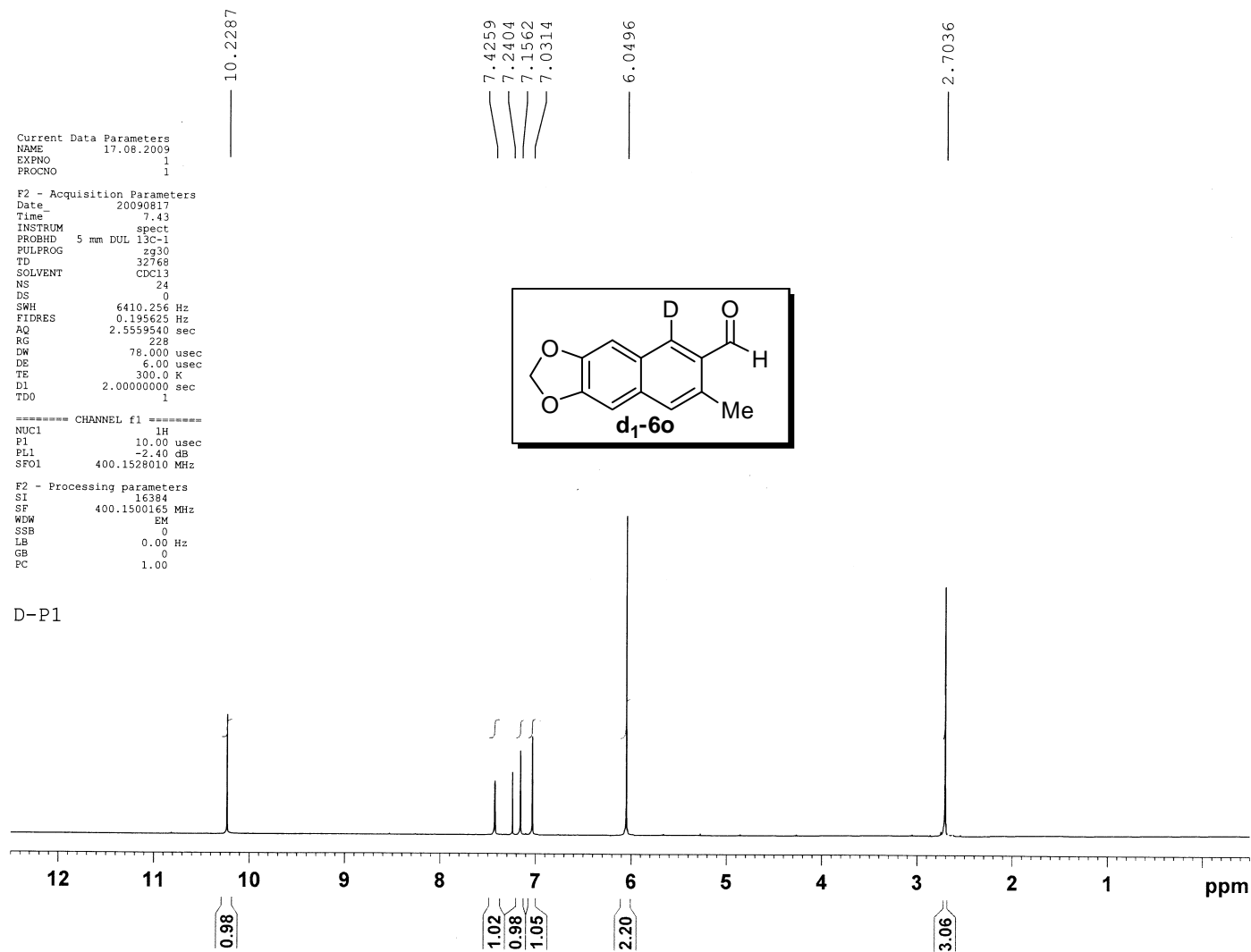
===== CHANNEL f2 =====
DPRG2 waltz16
IC2 1H
PD2 92.00 usec
2 120.00 dB
12 11.30 dB
13 14.00 dB
V2 599.2029960 MHz

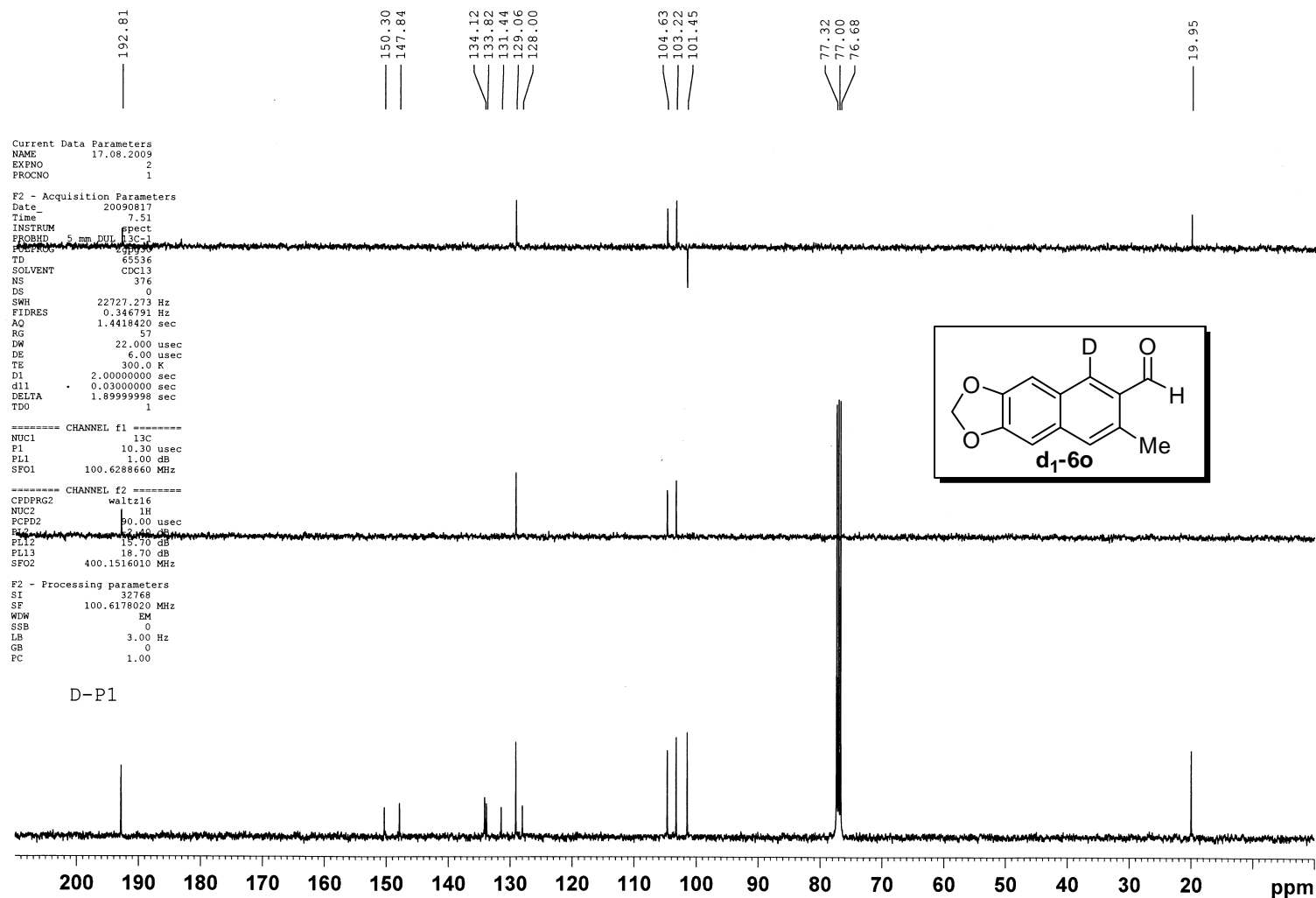
- Processing parameters
65536
150.6689620 MHz
M BM
1 0
1 3.00 Hz
1 0
1 0.50

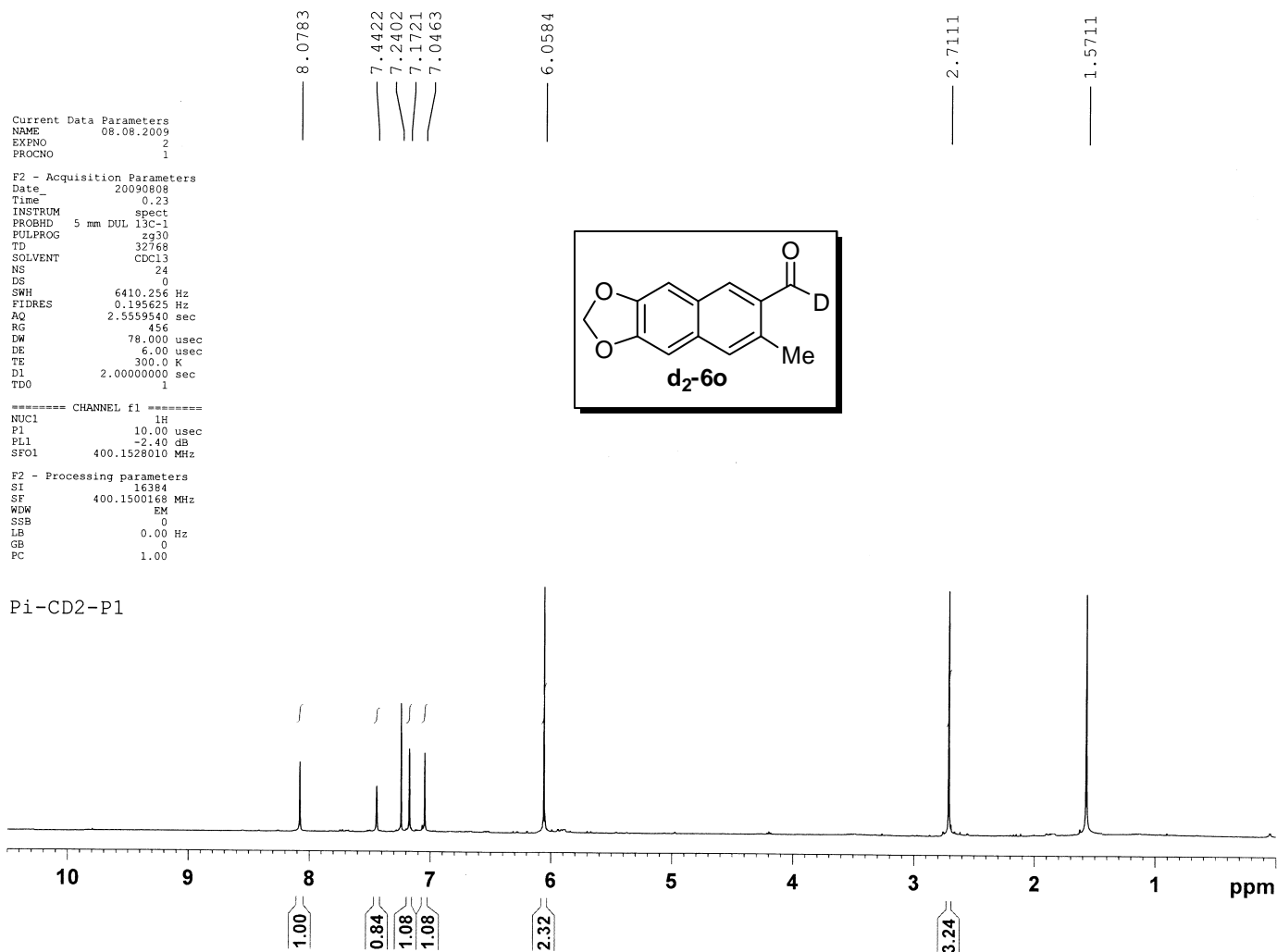
- NMR plot parameters
1 20.00 cm
1 20.00 cm
P 200.000 ppm
1P 30133.79 Hz
1P -5.000 ppm
1 753.34 Hz
MCM 10.25000 ppm/cm
CM 1544.35693 Hz/cm

```









```

Current Data Parameters
=====
F1  RCS-54-P1
PNO  2
JCNO  1

- Acquisition Parameters
=====
re_  20090807
ne  16.37
STRUM  spect
SFO  5 mm QNP 1H/1
LPROG  zgpg
32768
LVENT  CDCl3
10240
0

f1  45045.047 Hz
DRBS  1.374666 Hz
0.3637748 sec
1024
11.100 usec
6.50 usec
302.5 K
3.50000000 sec
1  0.03000000 sec
LTA  3.40000010 sec
REST  0.00000000 sec
KRC  0.01500000 sec

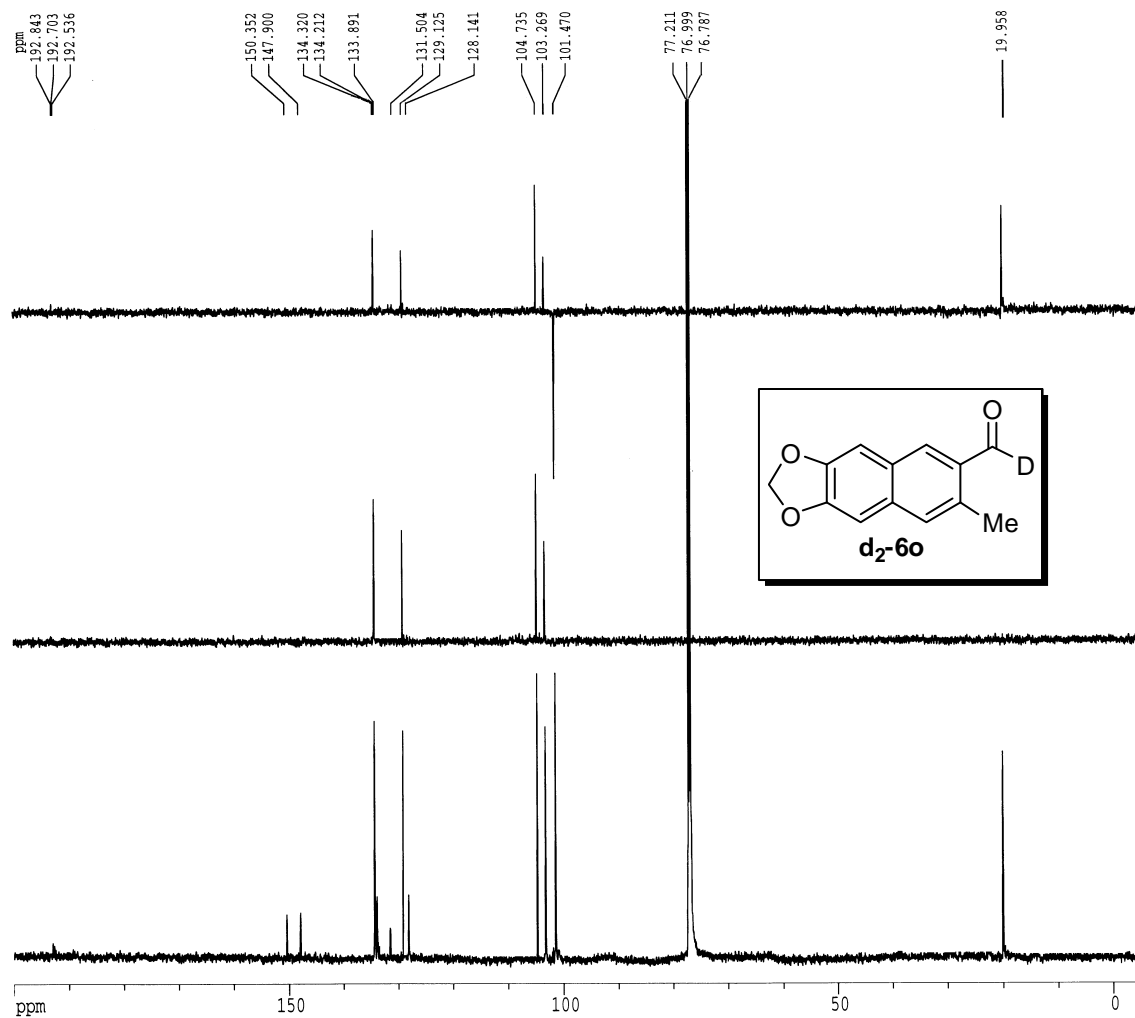
===== CHANNEL f1 =====
C1  13C
4.50 usec
1  0.00 dB
O1  150.6855336 MHz

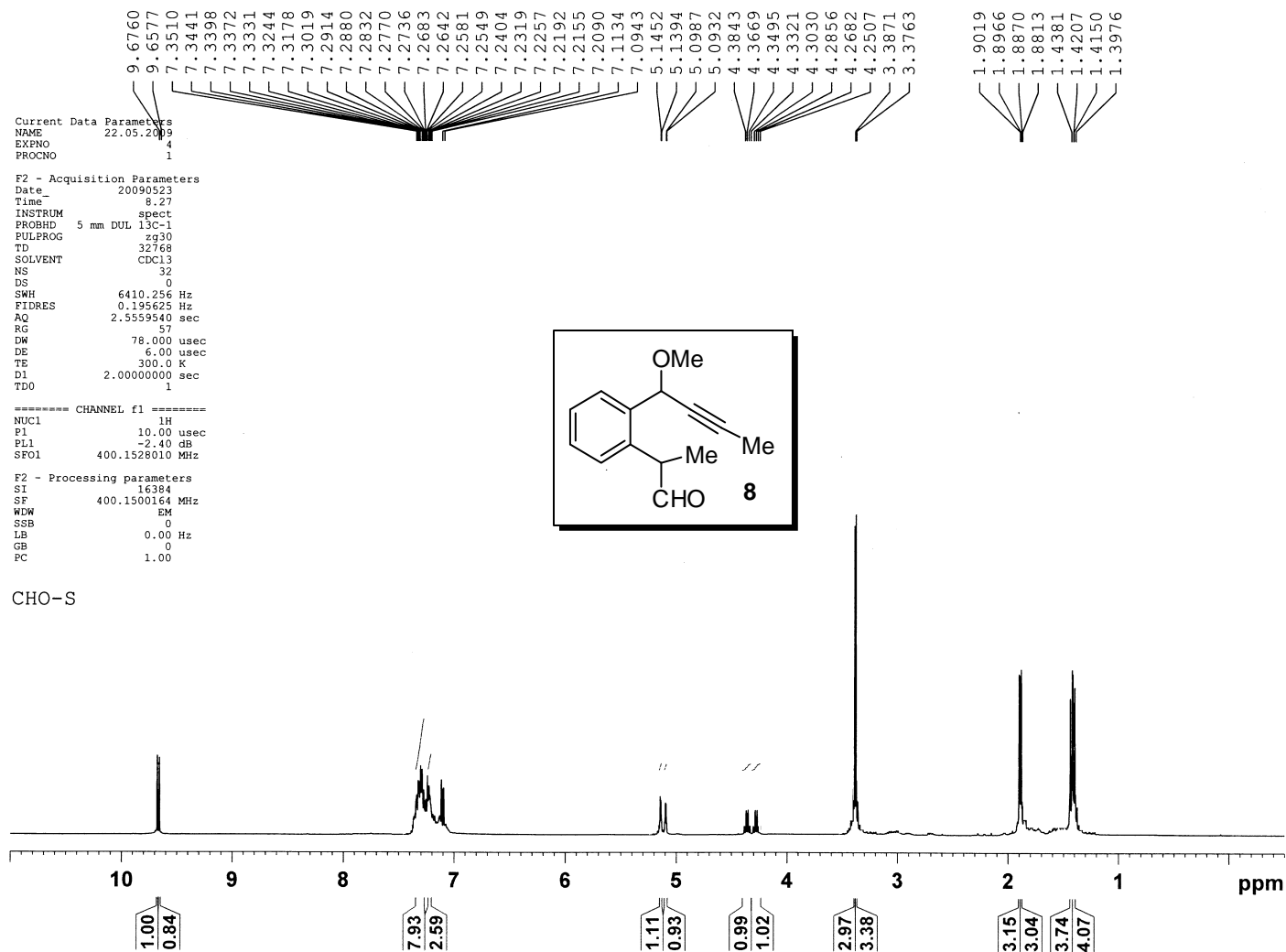
===== CHANNEL f2 =====
DPRG2  waltz16
C2  1H
PD2  92.00 usec
2  120.00 dB
12  11.30 dB
13  14.00 dB
O2  599.2029960 MHz

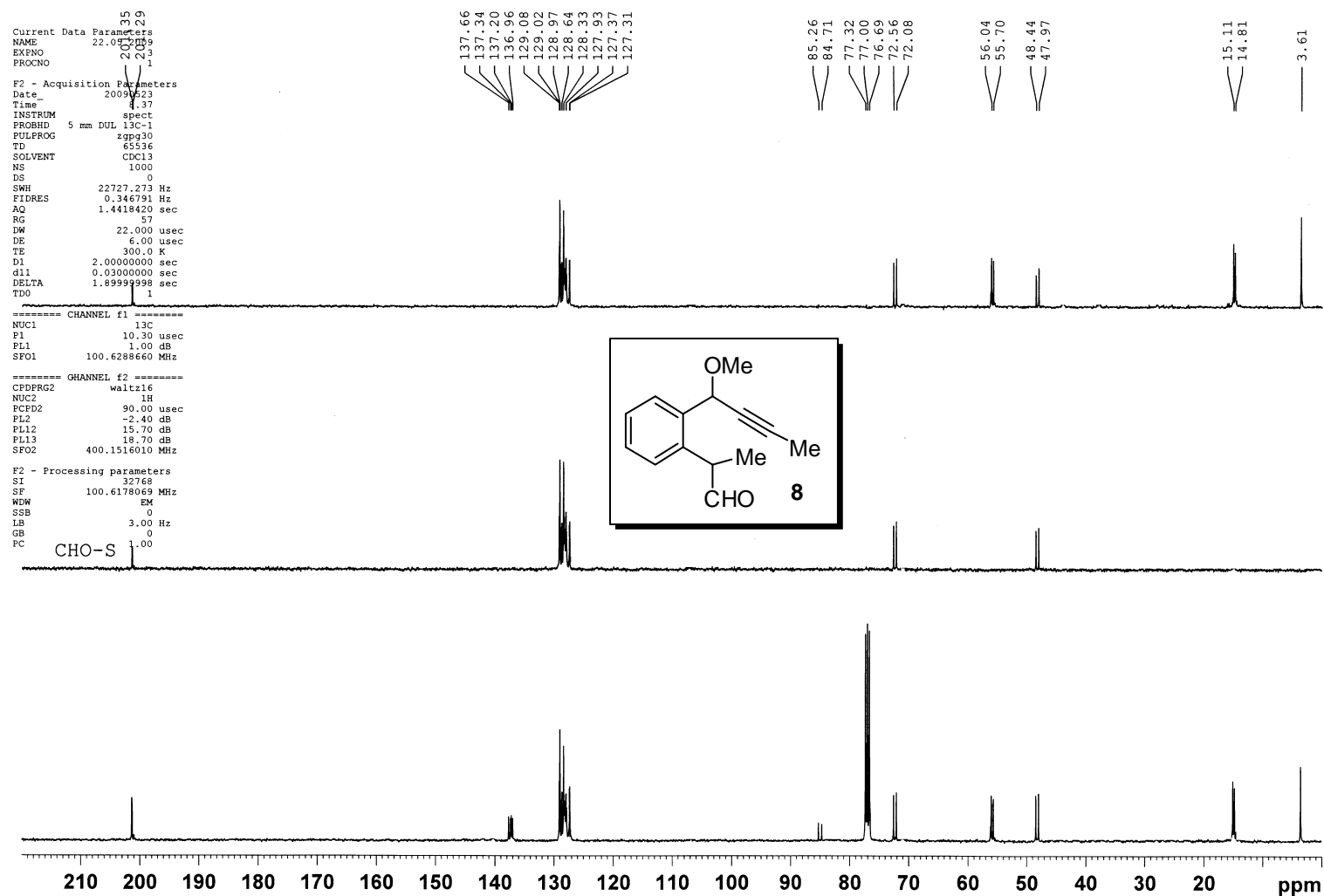
- Processing parameters
=====
65536
150.6689606 MHz
W  EN
B  0
3.00 Hz
0
0.50

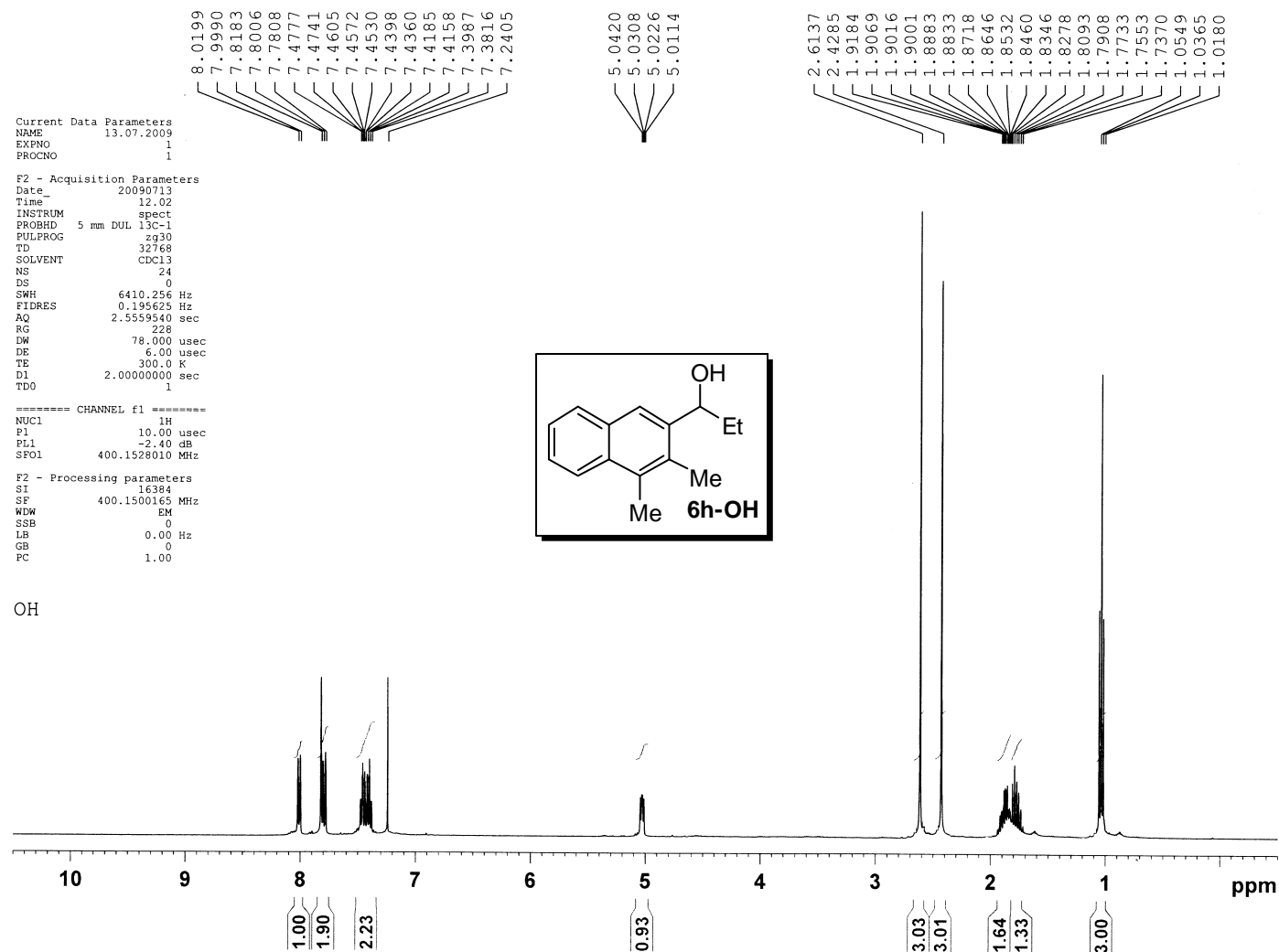
===== NMR plot parameters =====
20.00 cm
40.00 cm
P  200.000 ppm
30133.79 Hz
P  -5.000 ppm
-753.34 Hz
MCM  10.25000 ppm/cm
CM  1544.35693 Hz/cm

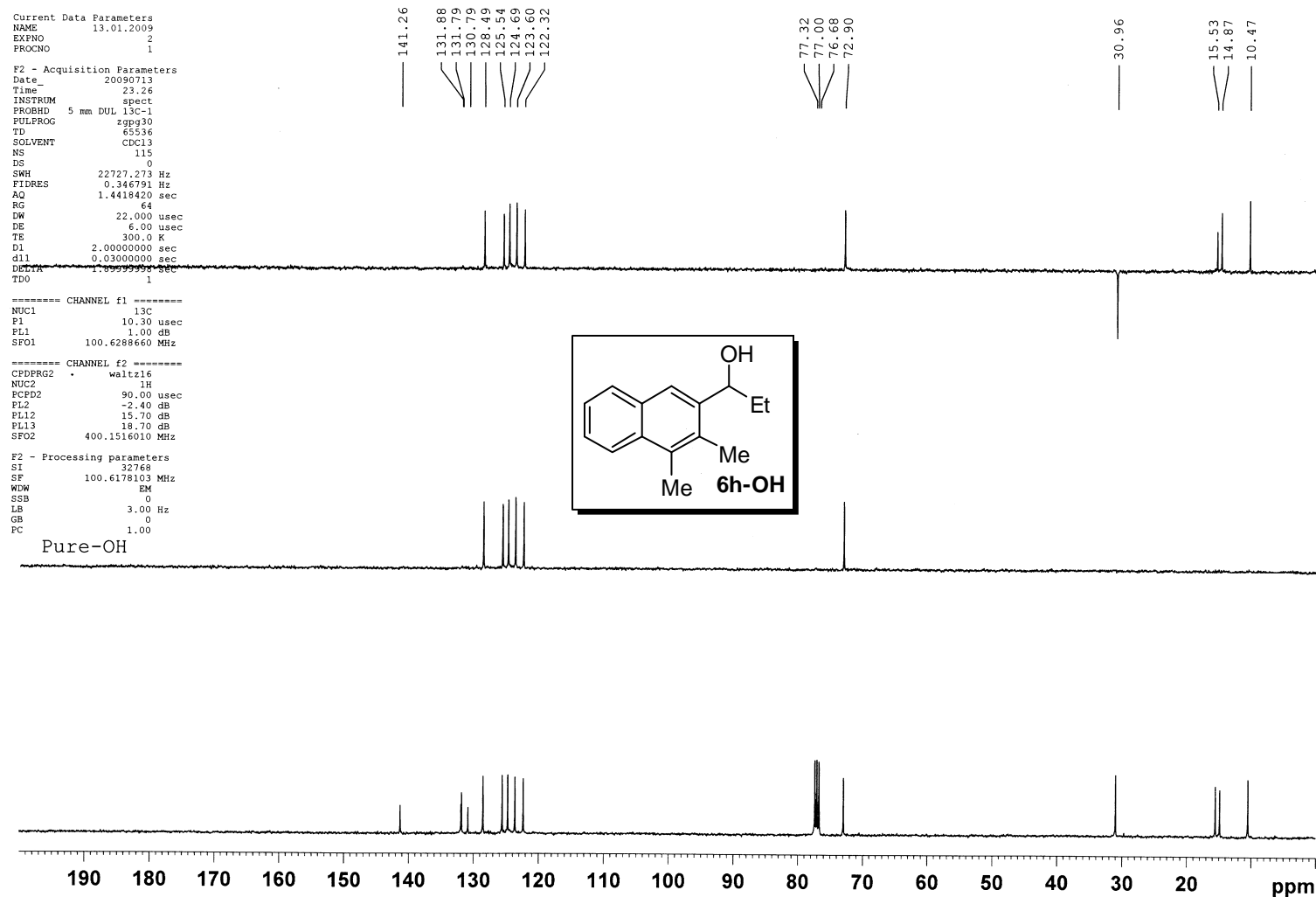
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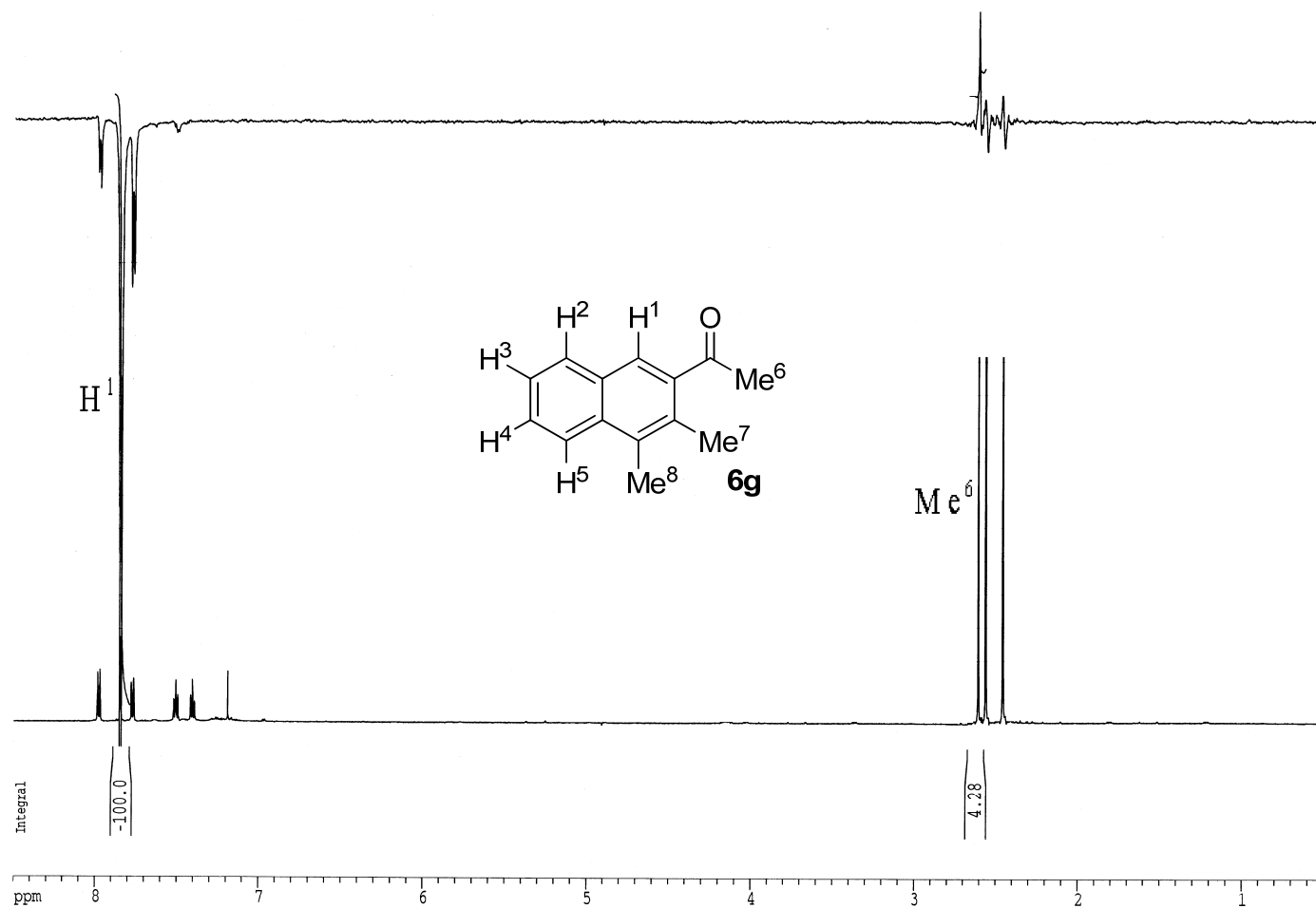


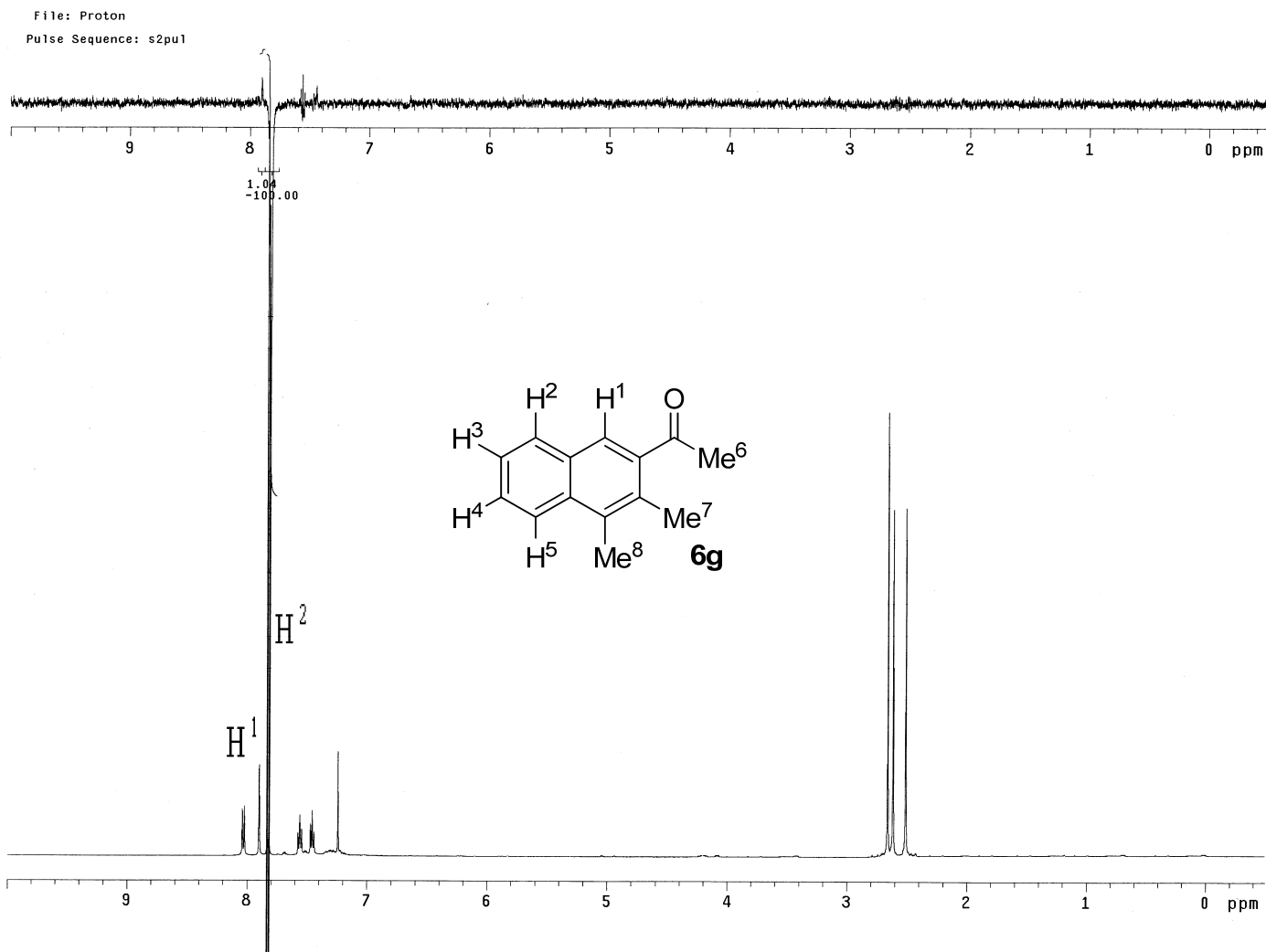


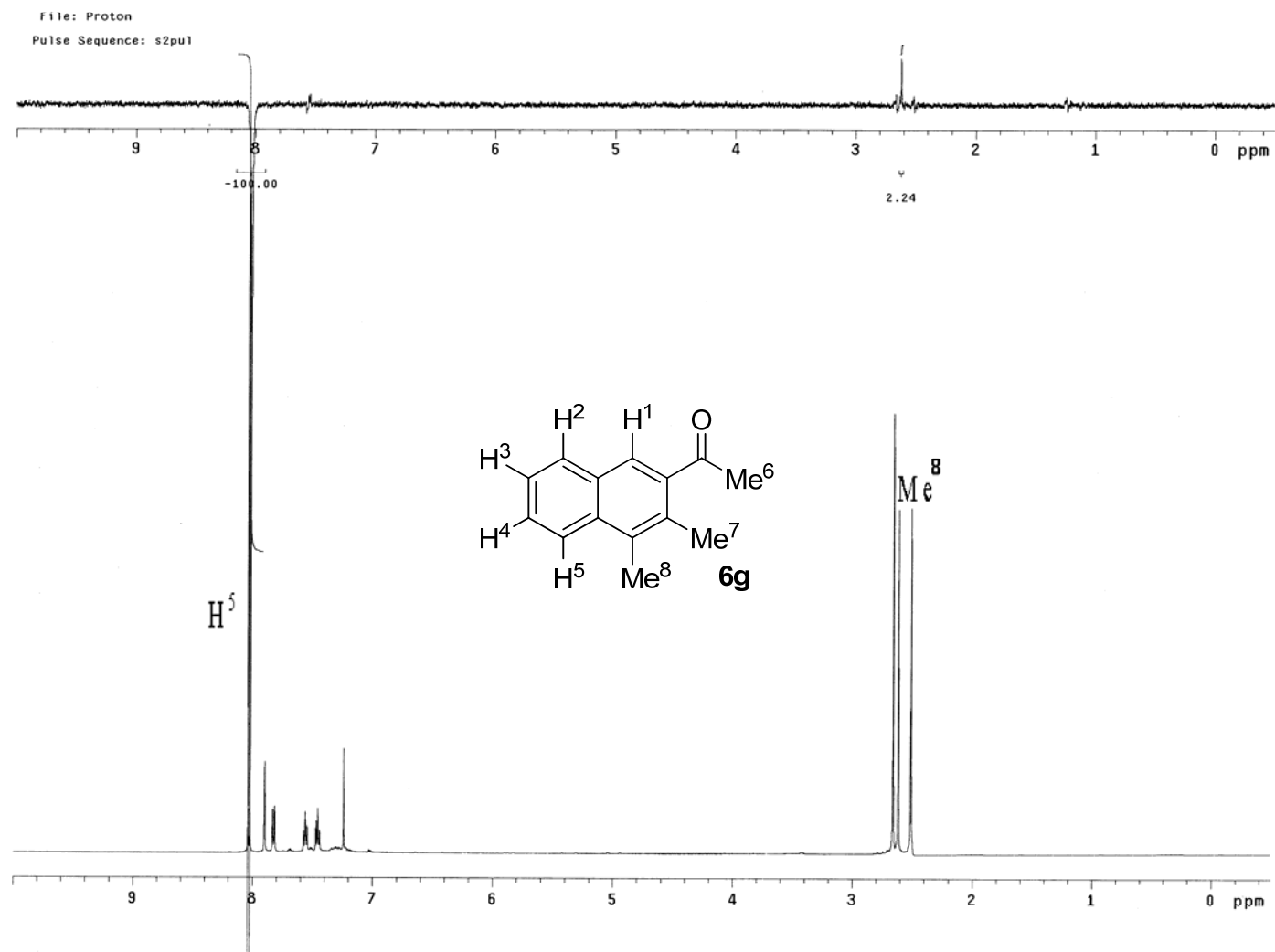


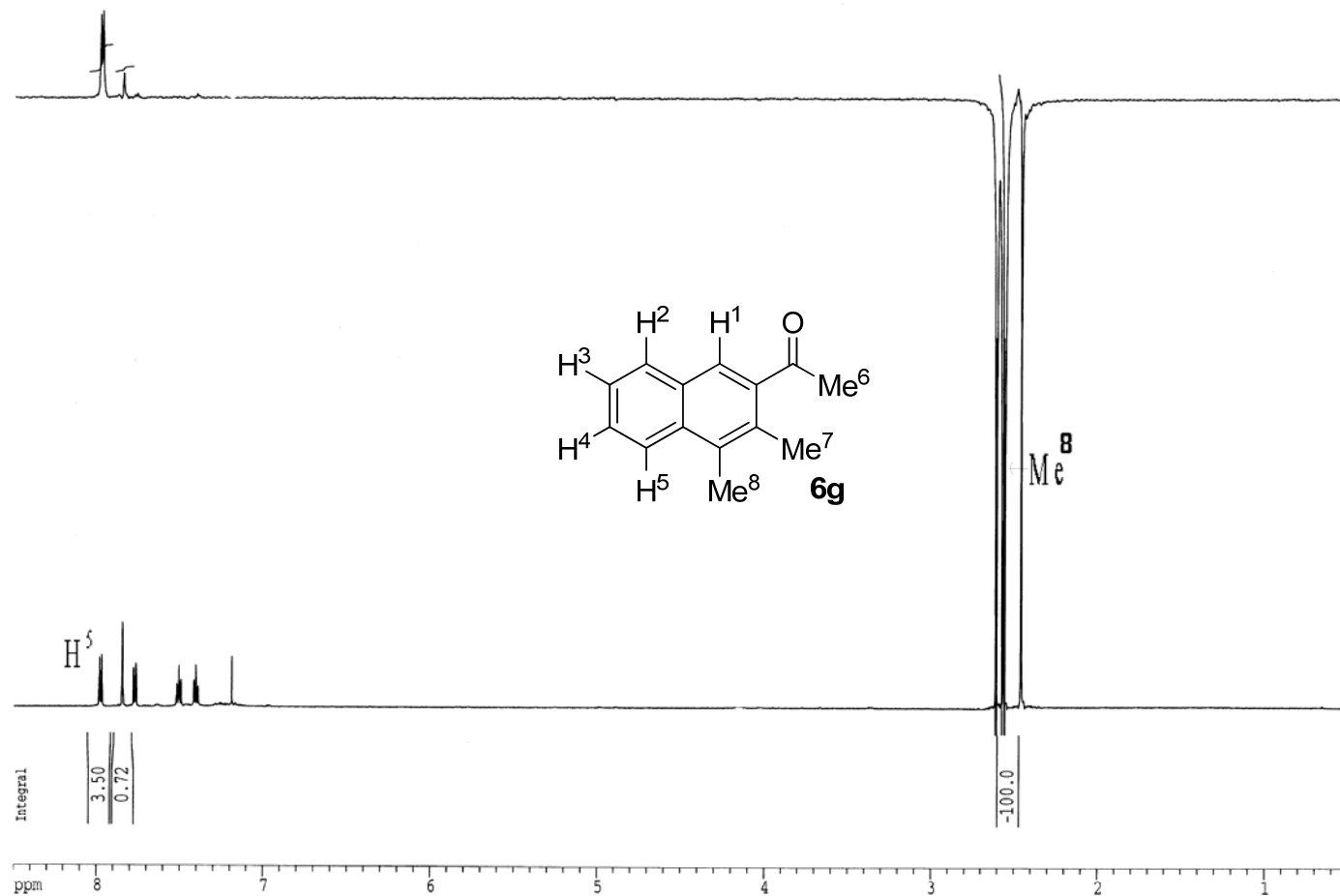


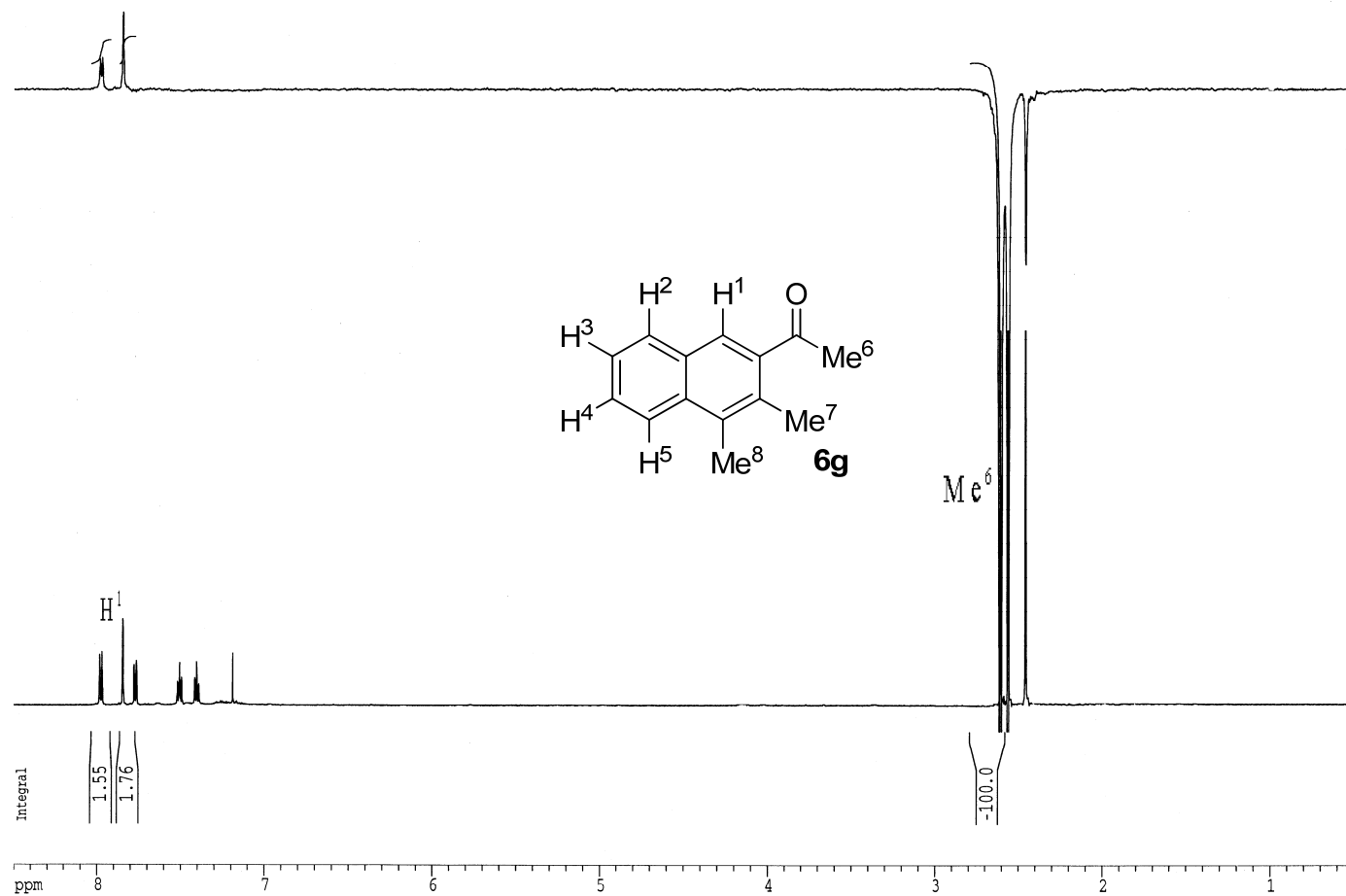


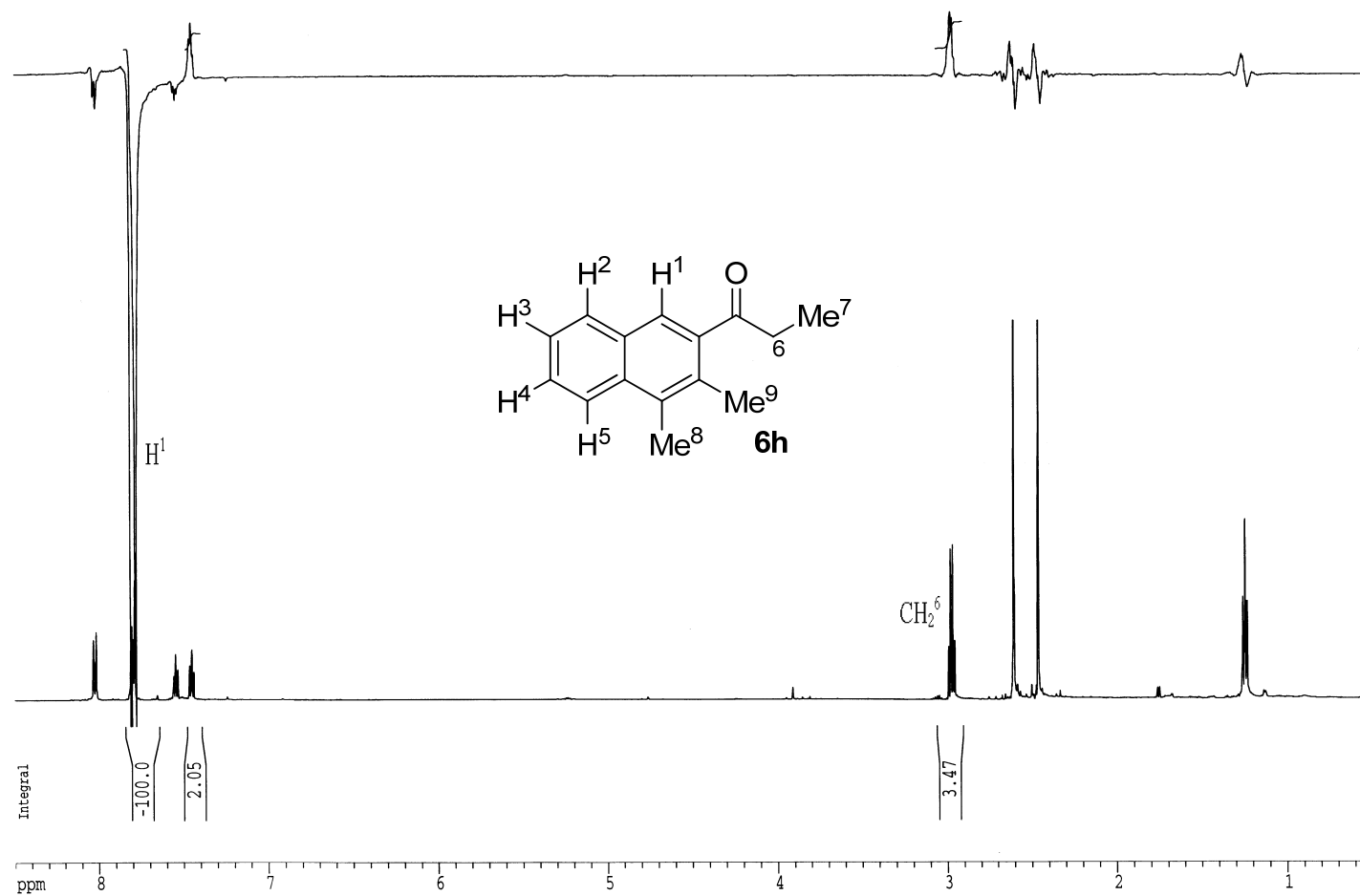


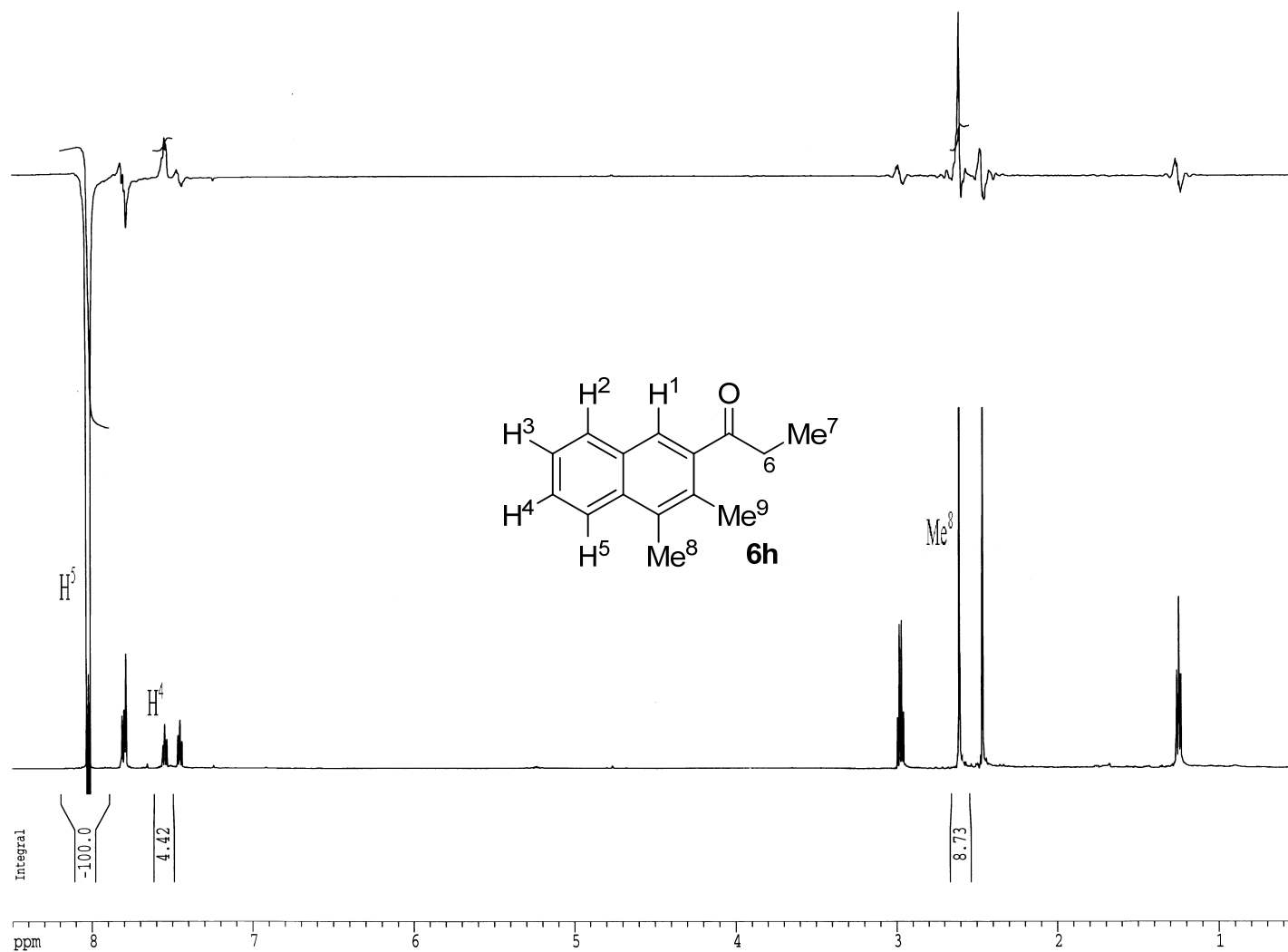


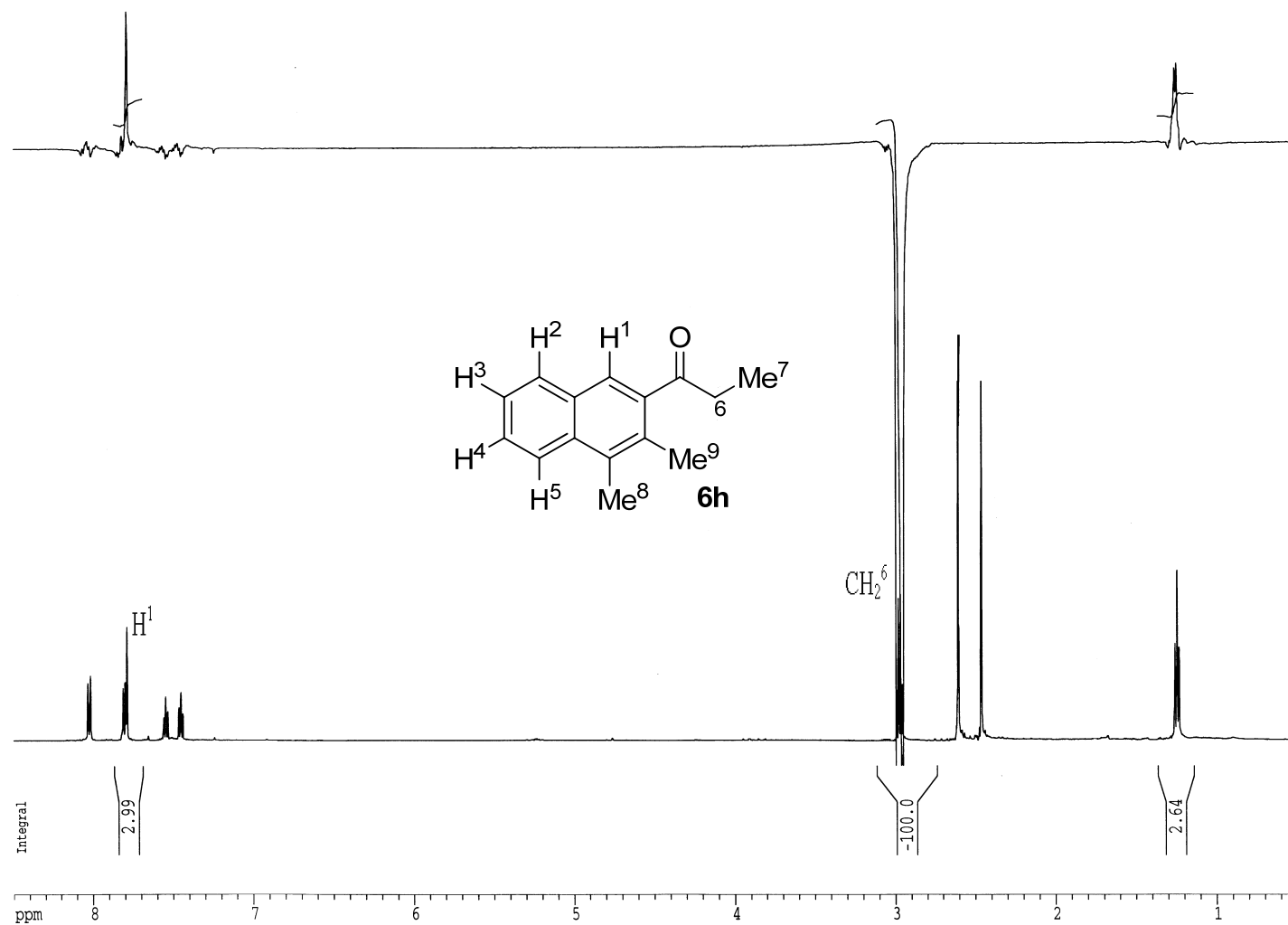


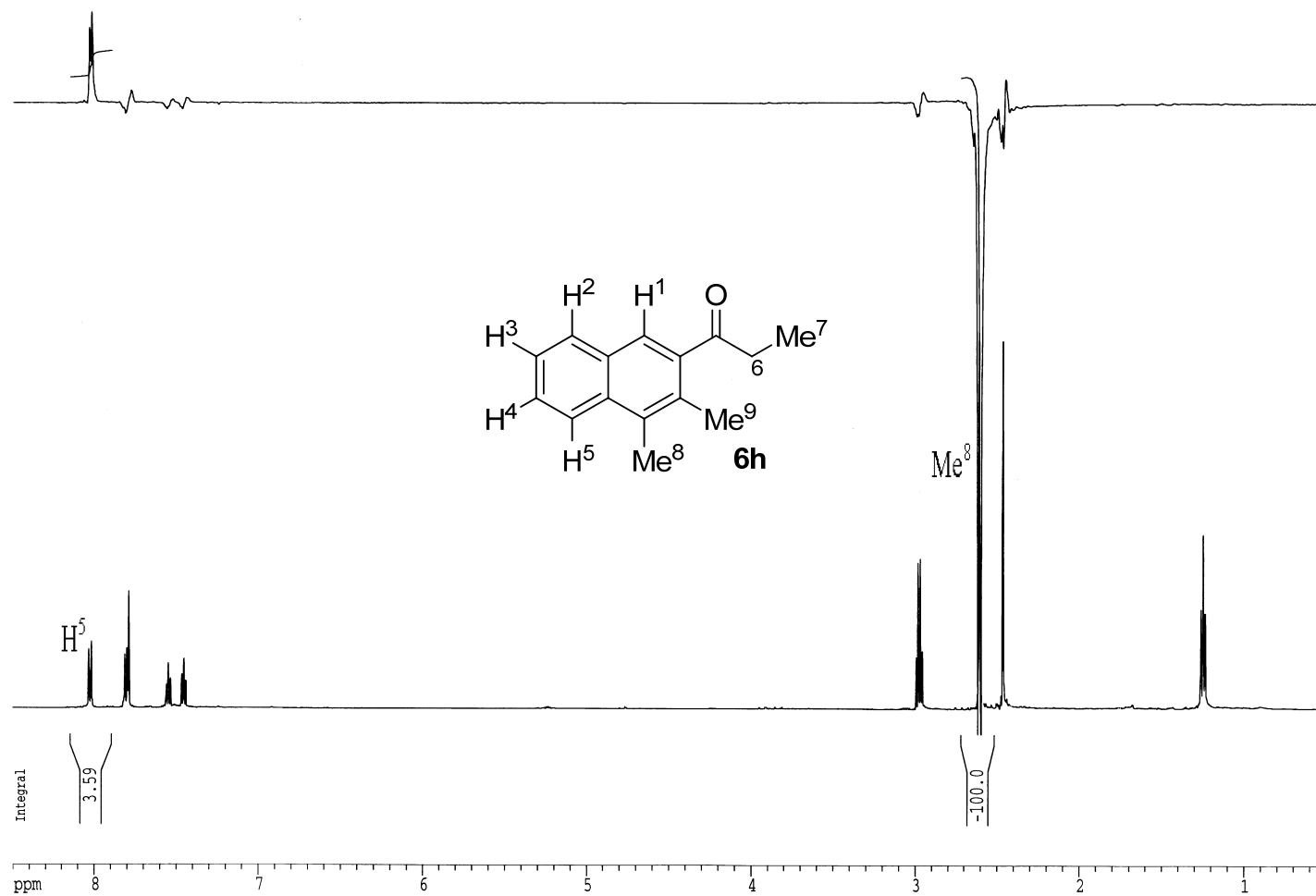


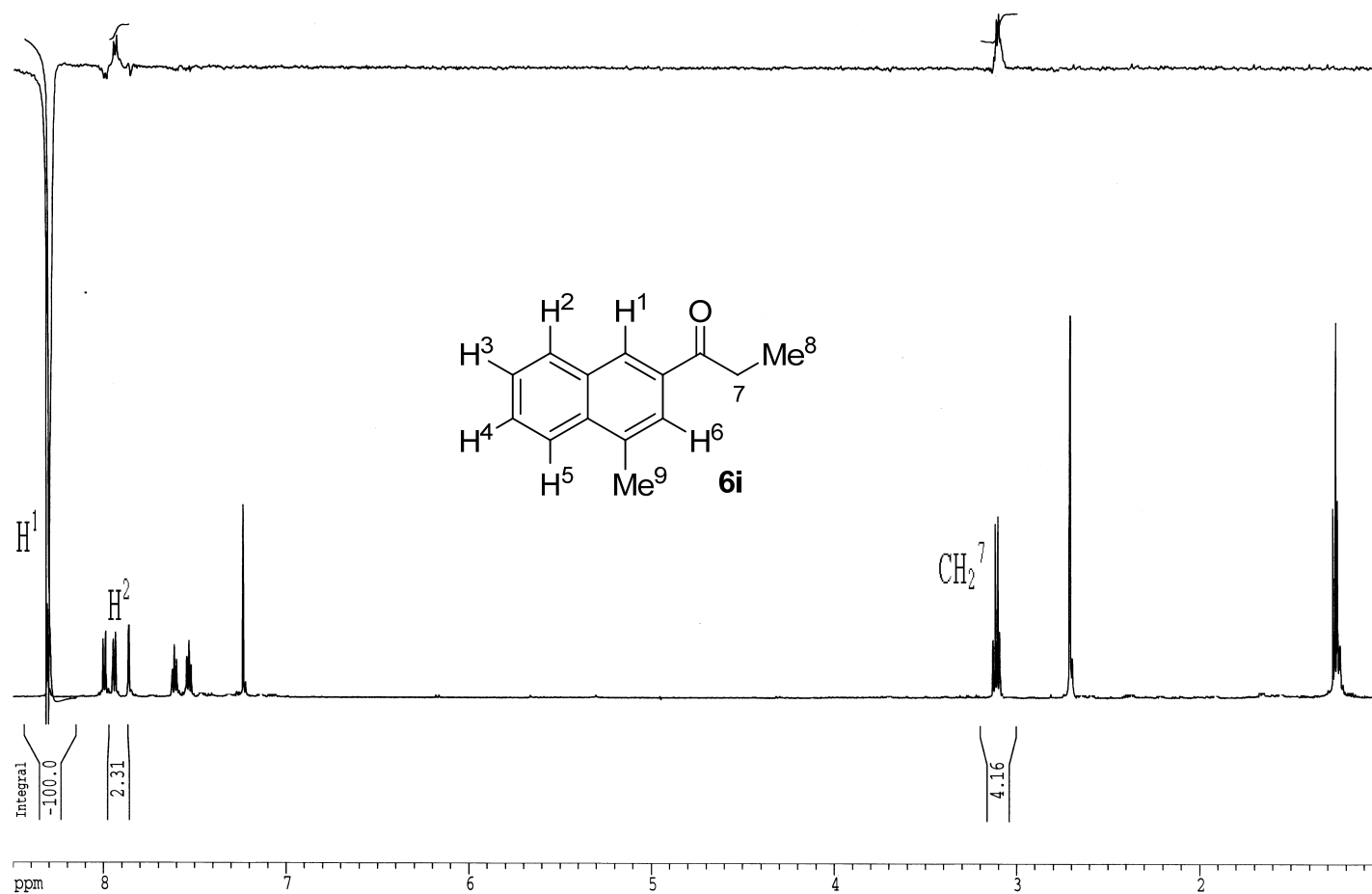


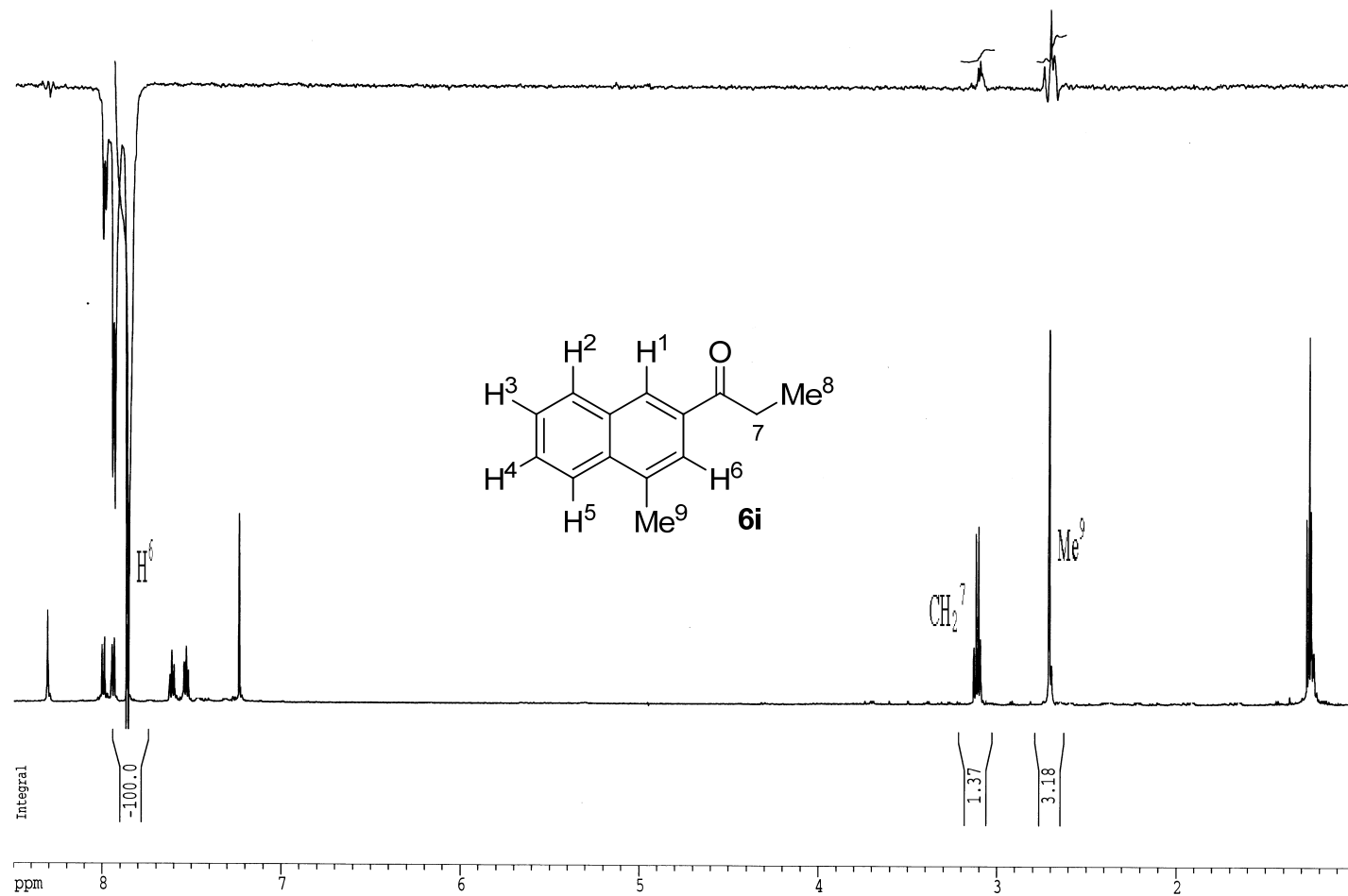


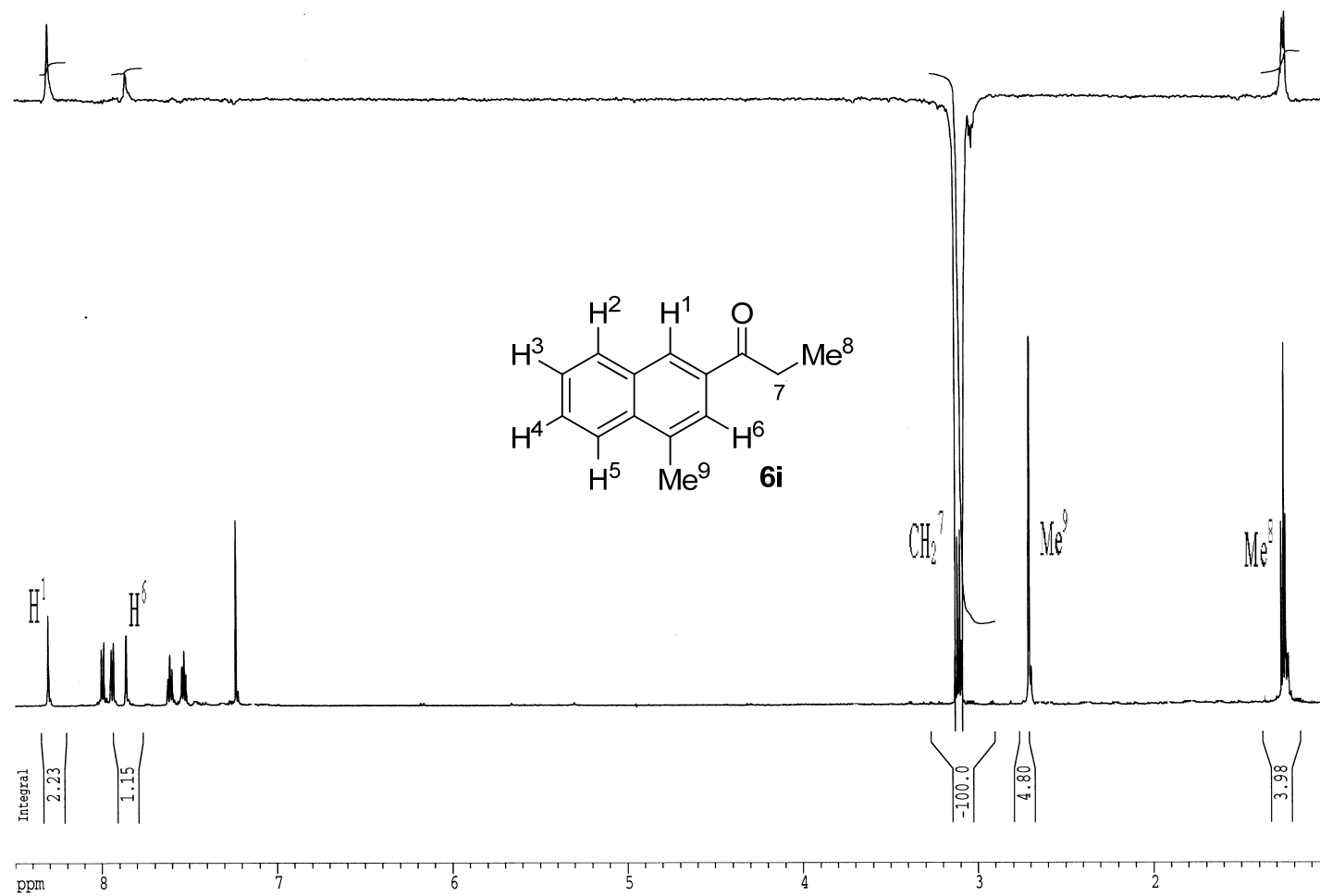


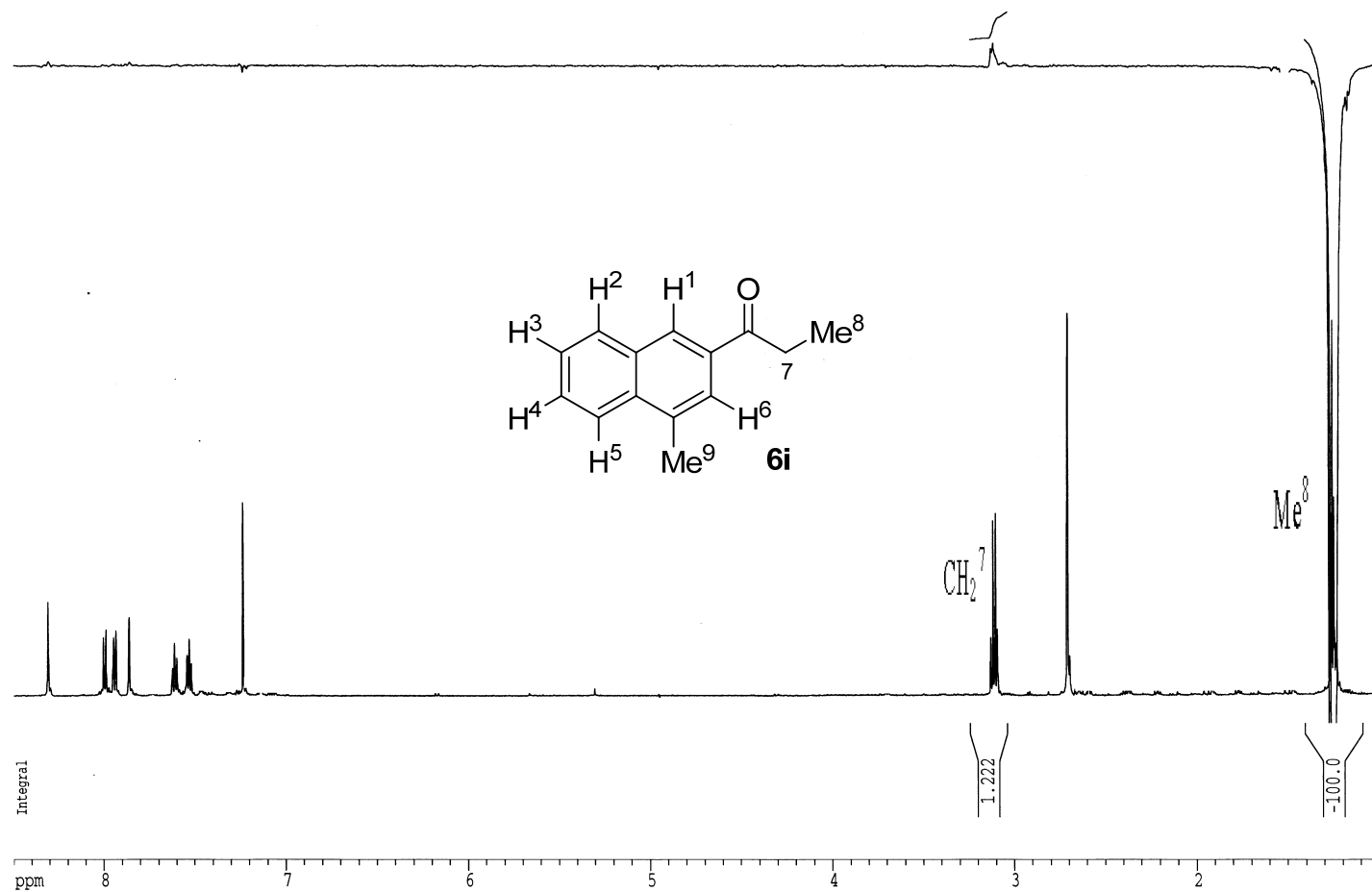


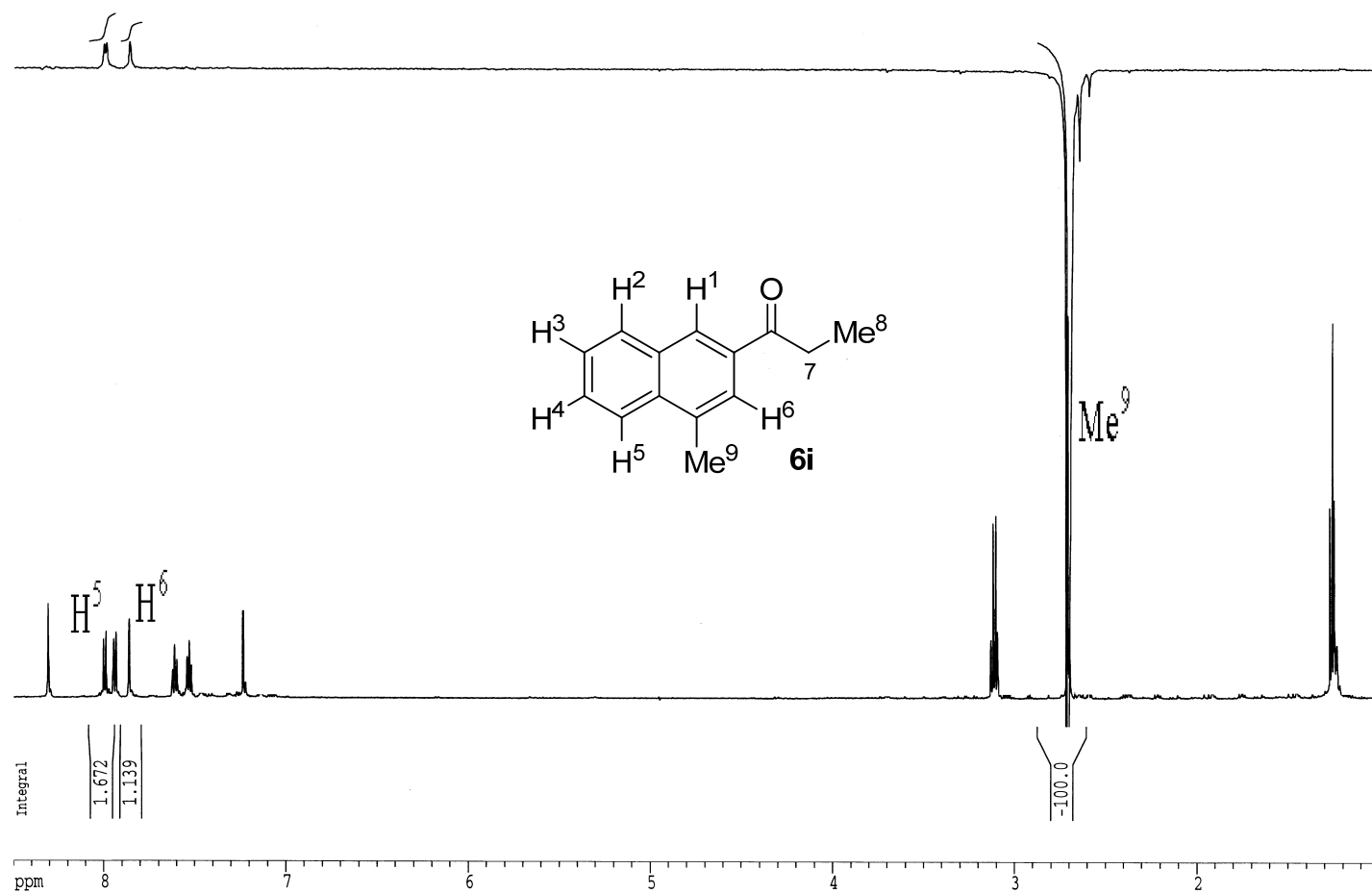












RC-4/256/P

File: Proton

Pulse Sequence: s2pu1

