

**Investigation on Amino-Heck Cyclization of 1-(2-Alkenylcyclohexyl)-ketone  
Diethyl Phosphinyloximes**

Sheng-Wei Cao and Jia-Liang Zhu\*

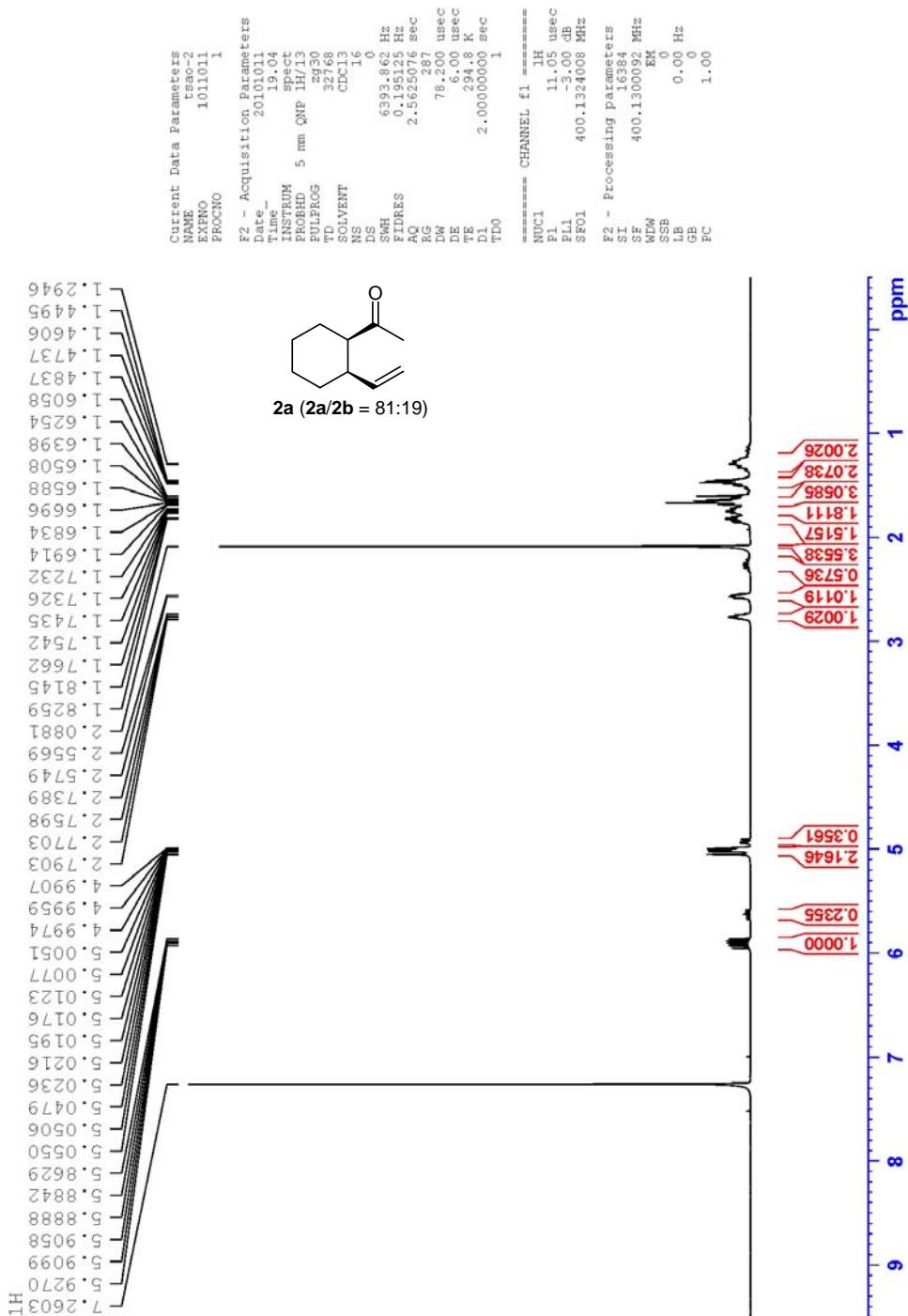
*Department of Chemistry, National Dong-Hwa University, Hualien 974, Taiwan*

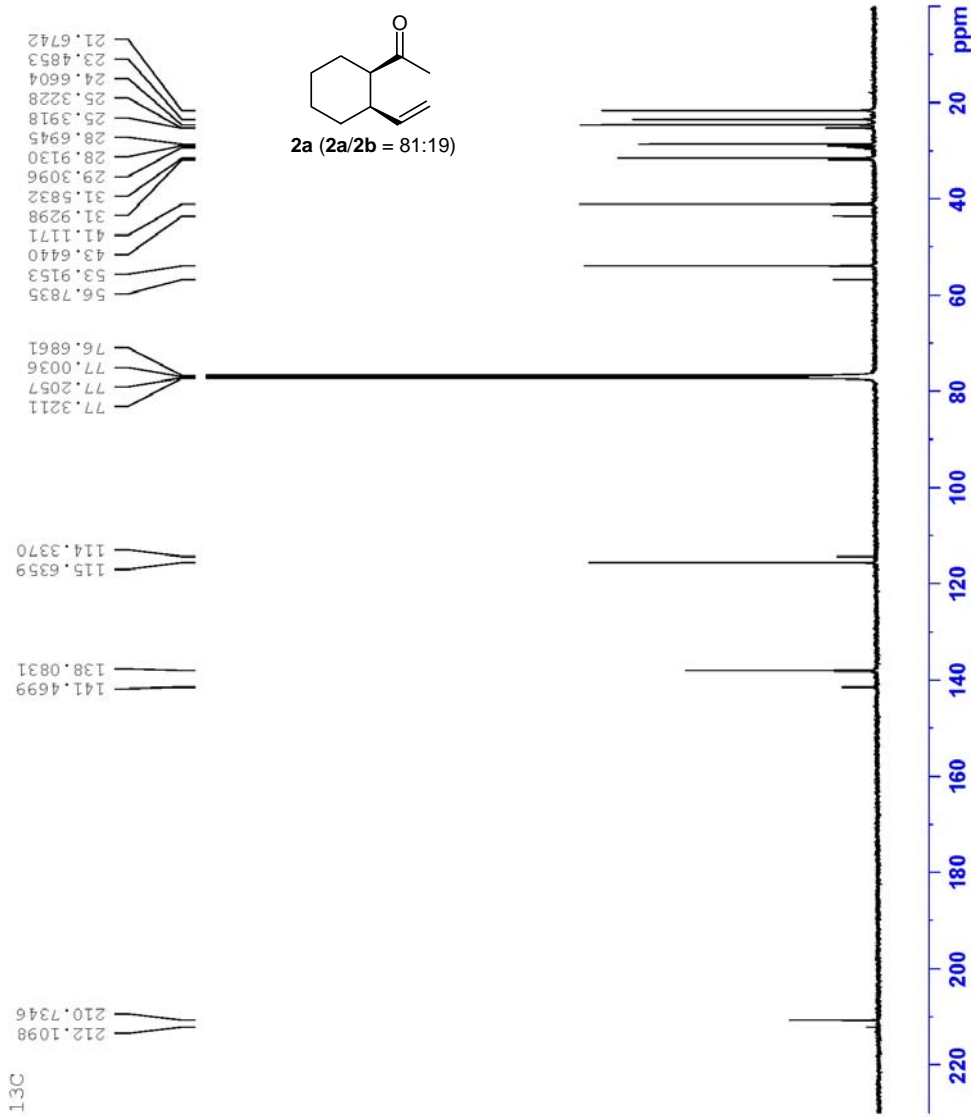
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***Support Information***

- A) <sup>1</sup>H and <sup>13</sup>C-NMR spectra of compounds **2a-g**, **3a-h**, **5a-d**, **6a/b**, **4a-g**, **7** and  
<sup>1</sup>H-NMR spectrum of **2h** .....S2-S66
- B) 2D-NOESY spectrum of **E-3e**.....S67

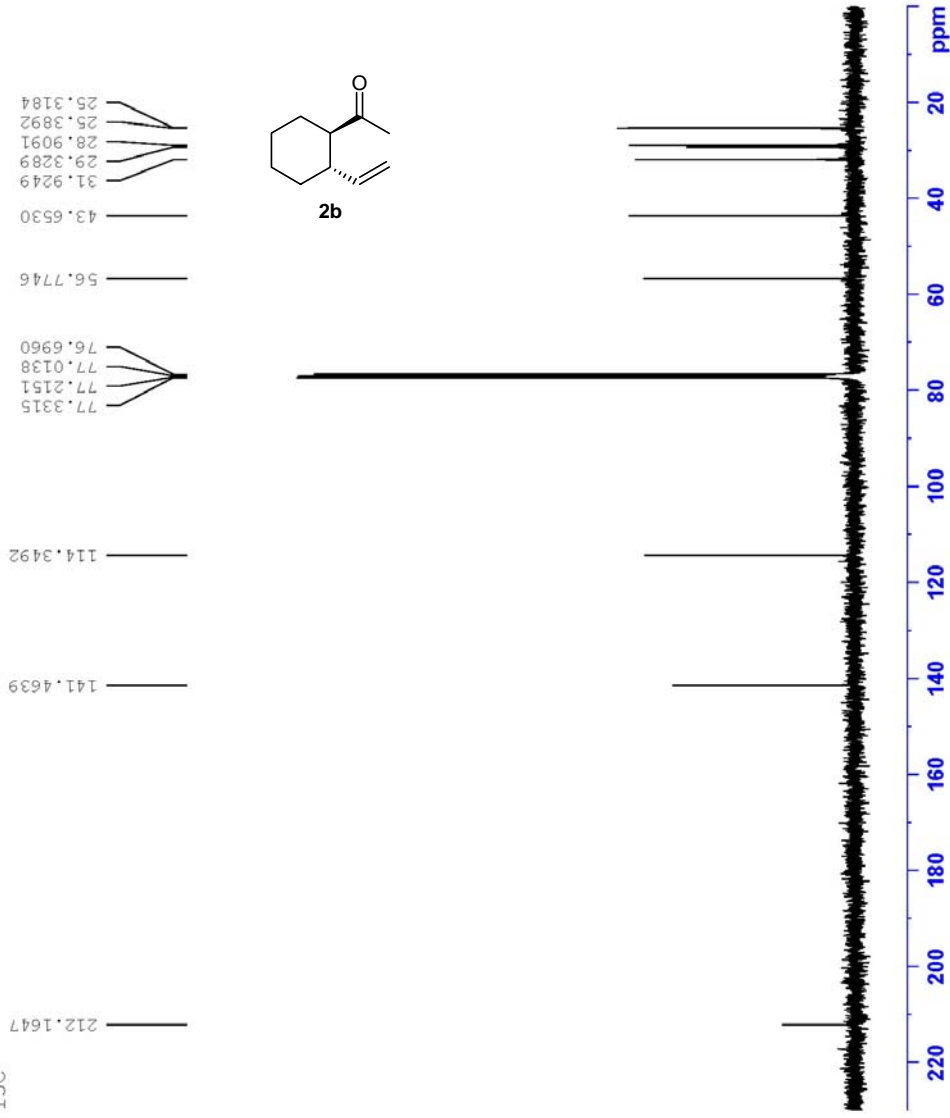
A)  
1) Compound 2a







13C



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PROCNO   1

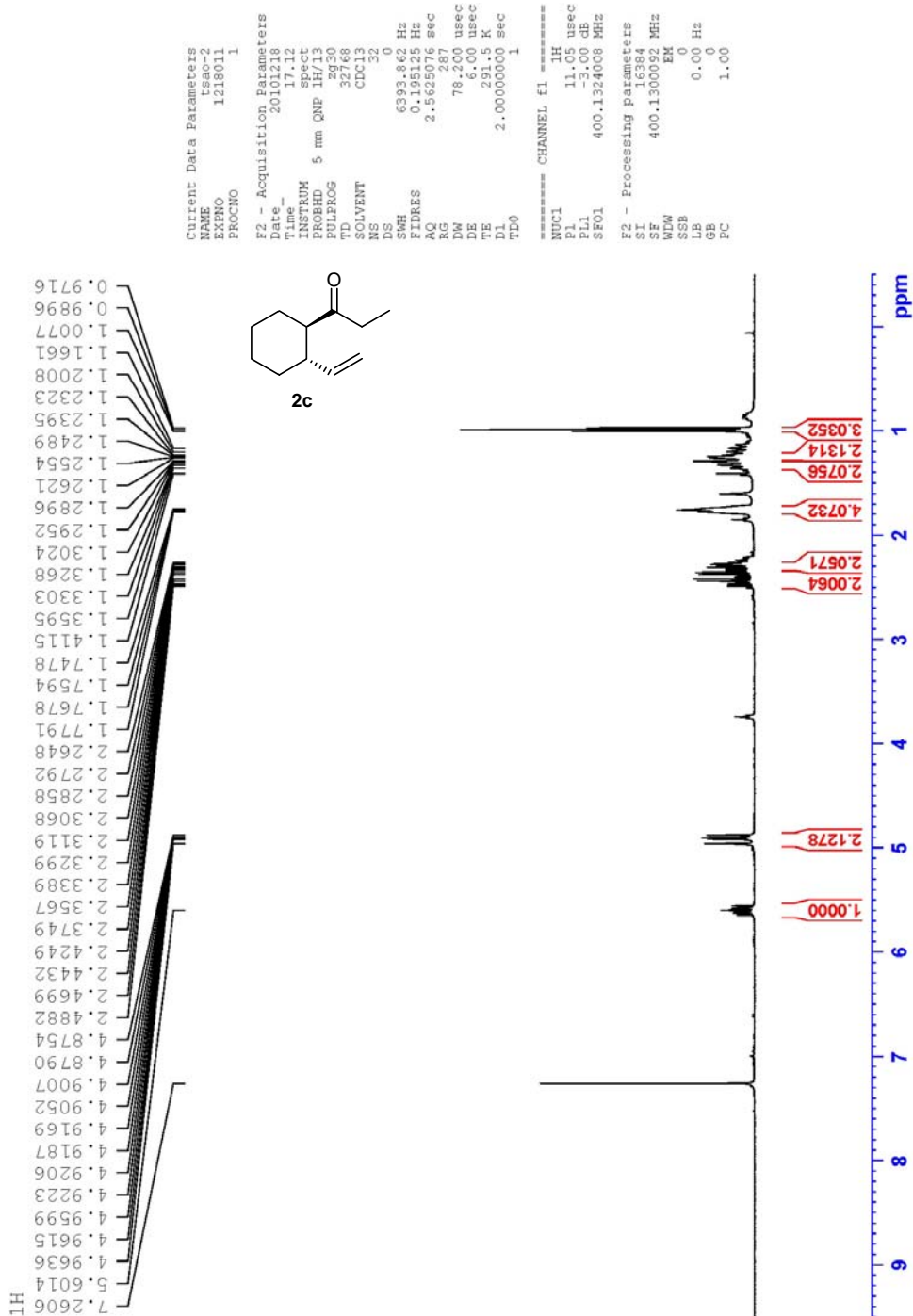
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PROBHD   5 mm QNP 1H/13
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TD       65536
SOLVENT  CDCl3
DS       51
DE       0
SWH      25510.203 Hz
FIDRES   0.389255 Hz
AQ       1.284556 sec
RG       4
DW       19.600 usec
DE       7.00 usec
TE       302.5 K
D1       2.0000000 sec
d11      0.0300000 sec
DELTA    1.8999998 sec
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NUC1     13C
P1       9.00 usec
PL1      0.00 dB
SFO1     100.6248425 MHz

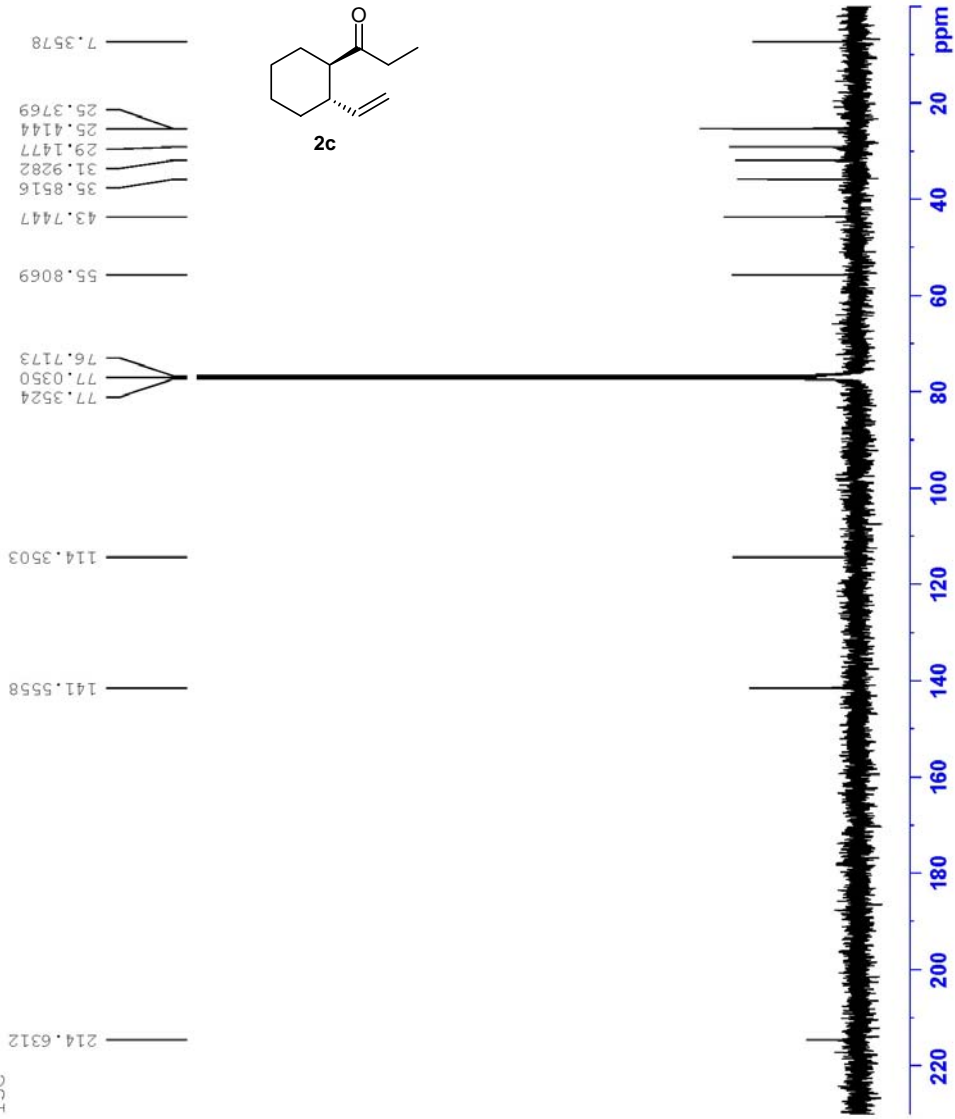
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NUC2     1H
PCPD2    90.00 usec
PL2      -3.00 dB
PL12     14.00 dB
PL13     17.00 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
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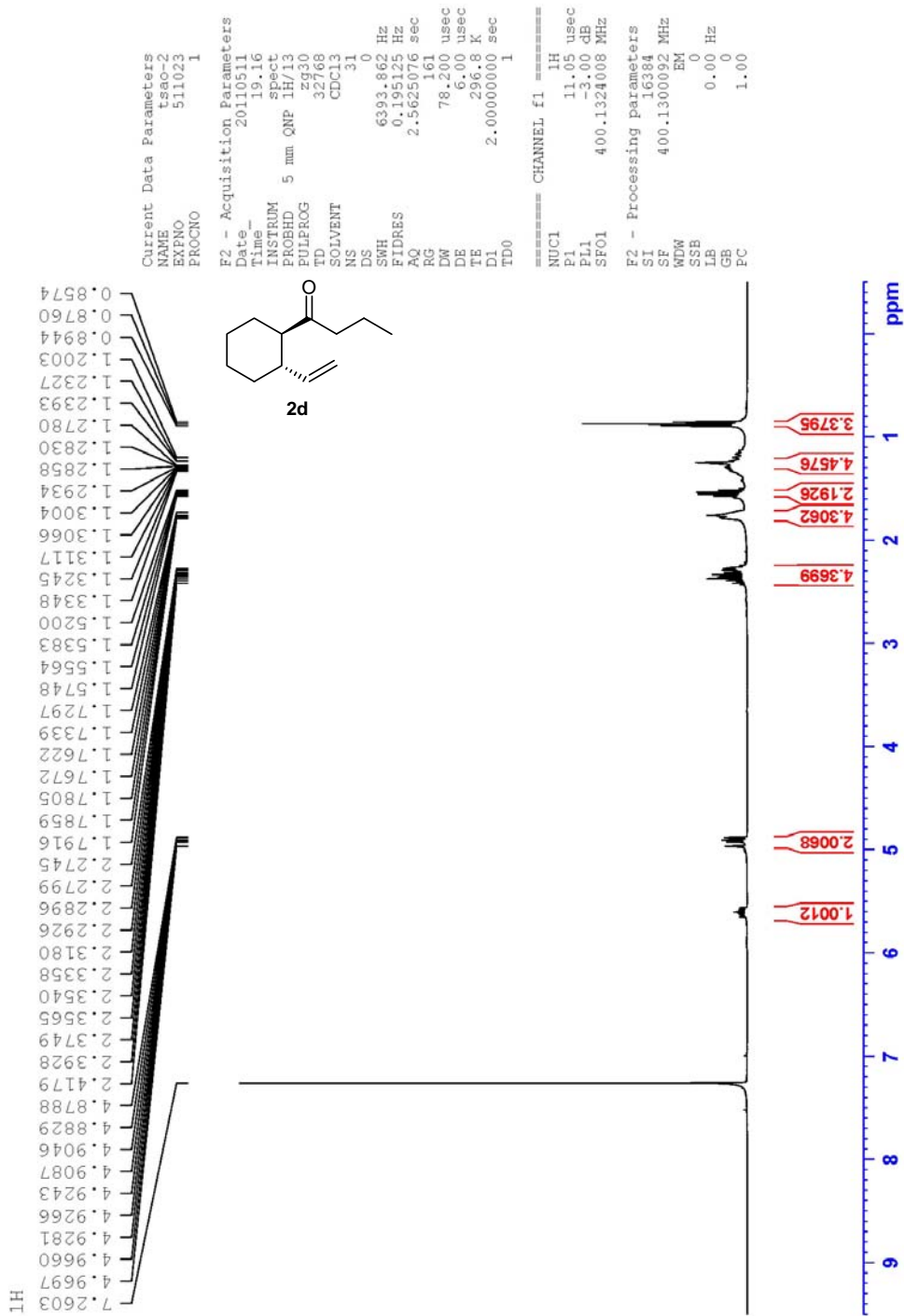
### 3) Compound 2c

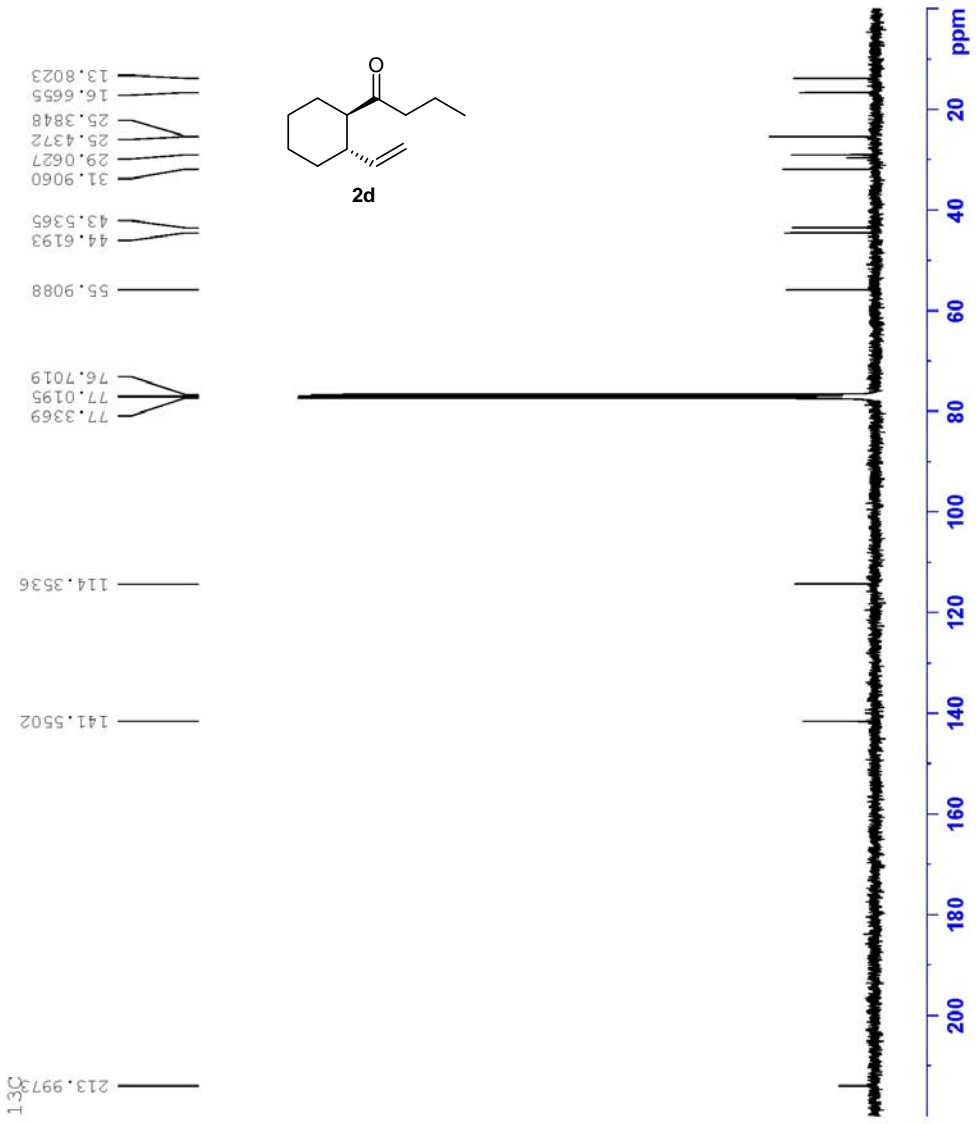


13C

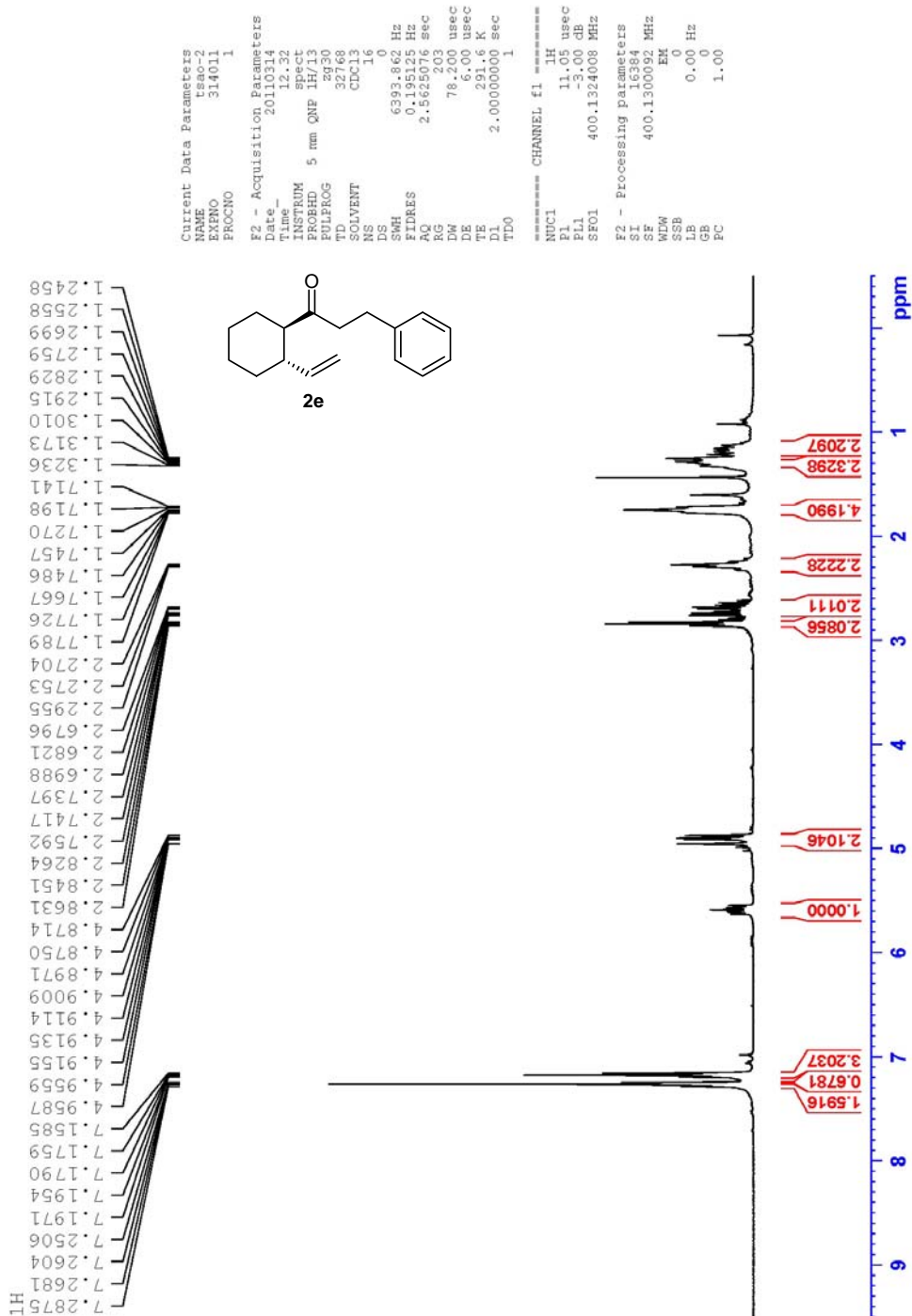


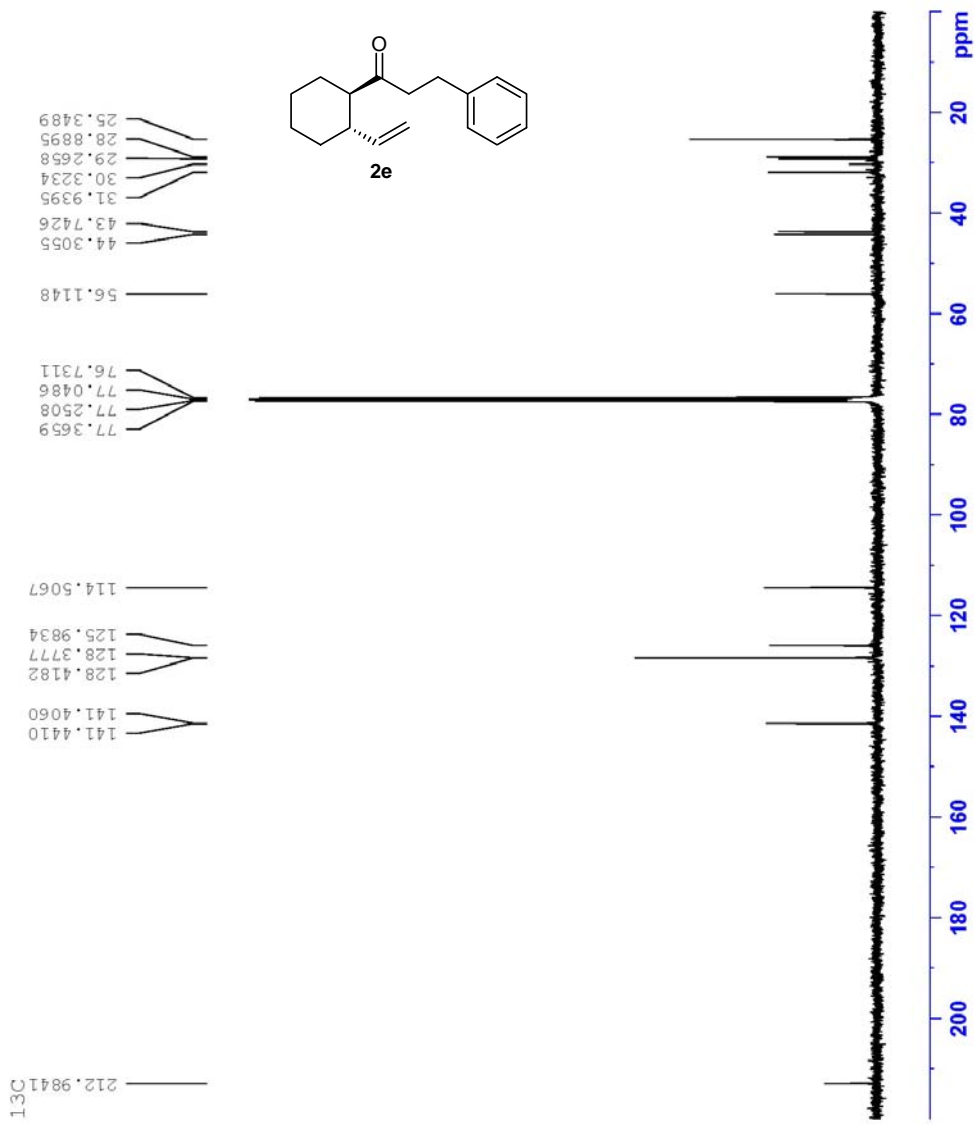
### 4) Compound 2d



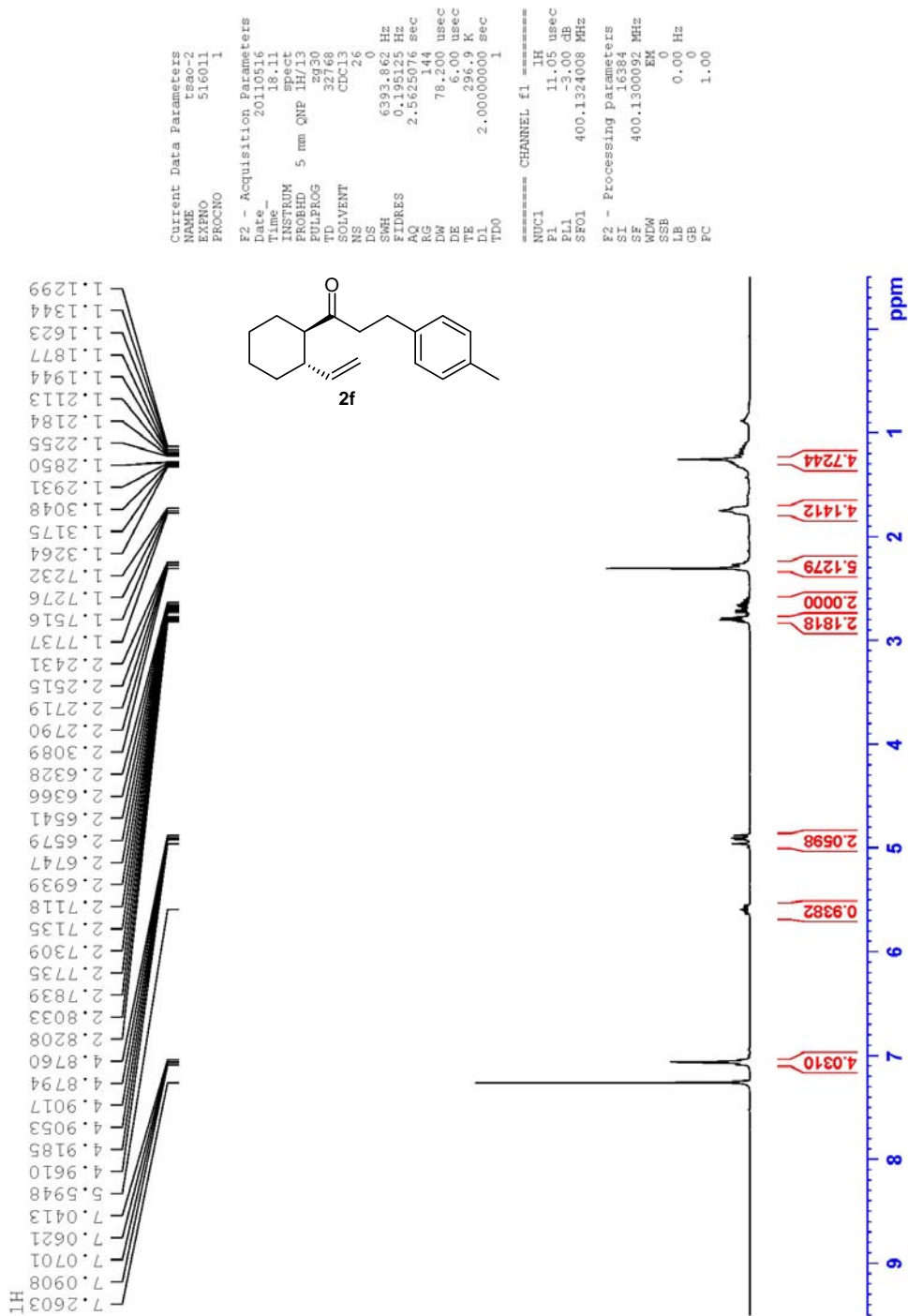


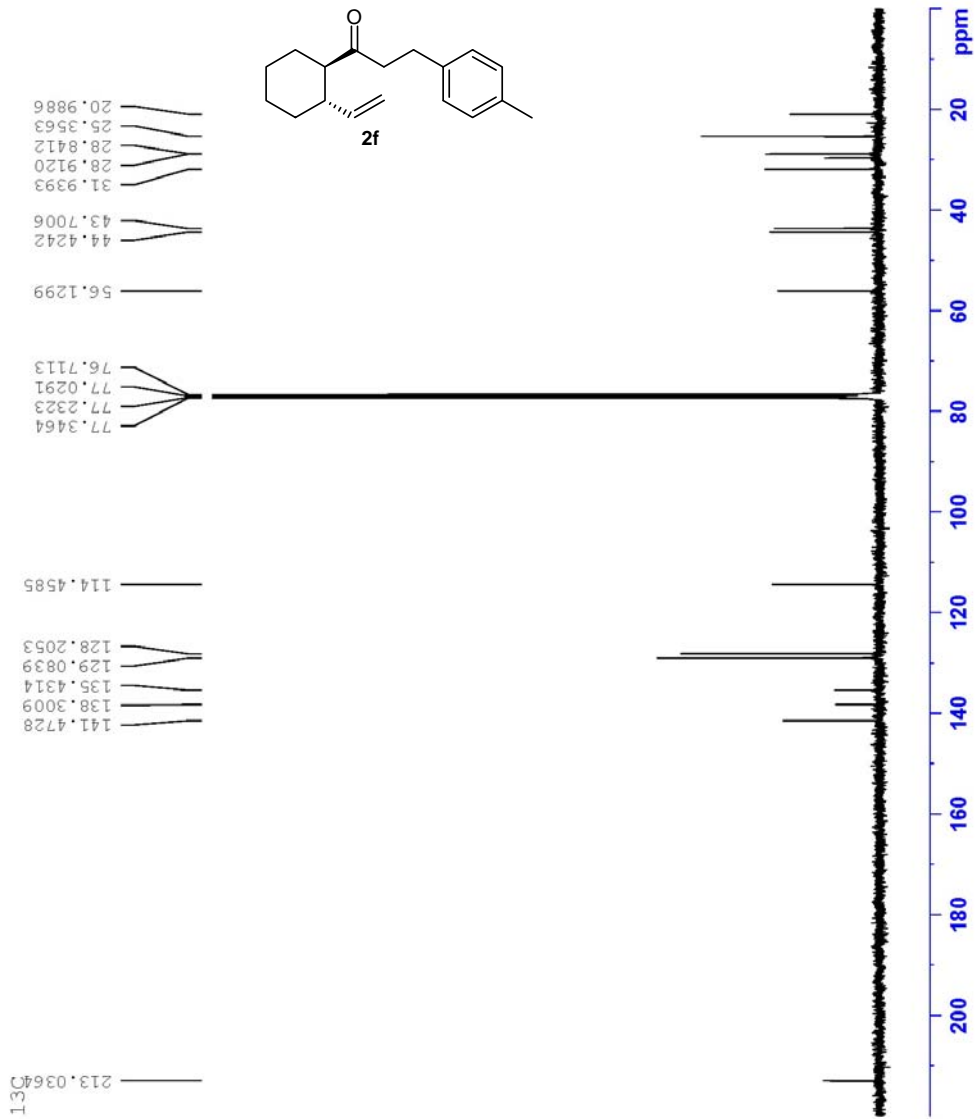
### 5) Compound 2e



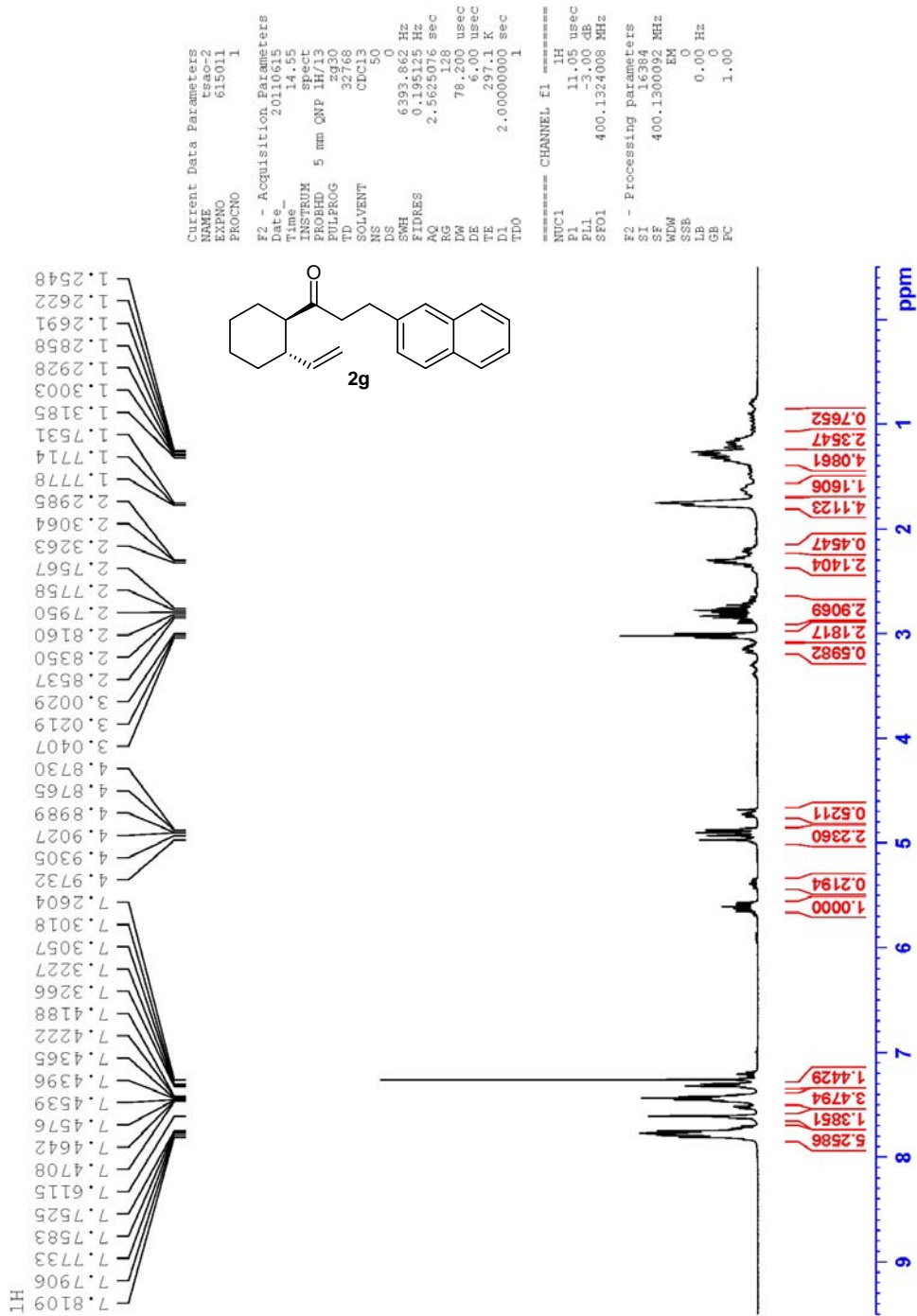


## 6) Compound 2f

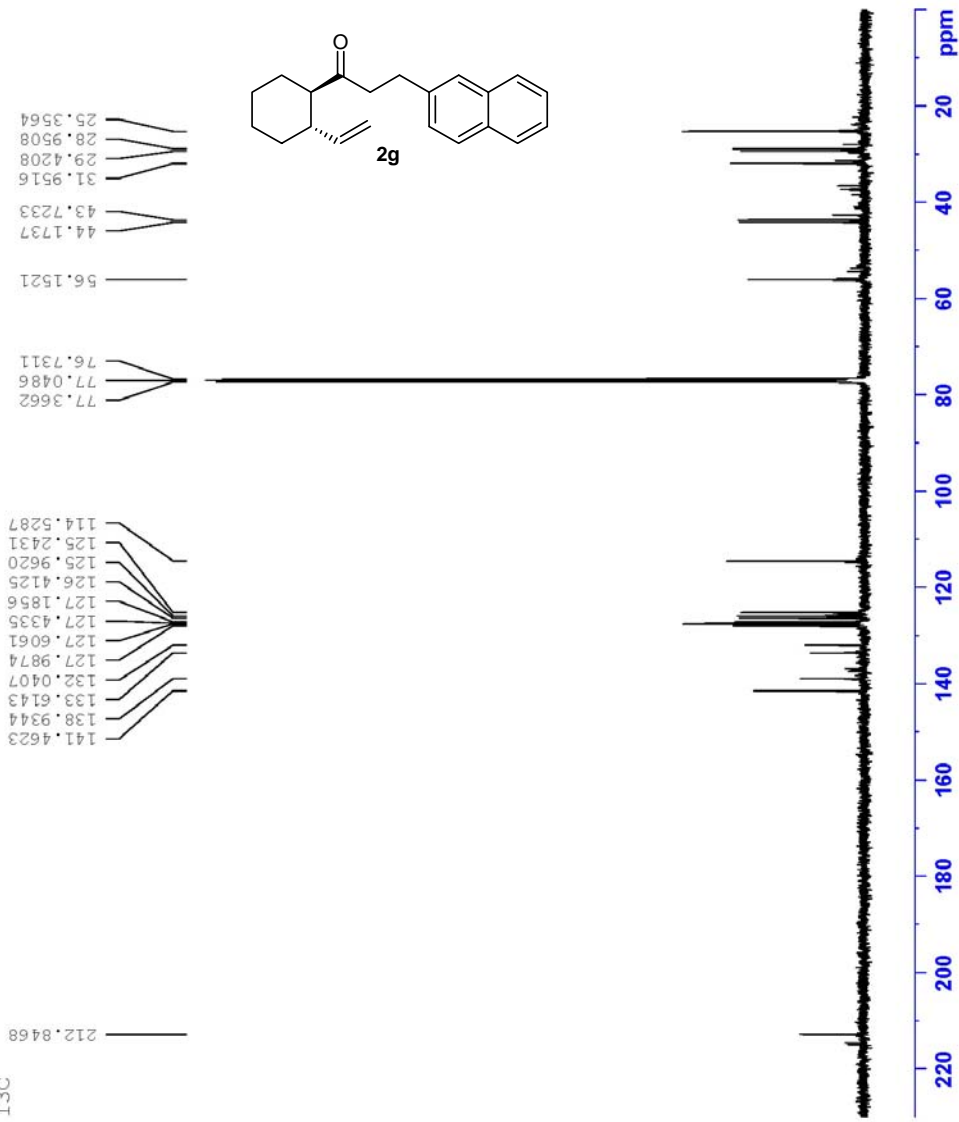




# 7) Compound 2g



13C



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PROCNO 1

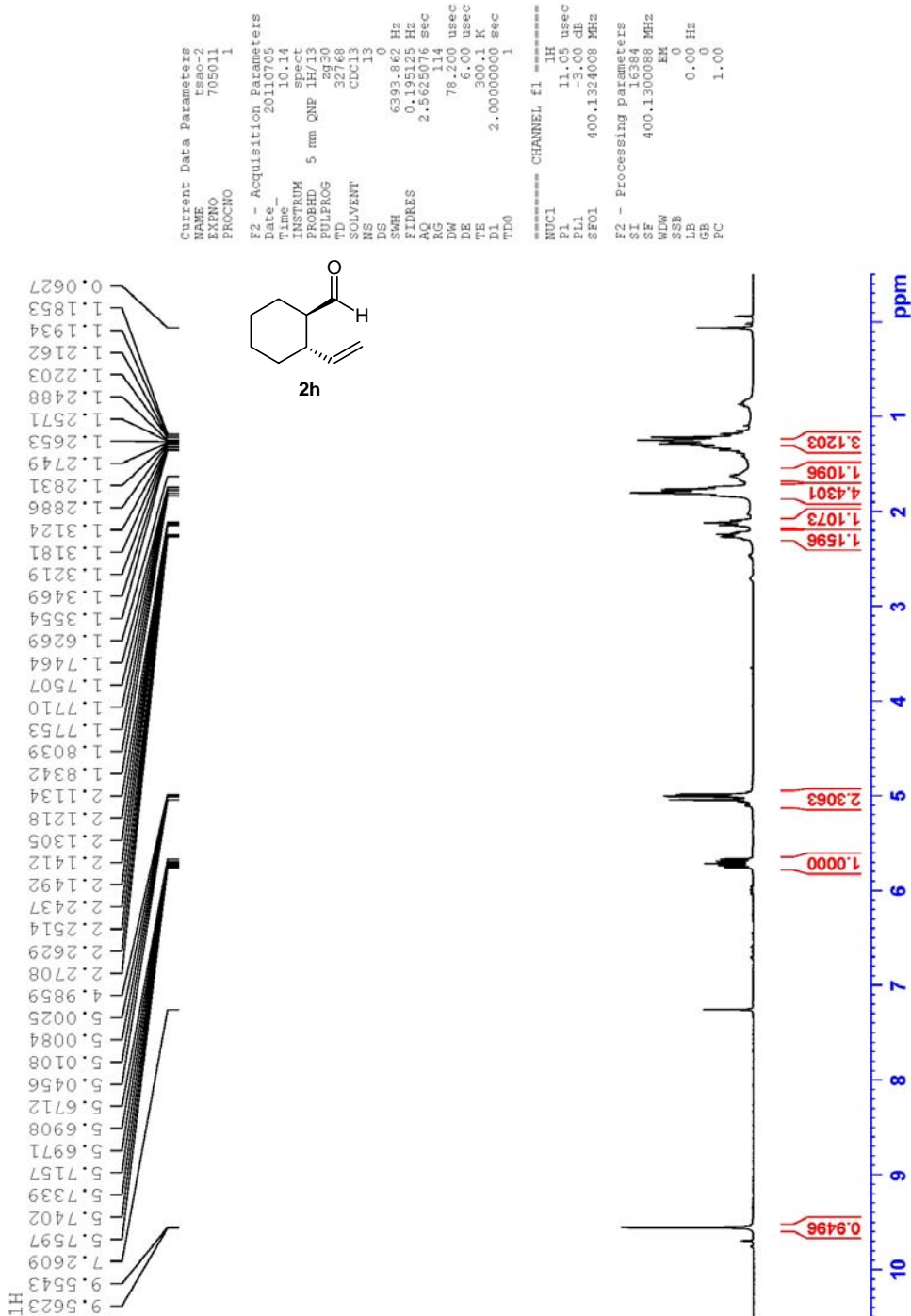
F2 - Acquisition Parameters  
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Time\_ 15.13  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 505  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2845556 sec  
RG 1820  
DE 19.820  
DM 7.00 usec  
TE 297.6 usec  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL F1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

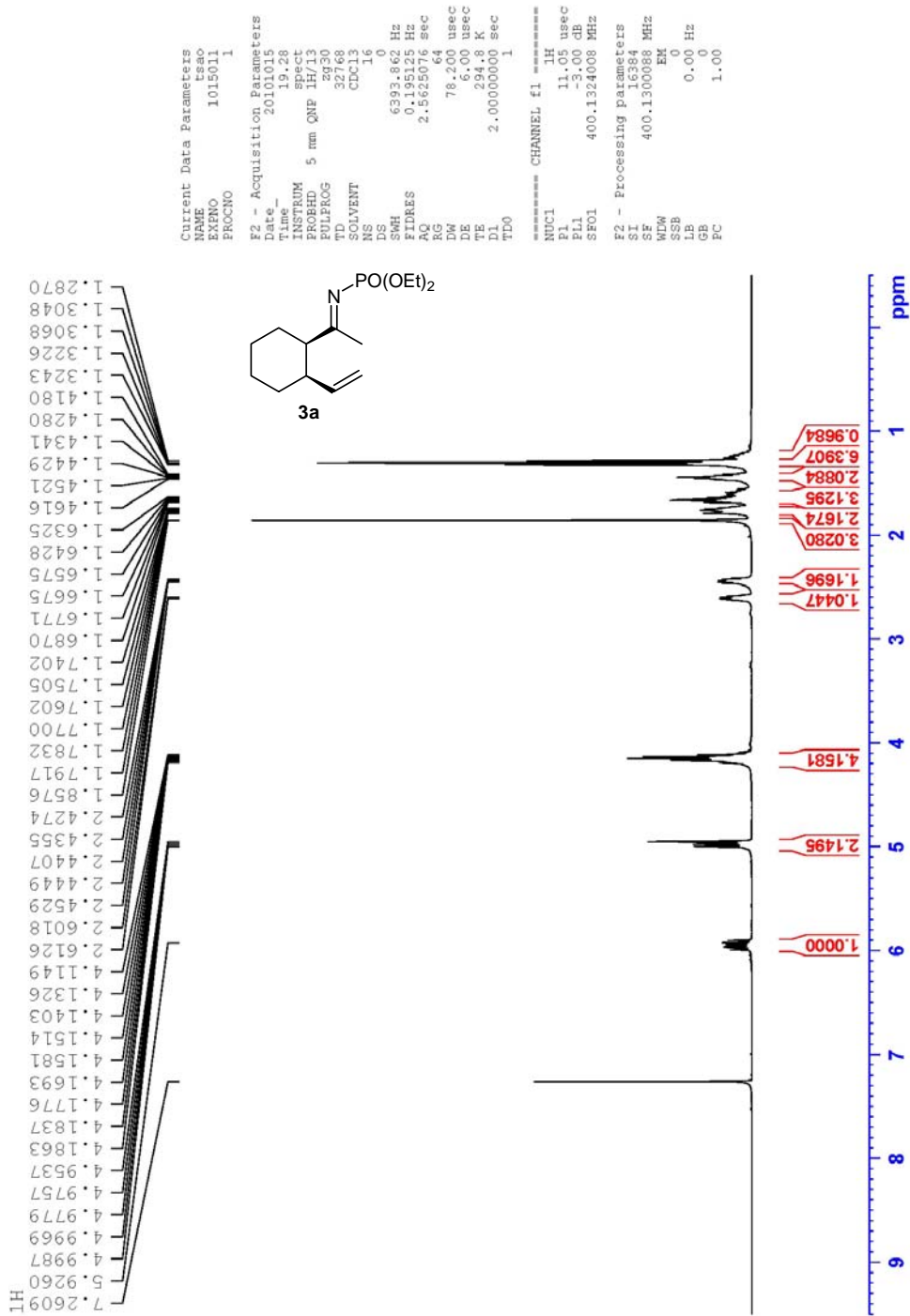
===== CHANNEL F2 =====  
CDEPRG2 waltz16  
NUC2 13C  
P2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
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SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.00

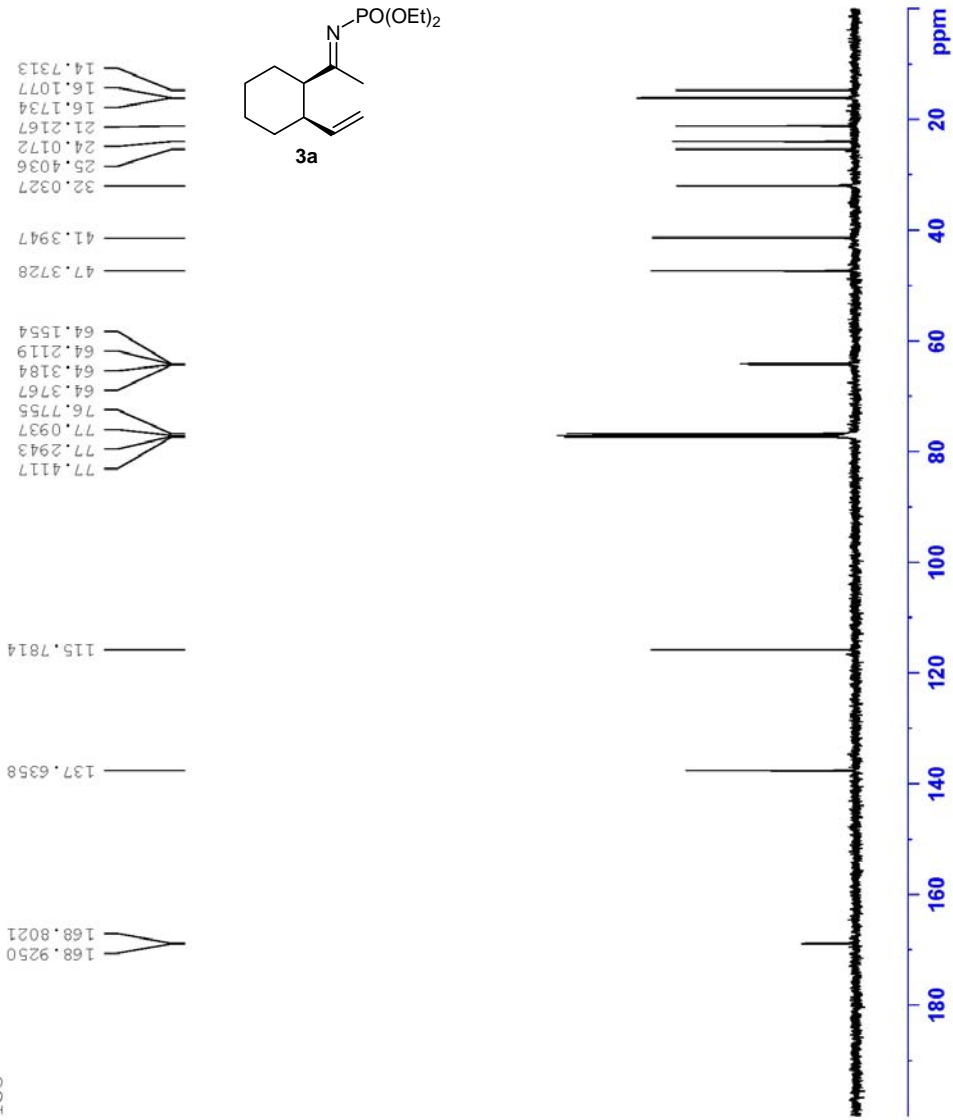
# 8) Compound 2h



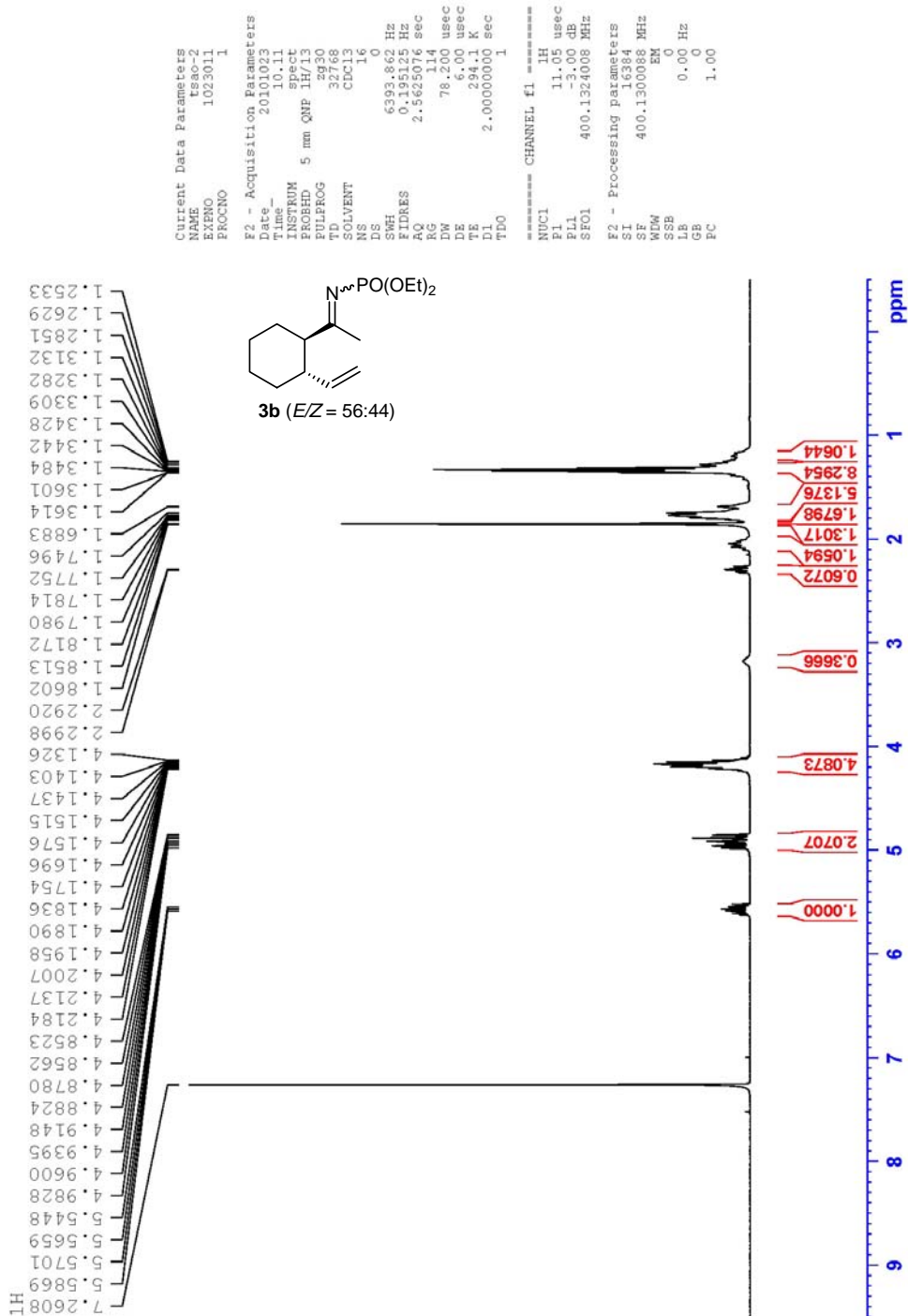
# 9) Compound 3a

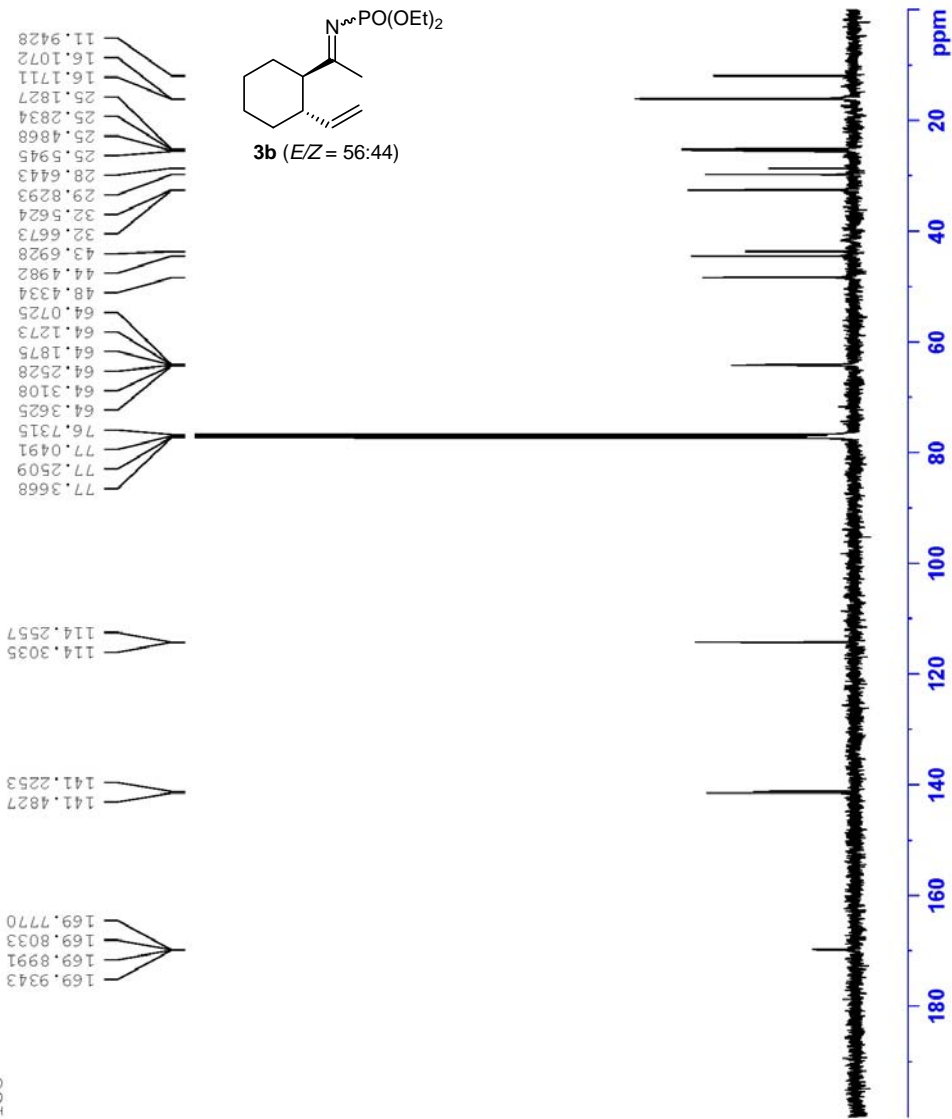


13C

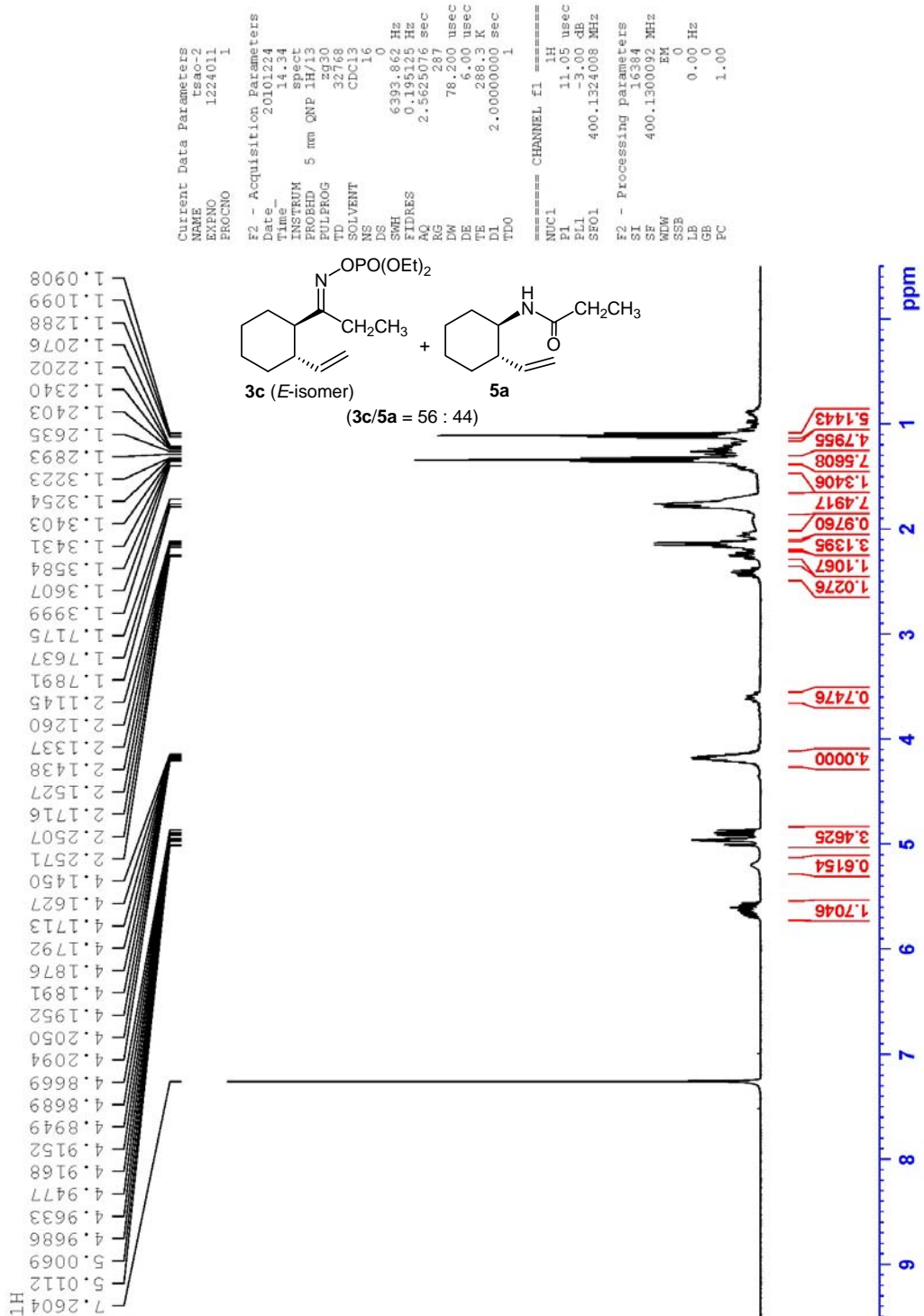


# 10) Compound 3b

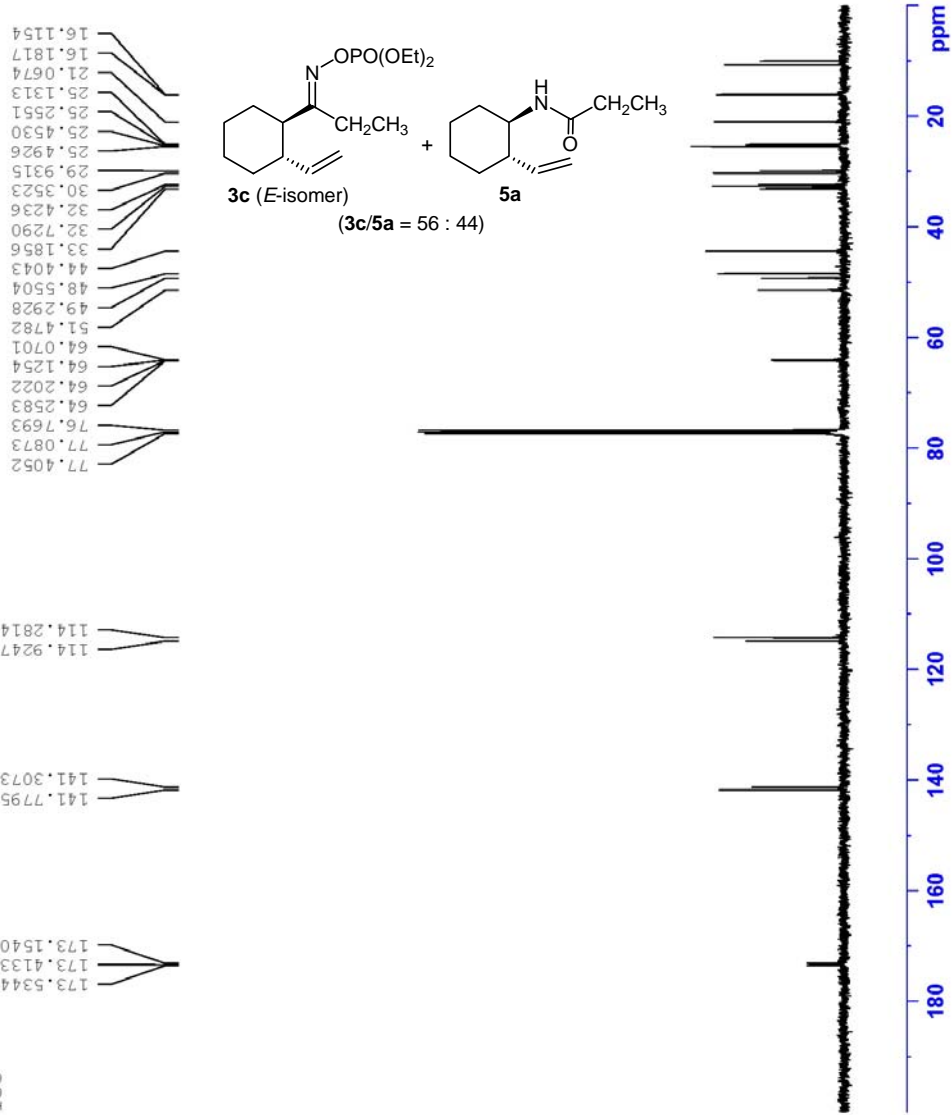




# 11) Compound 3c (in *E*-form mixed with 5a)



13C



Current Data Parameters  
 NAME tsao-2  
 EXRNO 1224012  
 PROCNO 1

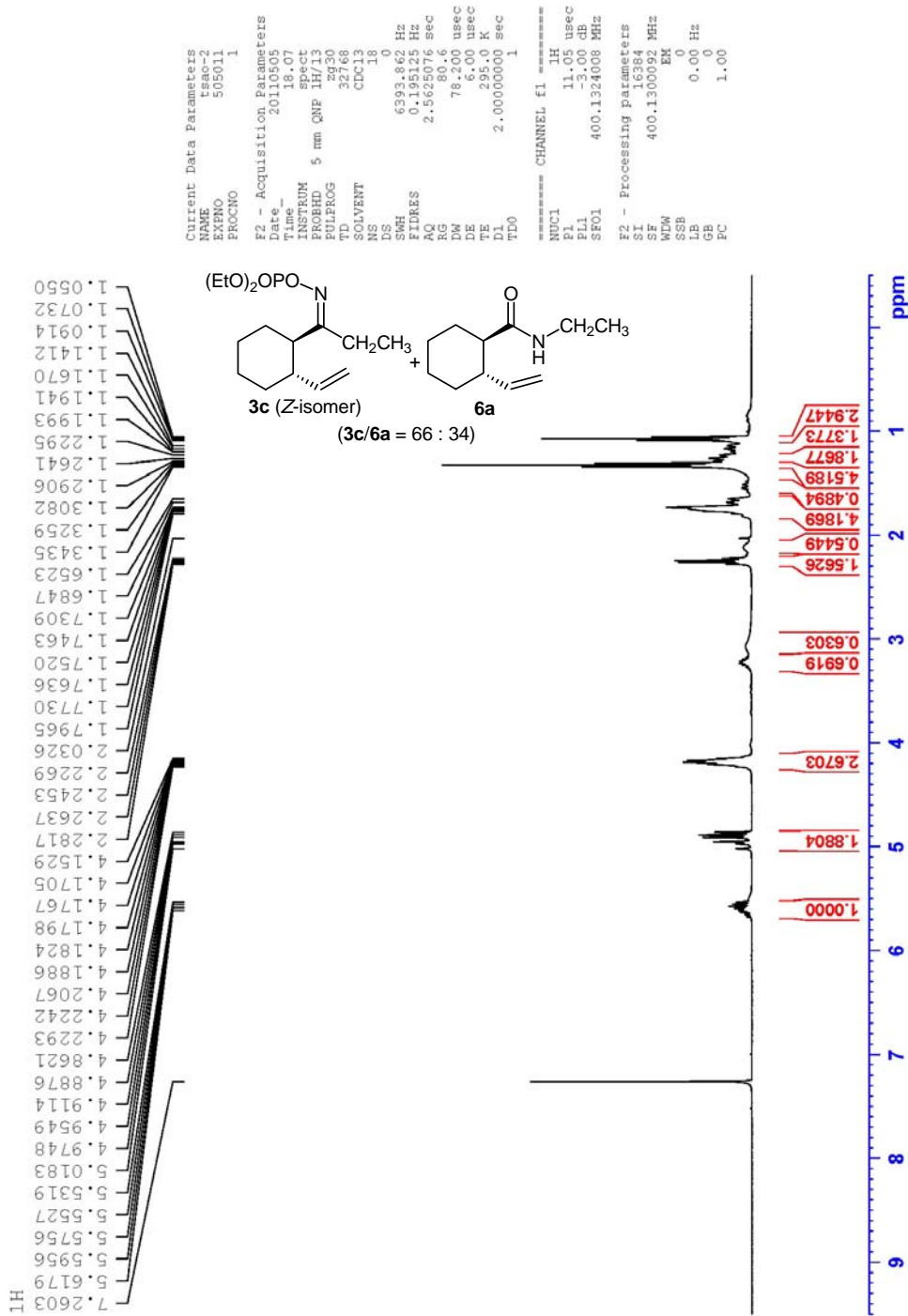
F2 - Acquisition Parameters  
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 Time\_ 15:02  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 212  
 DS 0  
 SWH 25510.203 Hz  
 FIDRES 0.389255 Hz  
 AQ 1.2845556 sec  
 RG 13.290  
 LE 13.00 usec  
 TE 288.8 K  
 DE 7.00 usec  
 DI 2.0000000 sec  
 d11 0.0300000 sec  
 DELTA 1.8999998 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.80 usec  
 PL1 0.00 dB  
 SFO1 100.6248425 MHz

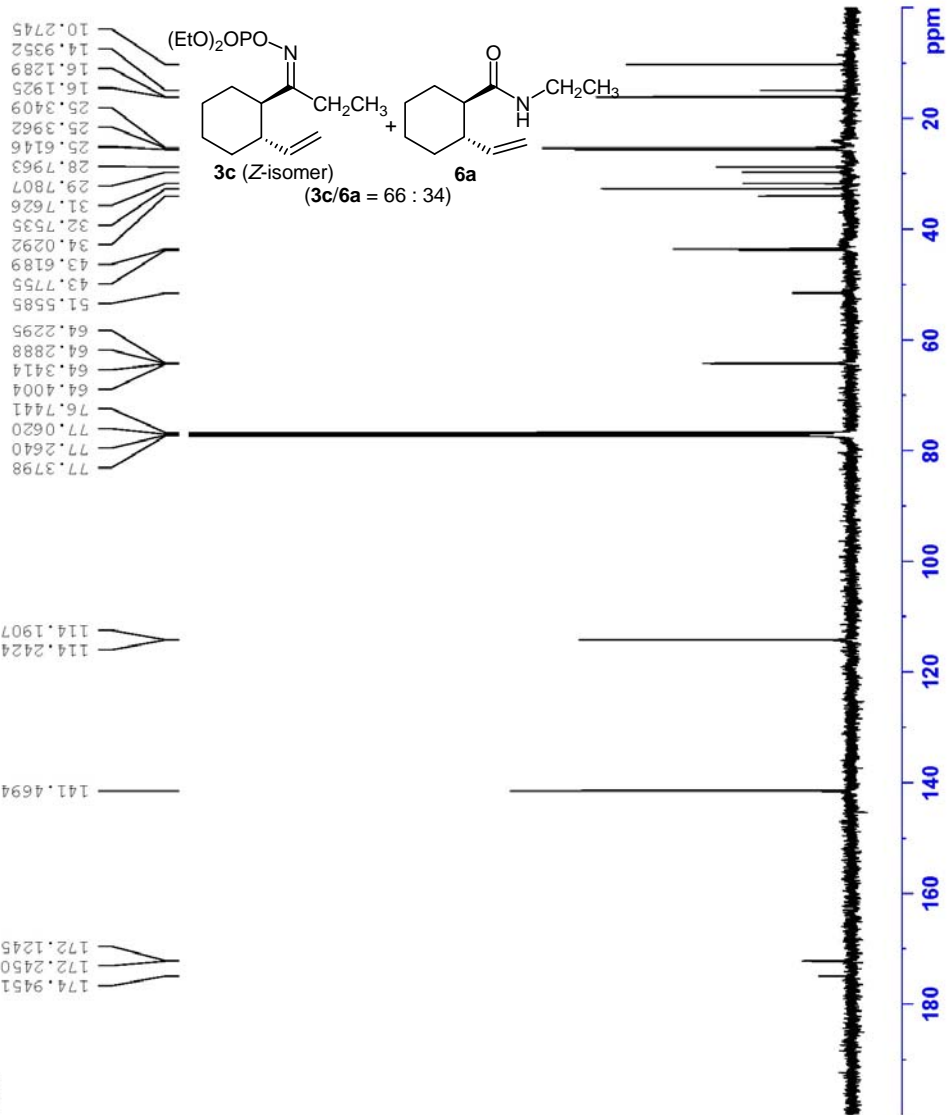
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P2 90.00 usec  
 PL2 -3.00 dB  
 PL12 14.00 dB  
 PL13 17.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127690 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 FC 1.00

Compound 3c (in Z-form mixed with 6a)



13C



Current Data Parameters  
 NAME tsso-2  
 EXNO 505012  
 PROCNO 1

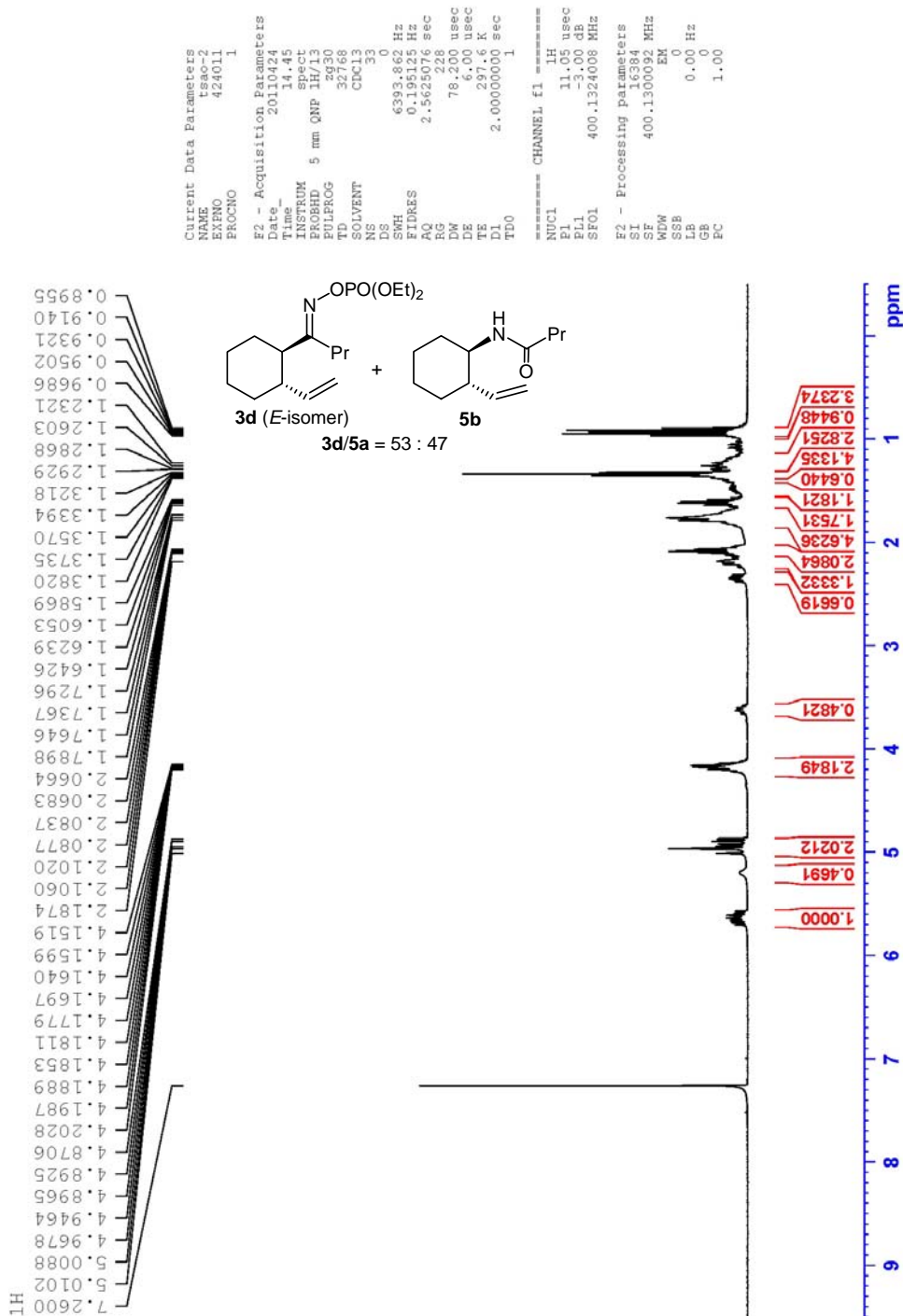
F2 - Acquisition Parameters  
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 Time 18.11  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 382  
 DS 0  
 SFO1 25510.203 Hz  
 FIDRES 0.389255 Hz  
 AQ 1.2845556 sec  
 RG 2050  
 DW 19.600 usec  
 DE 7.00 usec  
 TE 295.3 K  
 DL 2.0000000 sec  
 d11 0.0300000 sec  
 DELTA 1.8999998 sec  
 TD0 1

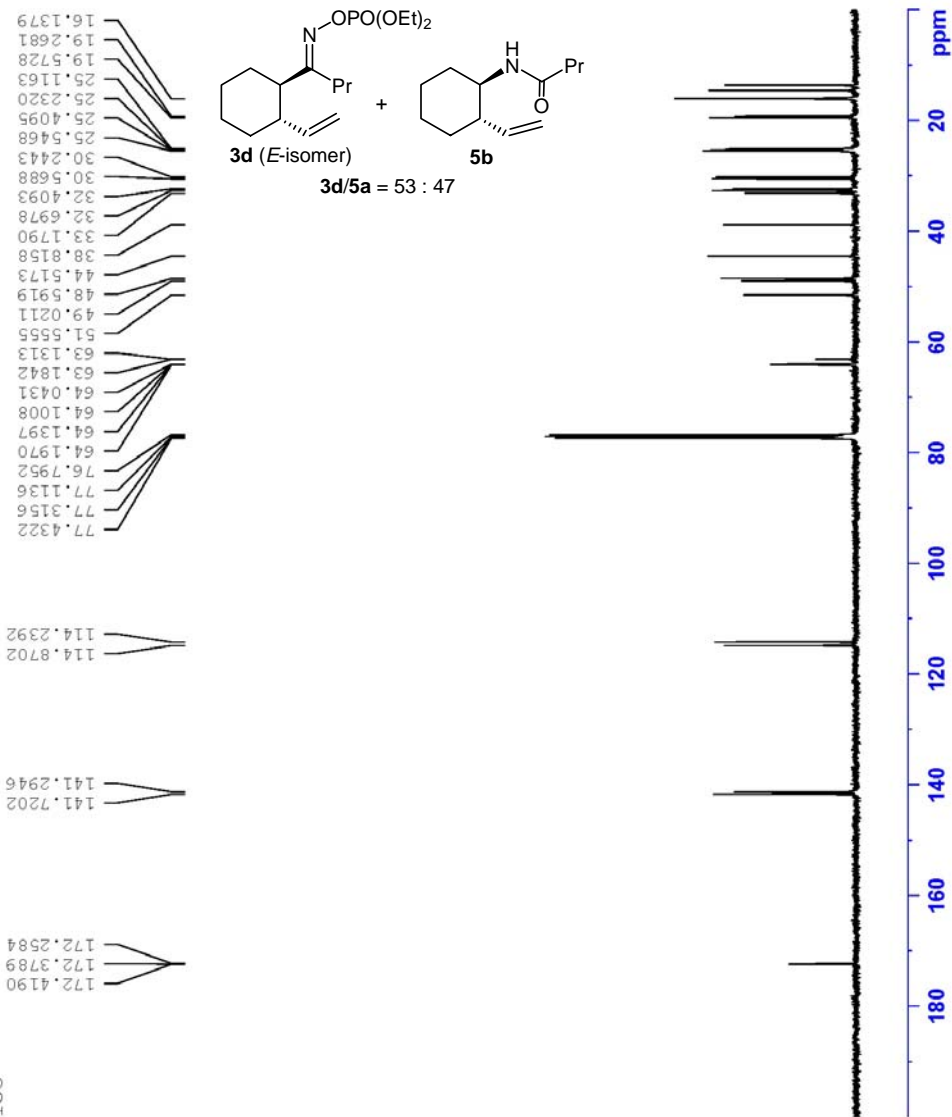
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.00 usec  
 PL1 0.00 dB  
 SFO1 100.6248425 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P2 90.00 usec  
 PL2 -3.00 dB  
 PL12 14.00 dB  
 PL13 17.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127690 MHz  
 EQ  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 1.00

## 12) Compound 3d (in *E*-form mixed with 5b)





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Current Data Parameters
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PROCNO   1

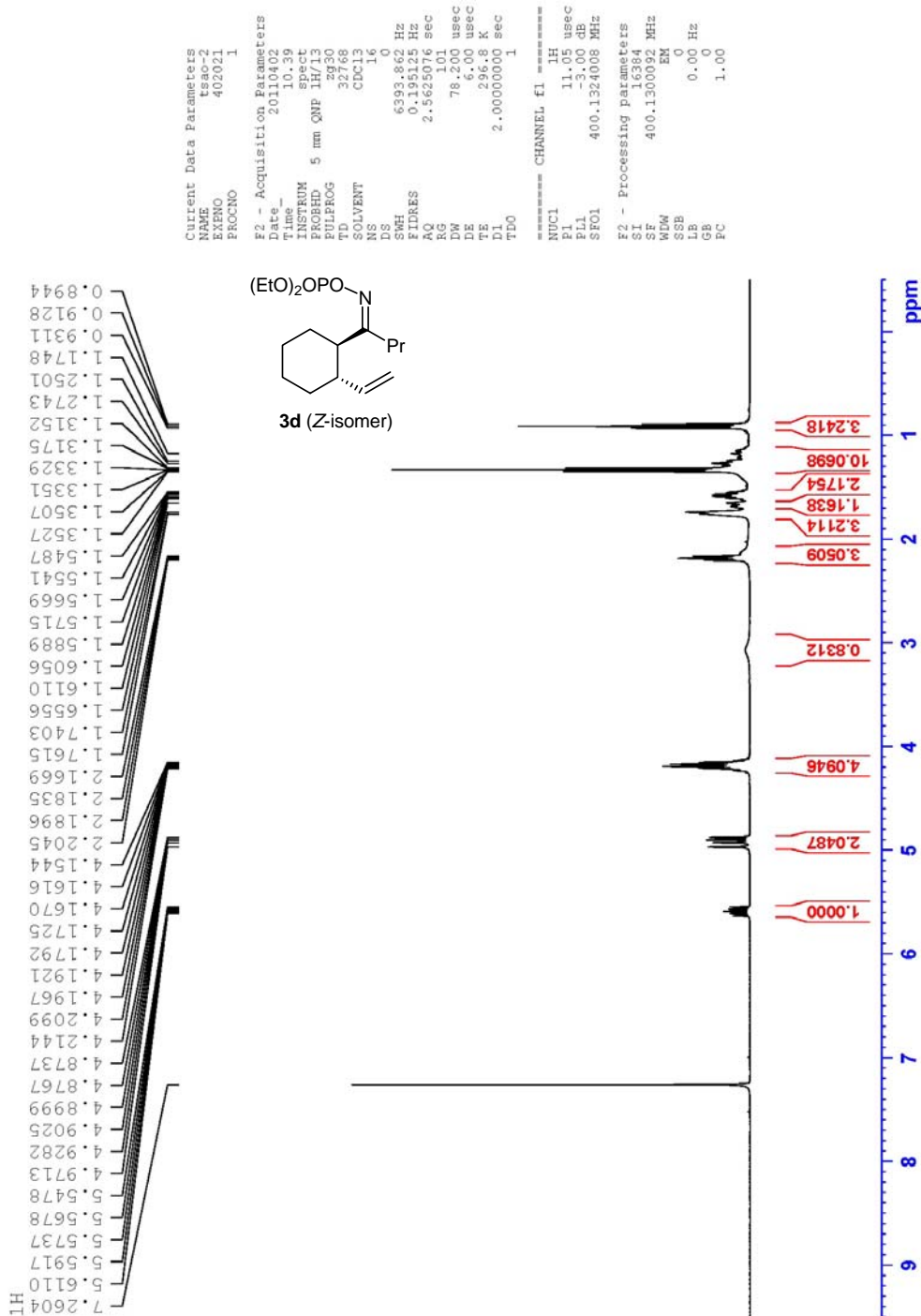
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Date_    20110330
Time     19.43
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       201
DS       4
SWH      25510.203 Hz
FIDRES   0.389255 Hz
AQ       1.2845556 sec
RG       2050
DW       19.600 usec
DE       7.00 usec
TE       294.1 K
D1       2.0000000 sec
d11      0.0300000 sec
DELTA    1.8999998 sec
TD0      1

===== CHANNEL f1 =====
NUC1     13C
P1       8.60 usec
PL1      0.00 dB
SFO1     100.6248425 MHz

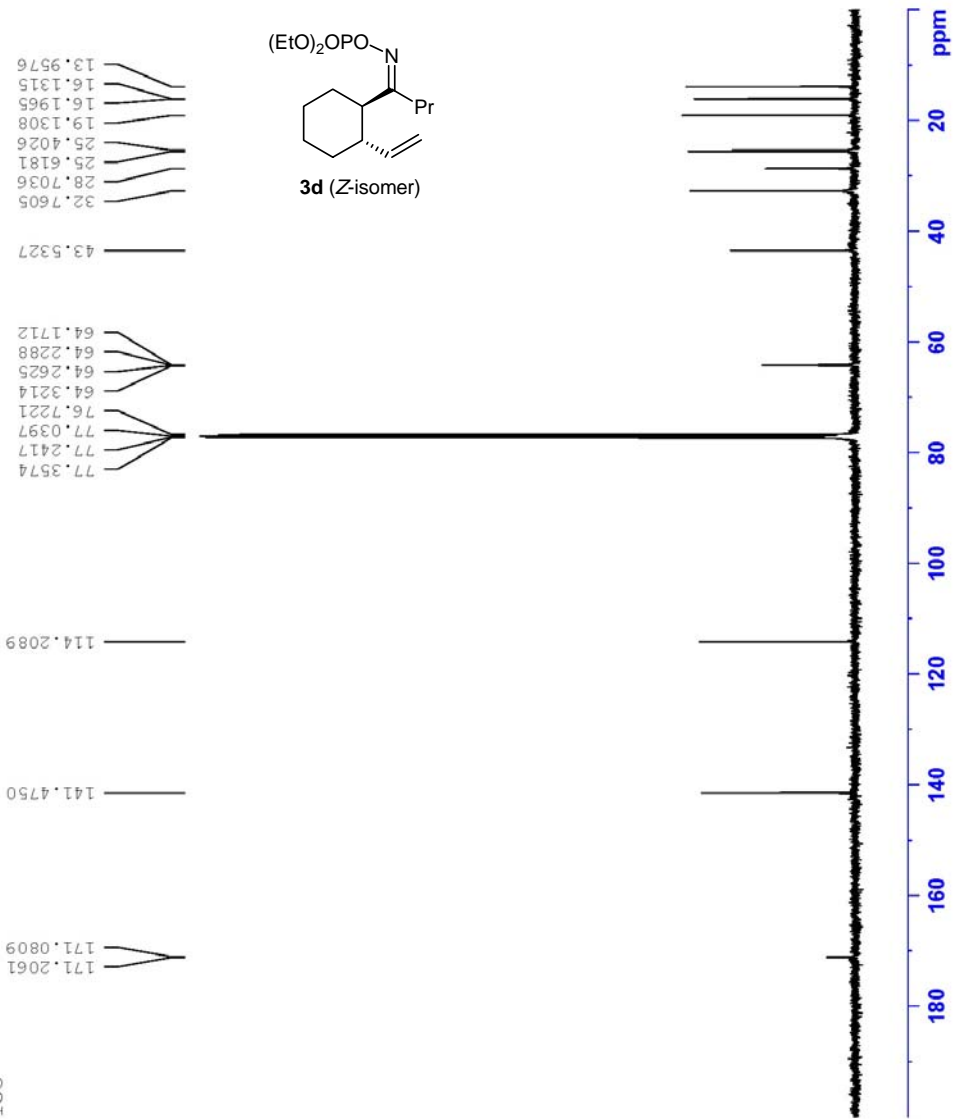
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    90.00 usec
PL2      -3.00 dB
PL12     14.00 dB
PL13     17.00 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI       32768
SF       100.6127690 MHz
WDW      EK
SSB      0
GB       2.00 Hz
PC       1.00
  
```

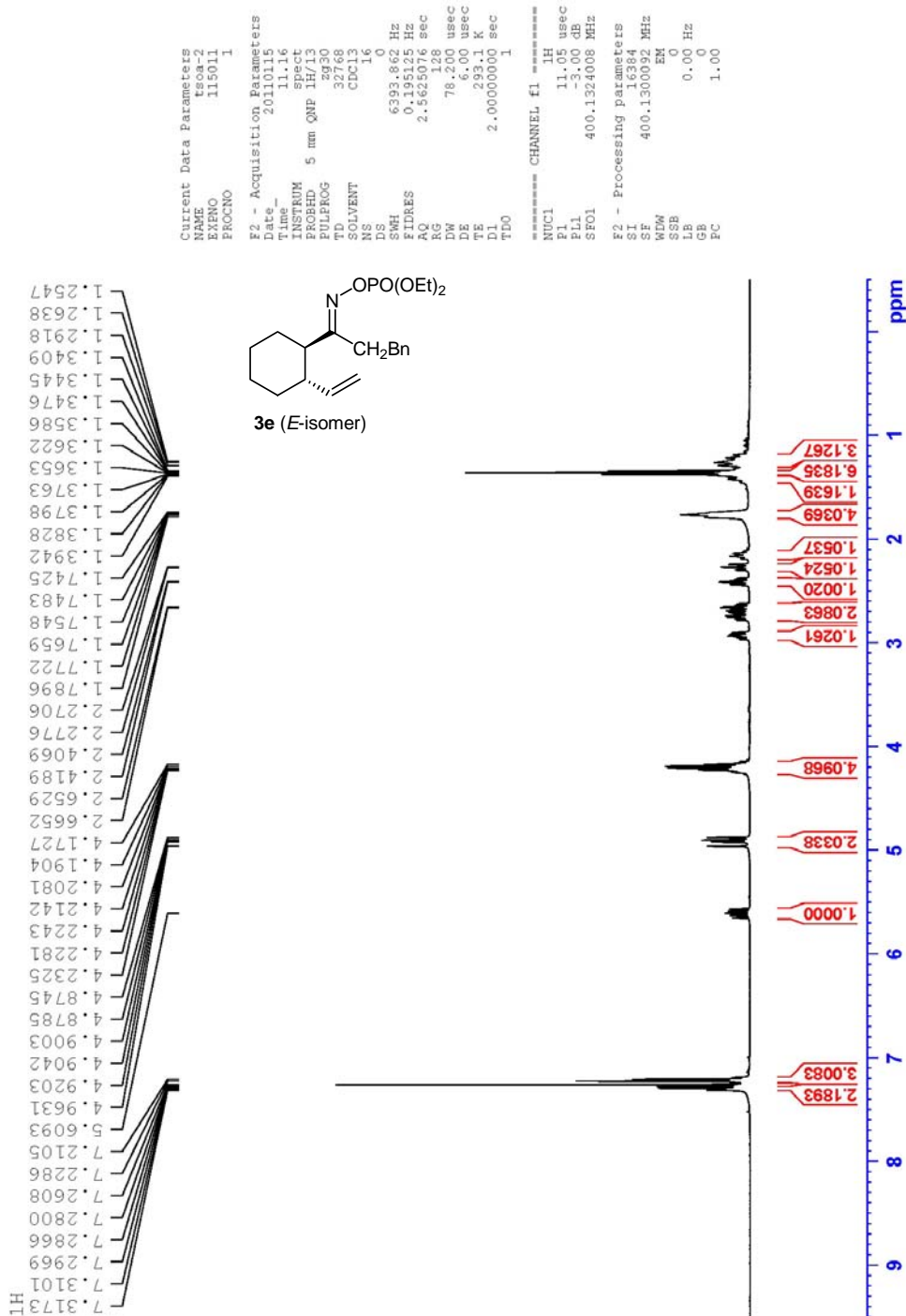
# Compound 3d (Z-form)

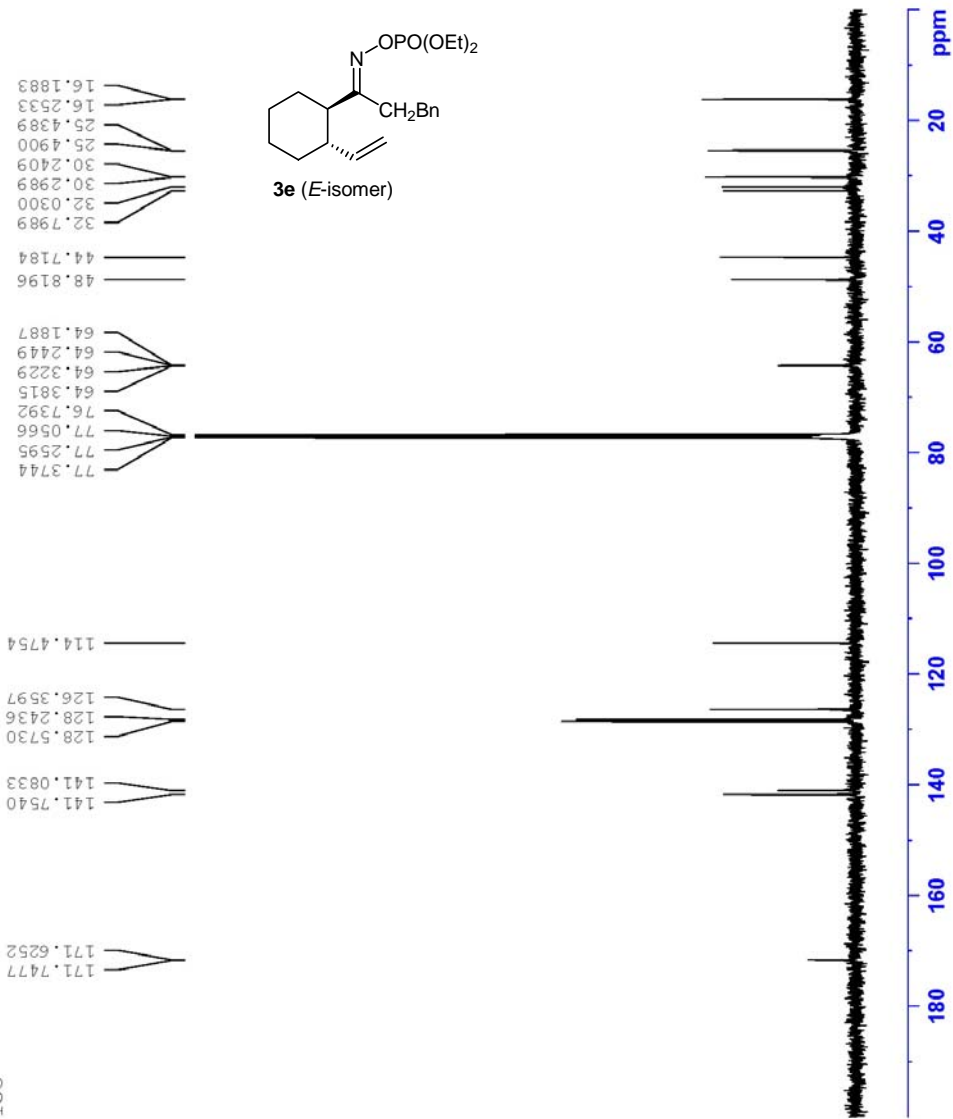


13C

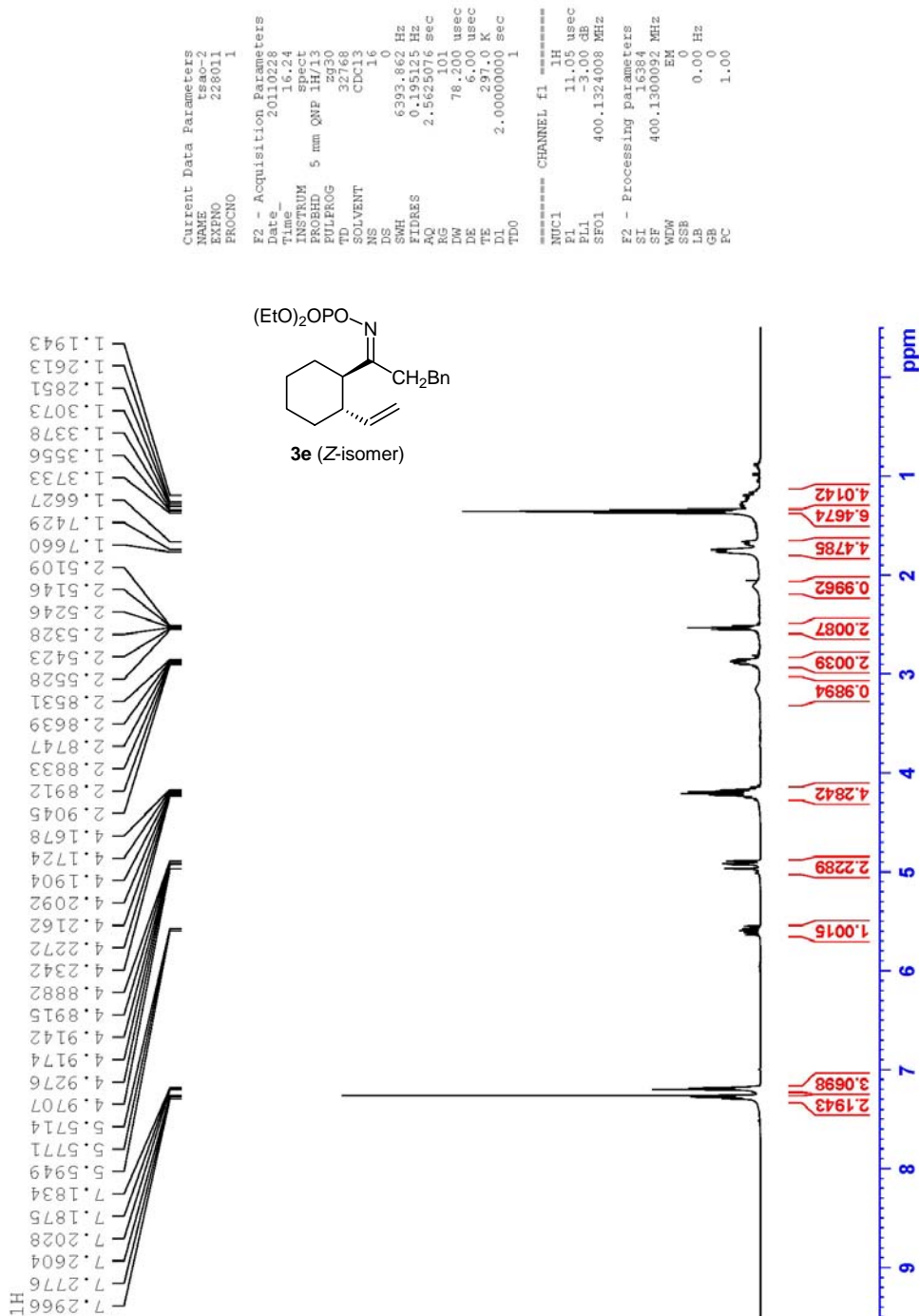


### 13) Compound 3e (*E*-isomer)

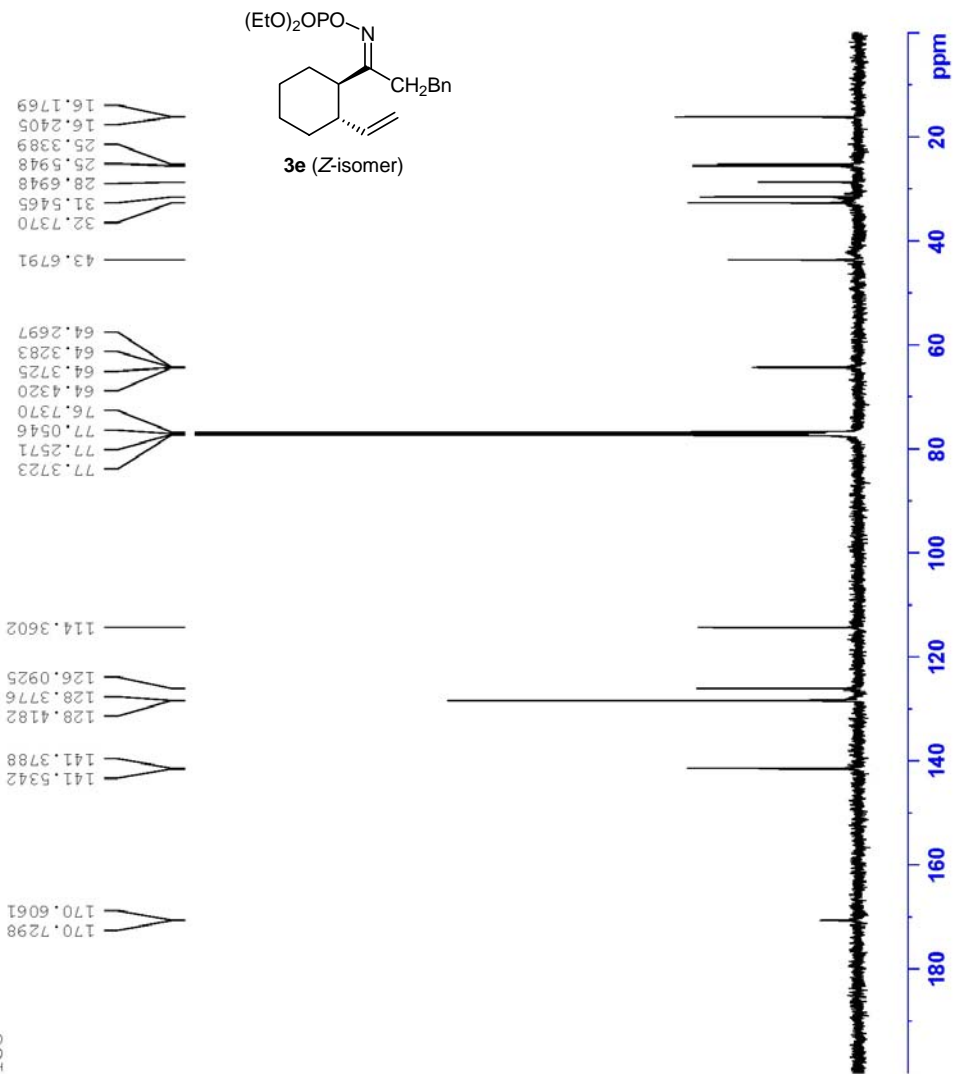




# Compound 3e (Z-isomer)



13C



Current Data Parameters  
NAME t8so-2  
EXPNO 228012  
PROCNO 1

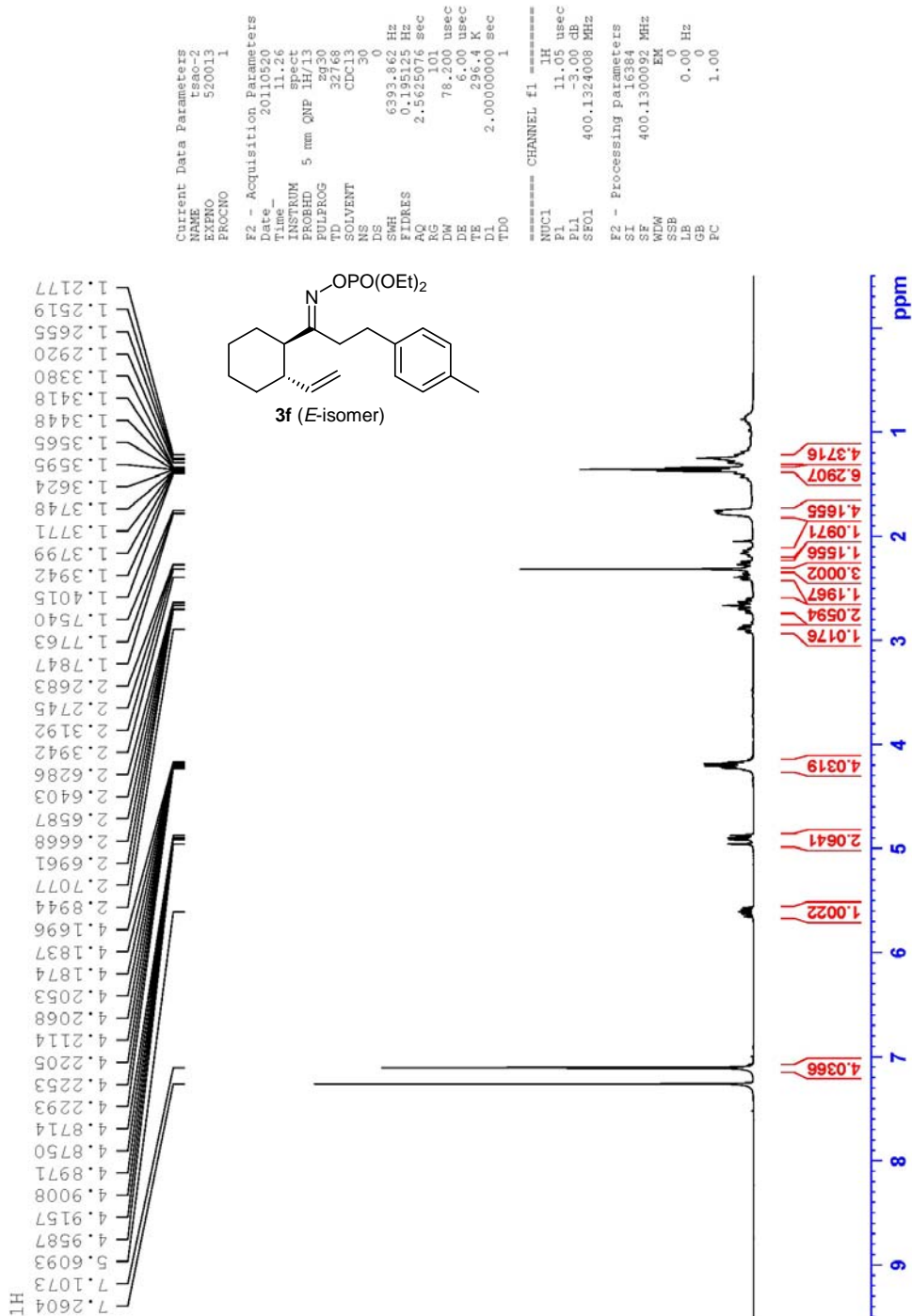
F2 - Acquisition Parameters  
Date\_ 20110228  
Time\_ 16.32  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 393  
DS 0  
SMH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2845556 sec  
RG 18.1440  
DE 19.000000 usec  
TE 297.5 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

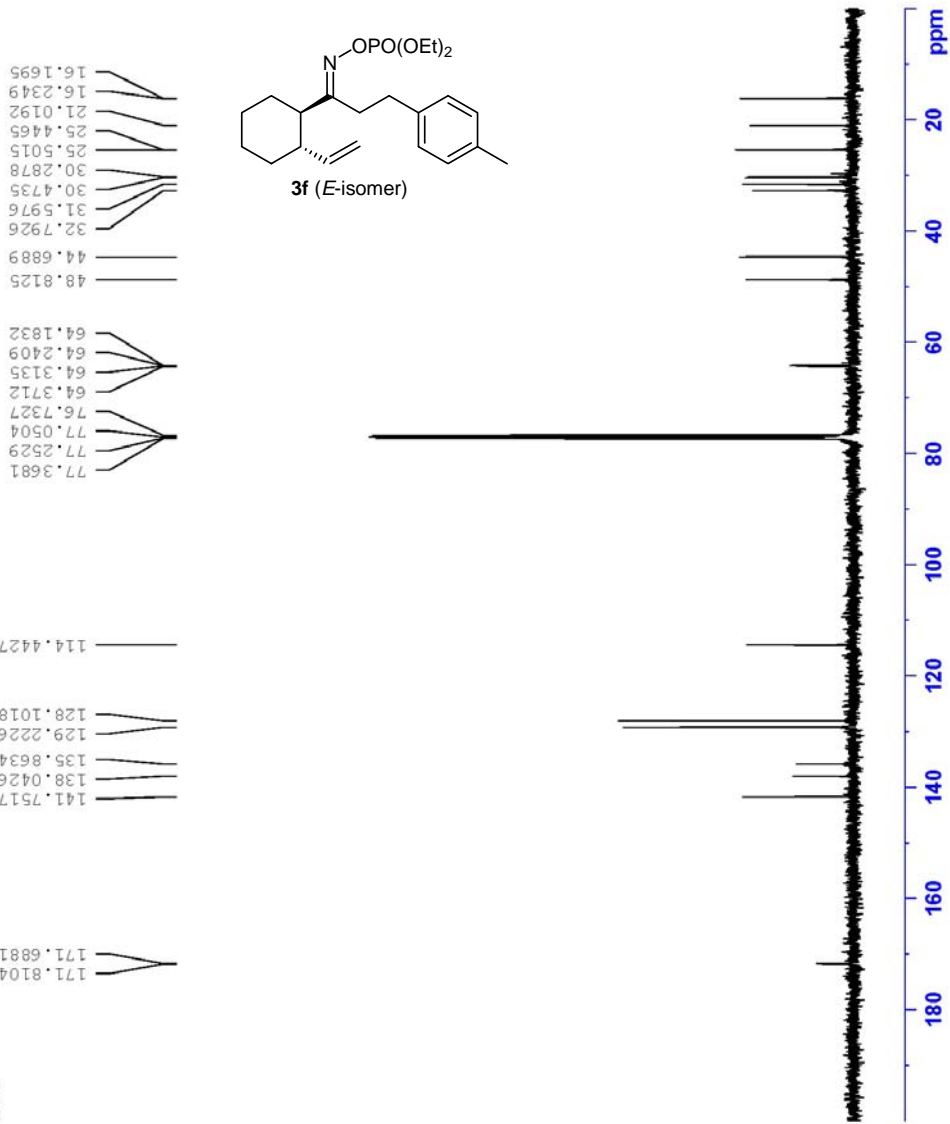
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
P2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
FC 1.00

# 14) Compound 3f (E-isomer)



13C



Current Data Parameters  
NAME tsao-2  
EXNO 520014  
PROCNO 1

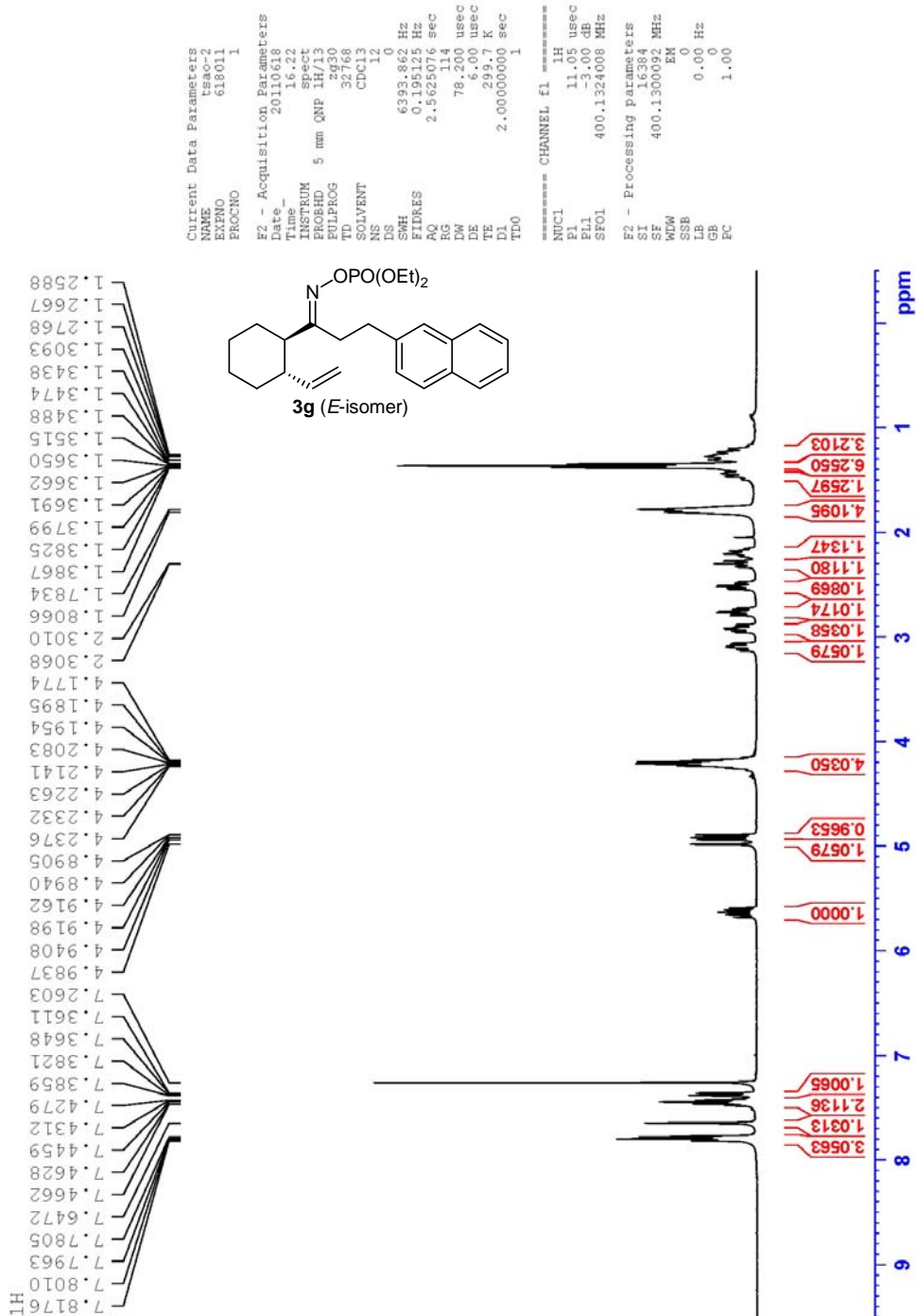
F2 - Acquisition Parameters  
Date\_ 20110520  
Time\_ 11.32  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 182  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389295 Hz  
AQ 1.2845556 sec  
RG 2050  
DQ 19.000 usec  
DE 7.000 usec  
TE 296.8 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL f1 =====  
NUCL 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

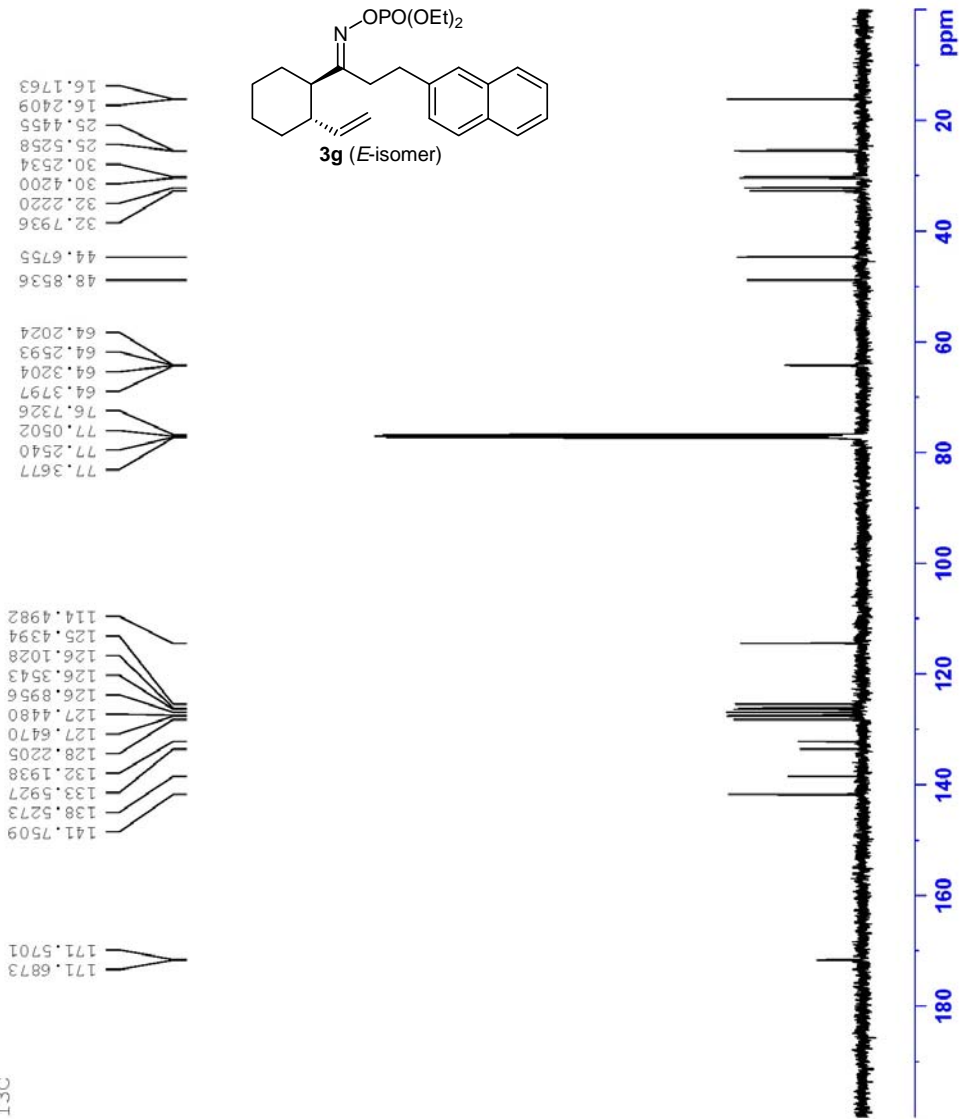
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NUC2 1H  
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PL2 0.00 dB  
PL12 -3.00 dB  
PL13 14.00 dB  
PL14 14.00 dB  
PL15 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
EC 1.00

# 15) Compound 3g (*E*-isomer)



13C



```
Current Data Parameters
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PROCNO    1

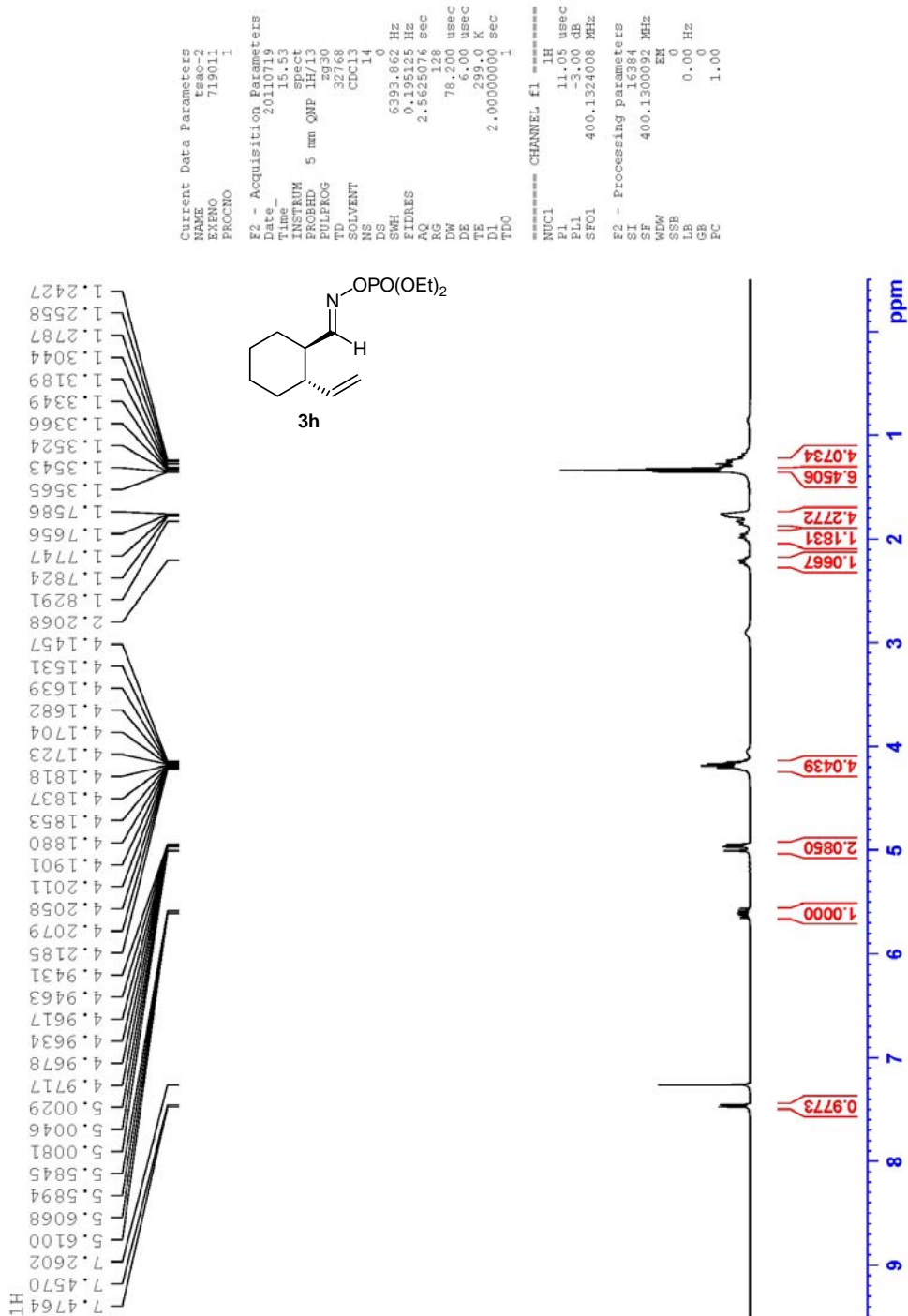
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Time      16.25
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PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         225
DS         4
SWH        25510.203 Hz
FIDRES     0.389255 Hz
AQ         1.2845556 sec
RG         2050
RG         2050
DM         19.600 usec
DE         7.00 usec
TE         299.8 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TDO        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.80 usec
PL1        0.00 dB
SFO1       100.6248423 MHz

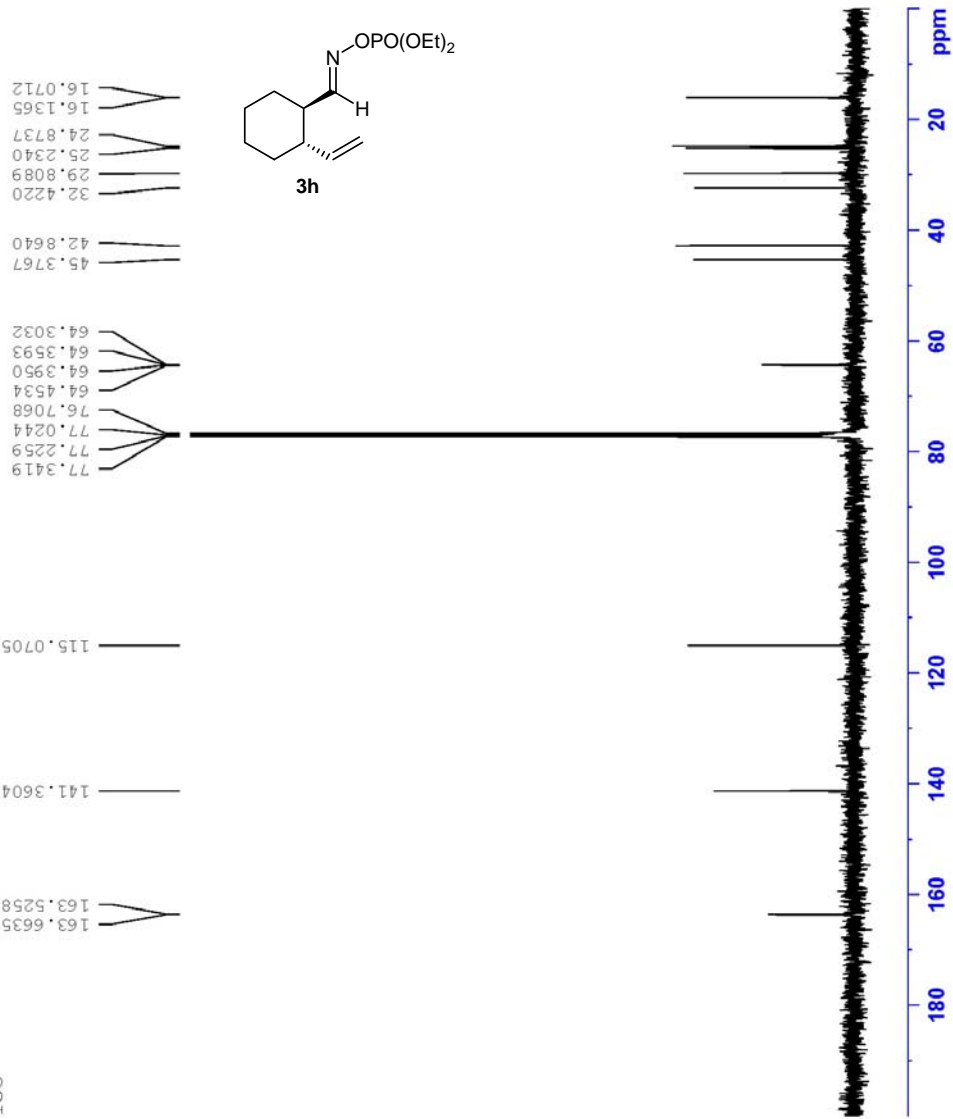
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CPDPRG2   waltz16
NUC2       1H
PCPD2     90.00 usec
PL2        -3.00 dB
PL12       14.00 dB
PL13       17.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         2.00 Hz
GB         0
PC         1.00
```

# 16) Compound 3h



13C



```
Current Data Parameters
NAME      tsao-2
EXPNO    719012
PROCNO   1

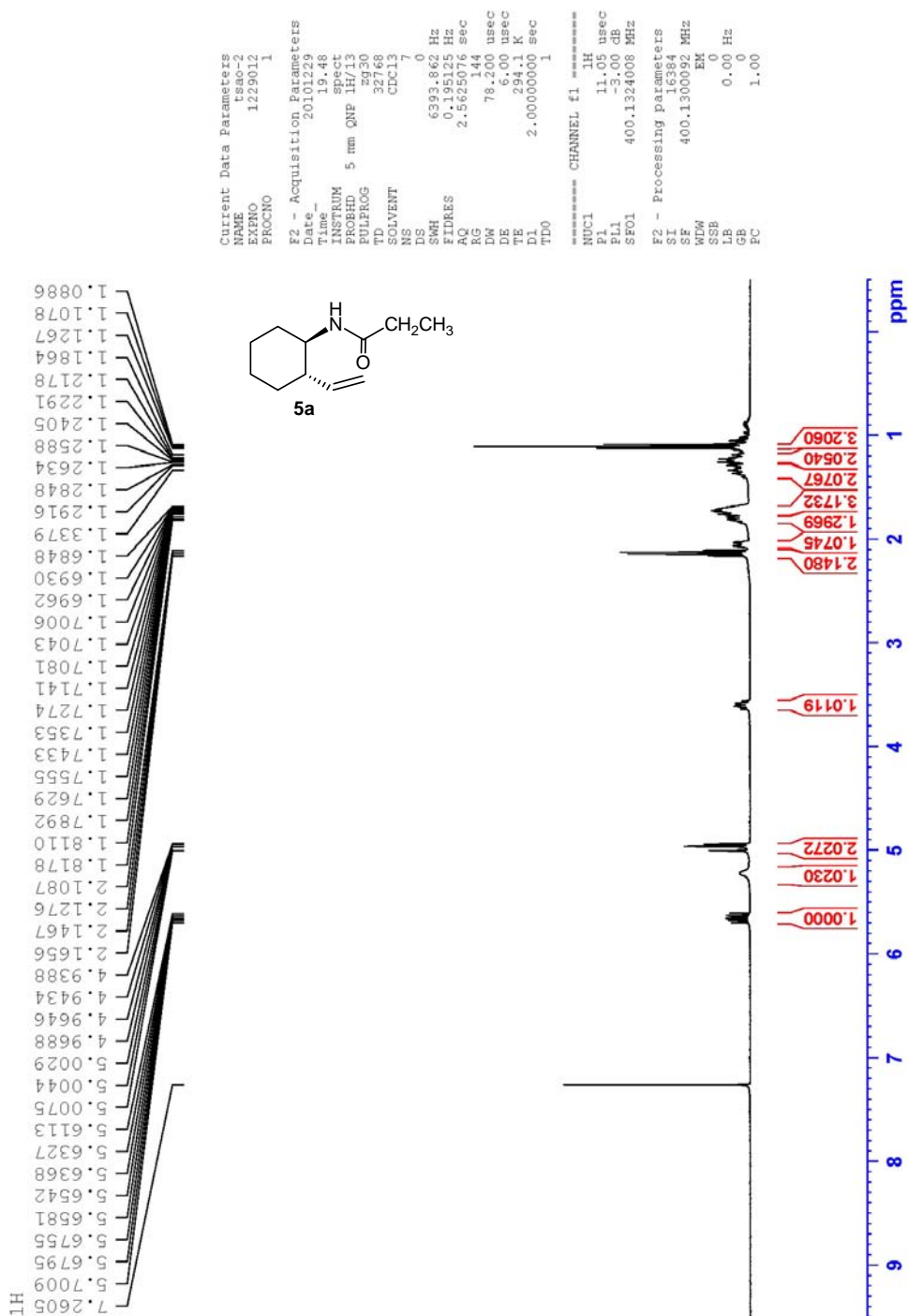
F2 - Acquisition Parameters
Date_    20110719
Time     16.04
INSTRUM spect
PROBHD   5 mm QNP 1H/13
PULPROG zgpg30
TD        65536
SOLVENT  CDCl3
NS        184
DS        4
SWH       25510.203 Hz
FIDRES    0.389255 Hz
AQ         1.2845556 sec
RG         2050
DW         19.600 usec
DE         7.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.8999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.80 usec
PL1        0.00 dB
SFO1       100.6248423 MHz

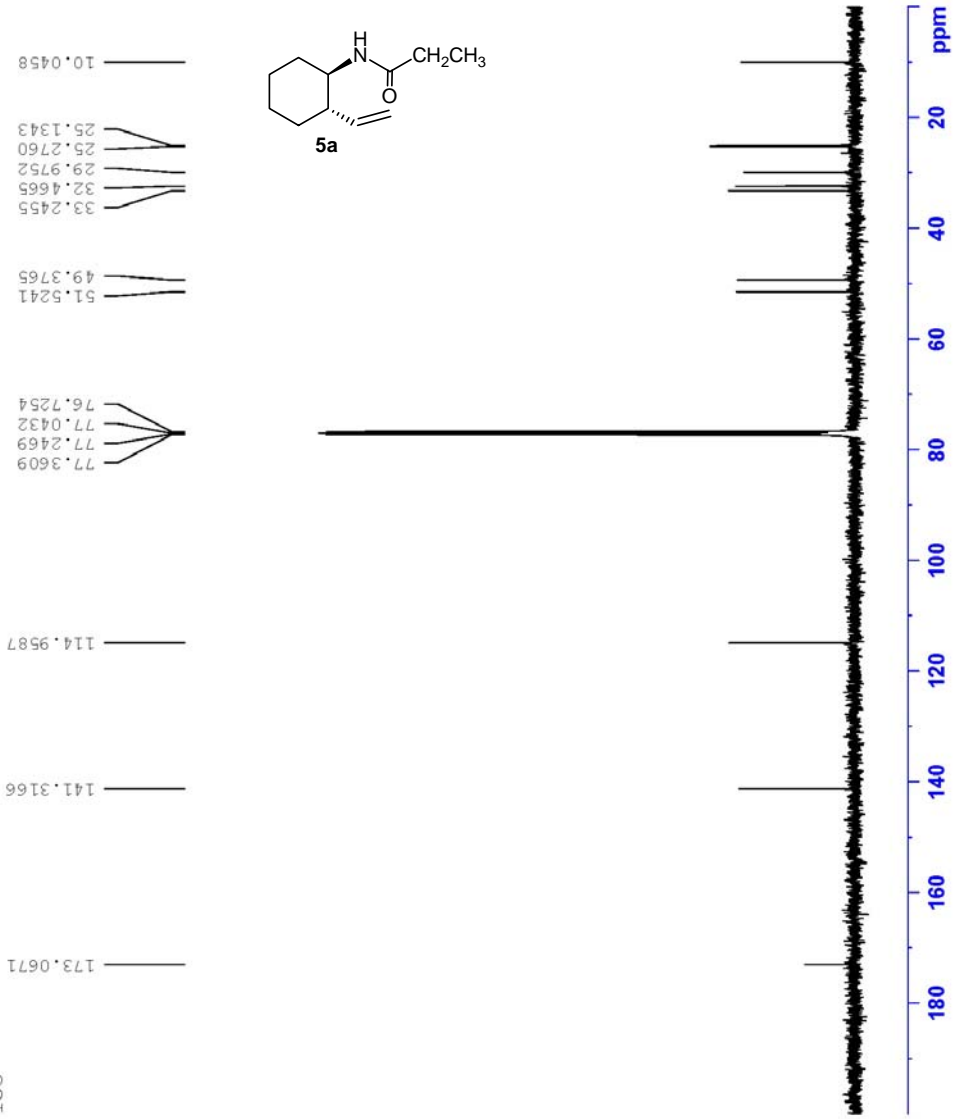
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CPDPRG2   waltz16
MUC2       1H
PCPD2      90.00 usec
PL2        -3.00 dB
PL12       14.00 dB
PL13       17.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         2.00 Hz
GB         0
PC         1.00
```

# 17) Compound 5a



13C



Current Data Parameters  
NAME tesao-2  
EXNO 1229013  
PROCNO 1

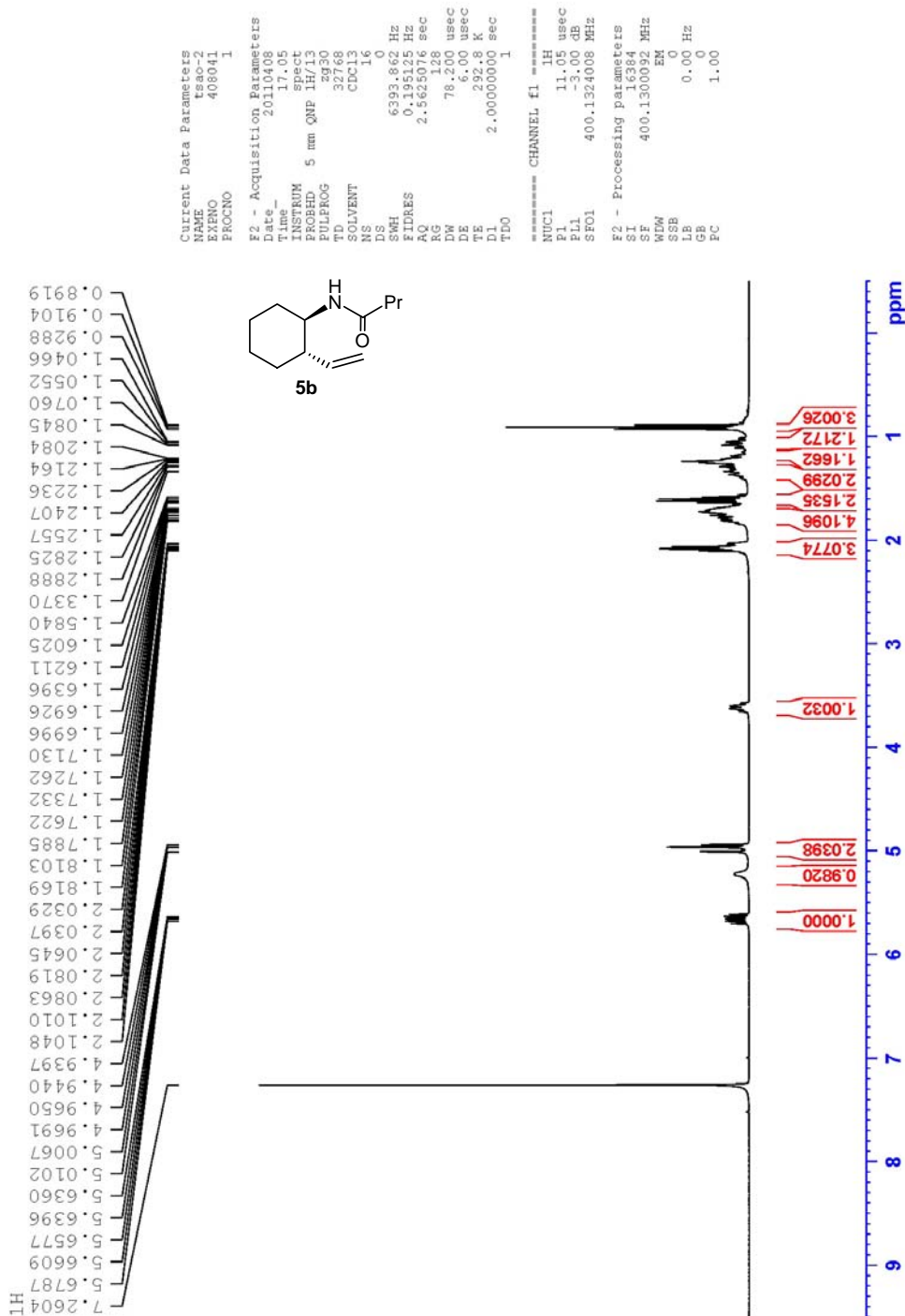
F2 - Acquisition Parameters  
Date\_ 20101229  
Time\_ 19.51  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 200  
DS 4  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2845556 sec  
RG 2050  
DW 19.600 usec  
DE 7.00 usec  
TE 294.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.8999998 sec  
TDO 1

===== CHANNEL F1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248423 MHz

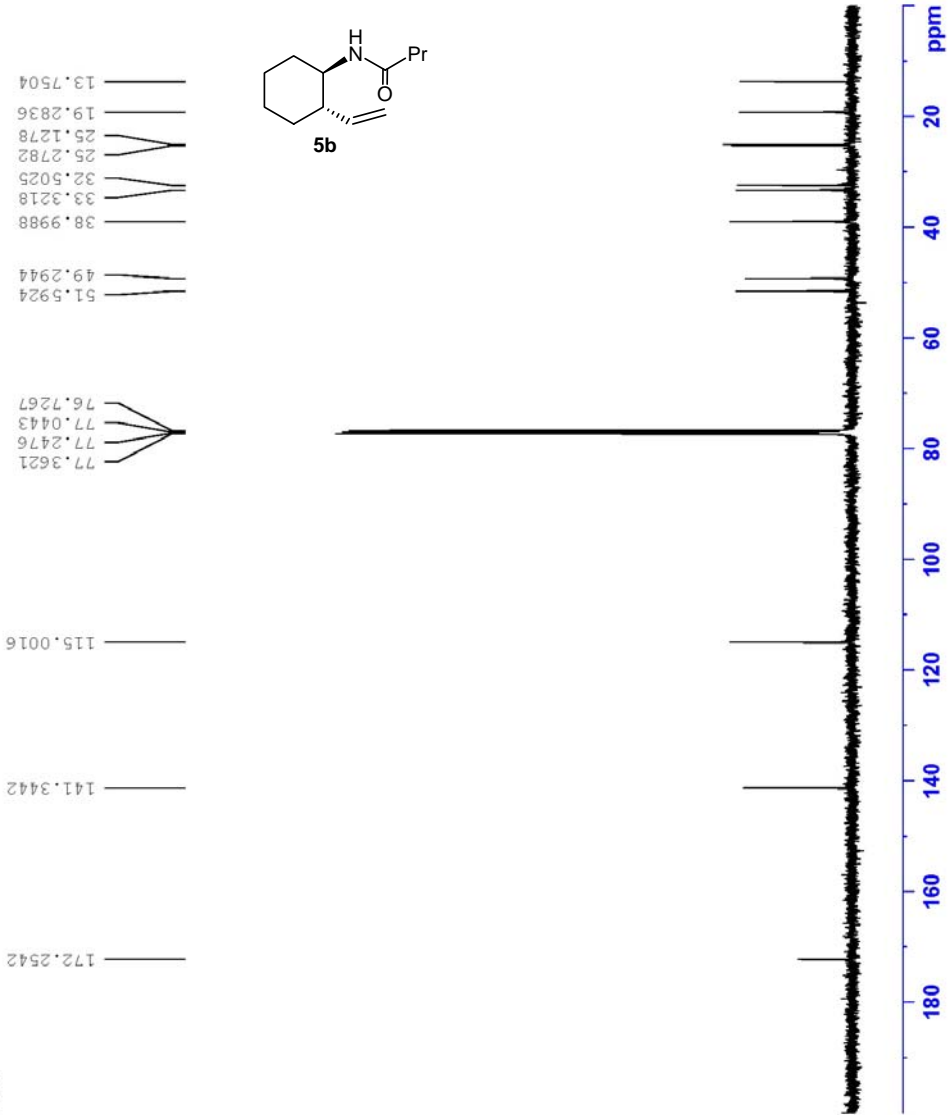
===== CHANNEL F2 =====  
CPDPRG2 waltz16  
MUC2 1H  
PCPD2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.00

# 18) Compound 5b



13C



Current Data Parameters  
NAME Tsao-2  
EXPNO 408042  
PROCNO 1

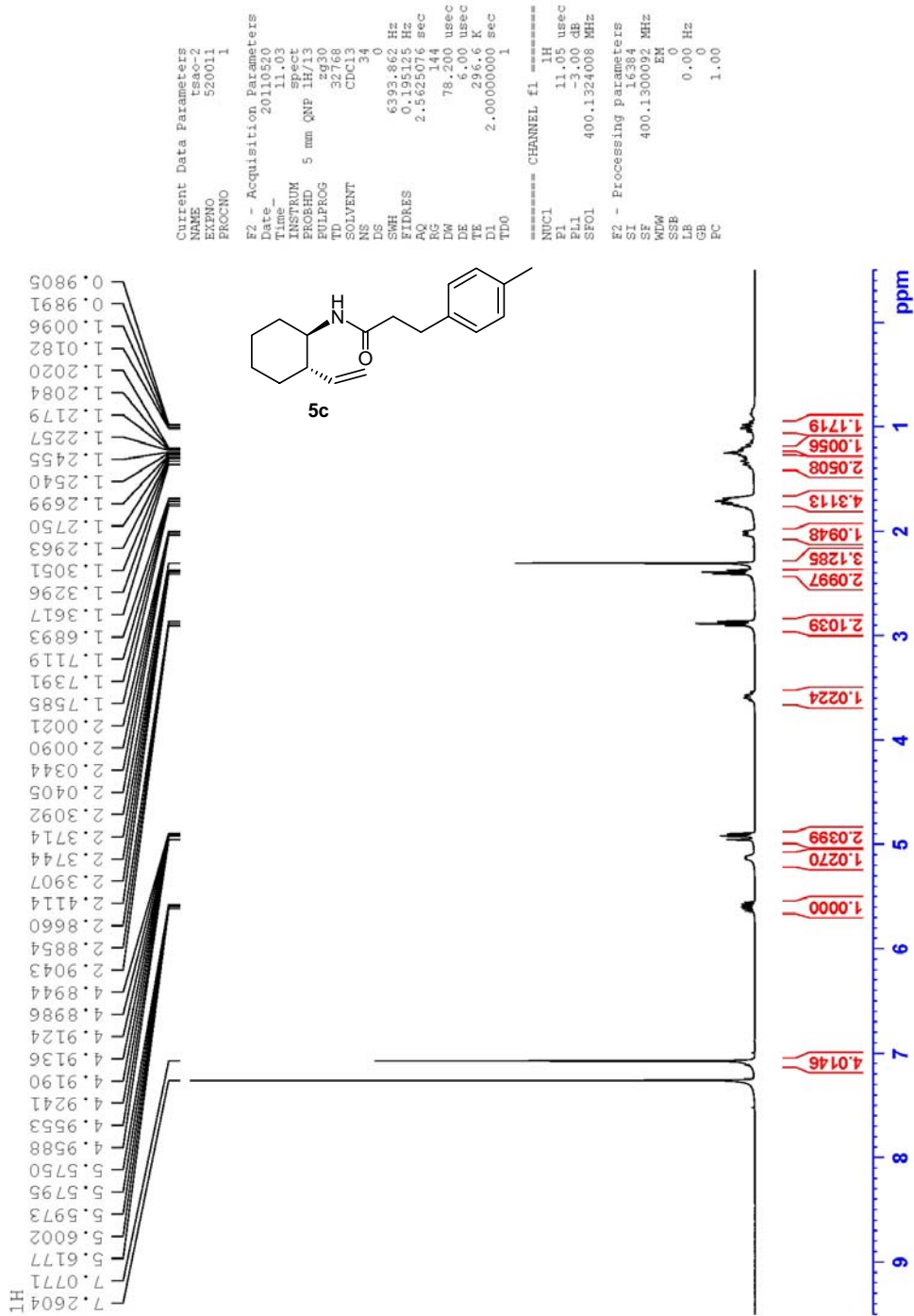
F2 - Acquisition Parameters  
Date\_ 20110408  
Time\_ 17.15  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 186  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2845556 sec  
RG 19.2050  
DW 19.700 usec  
DE 263.3 K  
TE 293.2 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999998 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

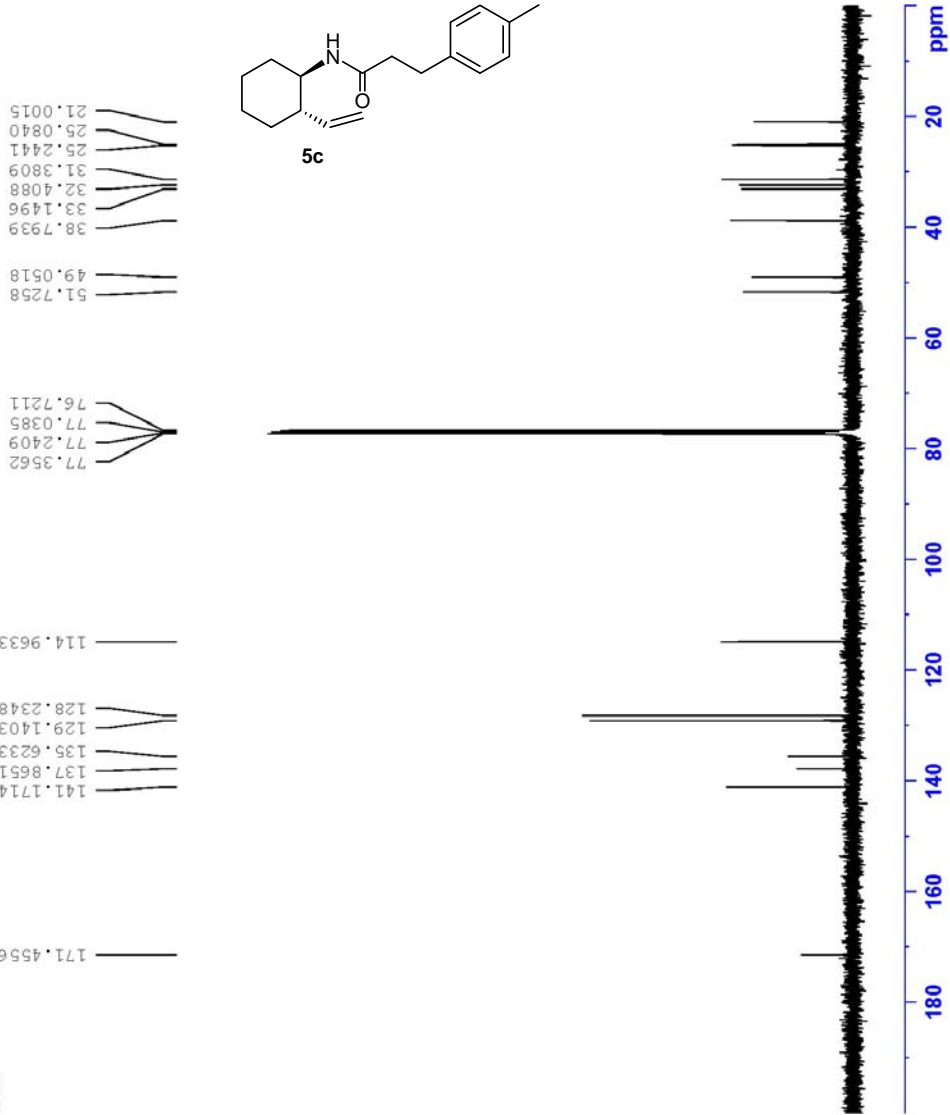
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 13C  
P2 9.80 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDM EM  
SSB 0  
LB 2.00 Hz  
GB 0  
FC 1.00

# 19) Compound 5c



13C



Current Data Parameters  
NAME Esao-2  
EXPNO 520012  
PROCNO 1

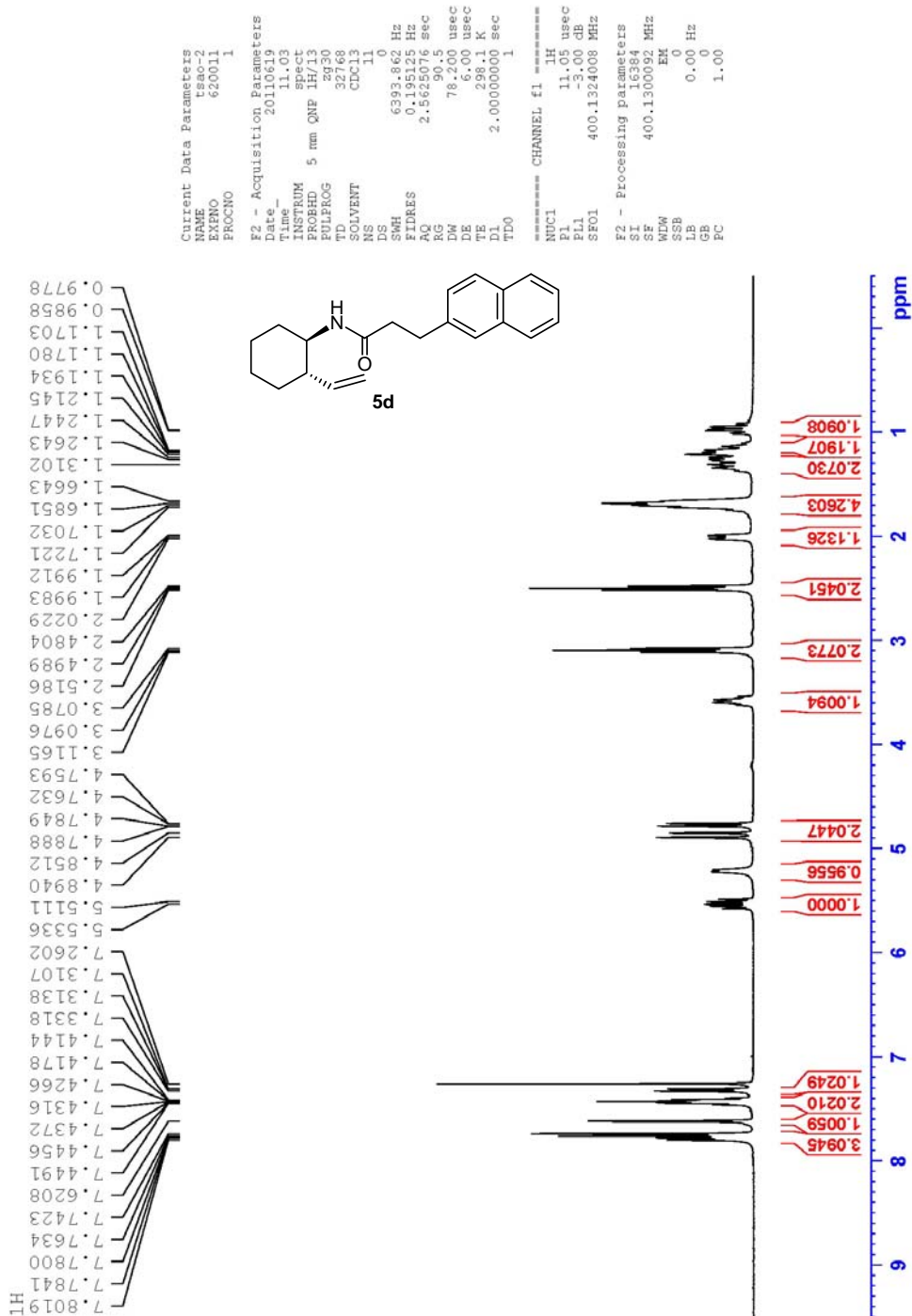
F2 - Acquisition Parameters  
Date\_ 20110520  
Time\_ 11.11  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 249  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.284556 sec  
RG 19.2050  
DW 19.600 usec  
DE 7.000 usec  
TE 296.2 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

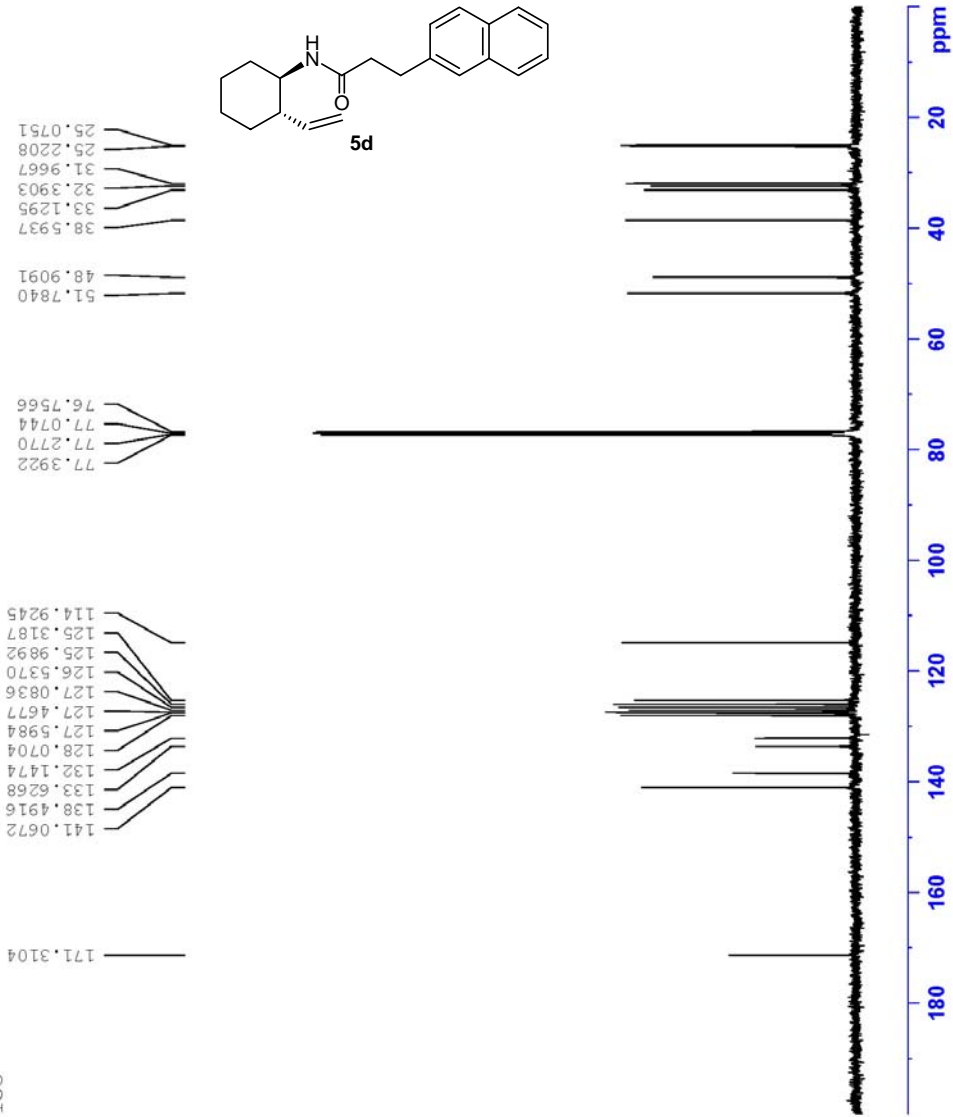
===== CHANNEL f2 =====  
CHPROG2 waltz16  
NUC2 13C  
P2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

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

## 20) Compound 5d



13C



Current Data Parameters  
NAME tsao-2  
EXPNO 620012  
PROCNO 1

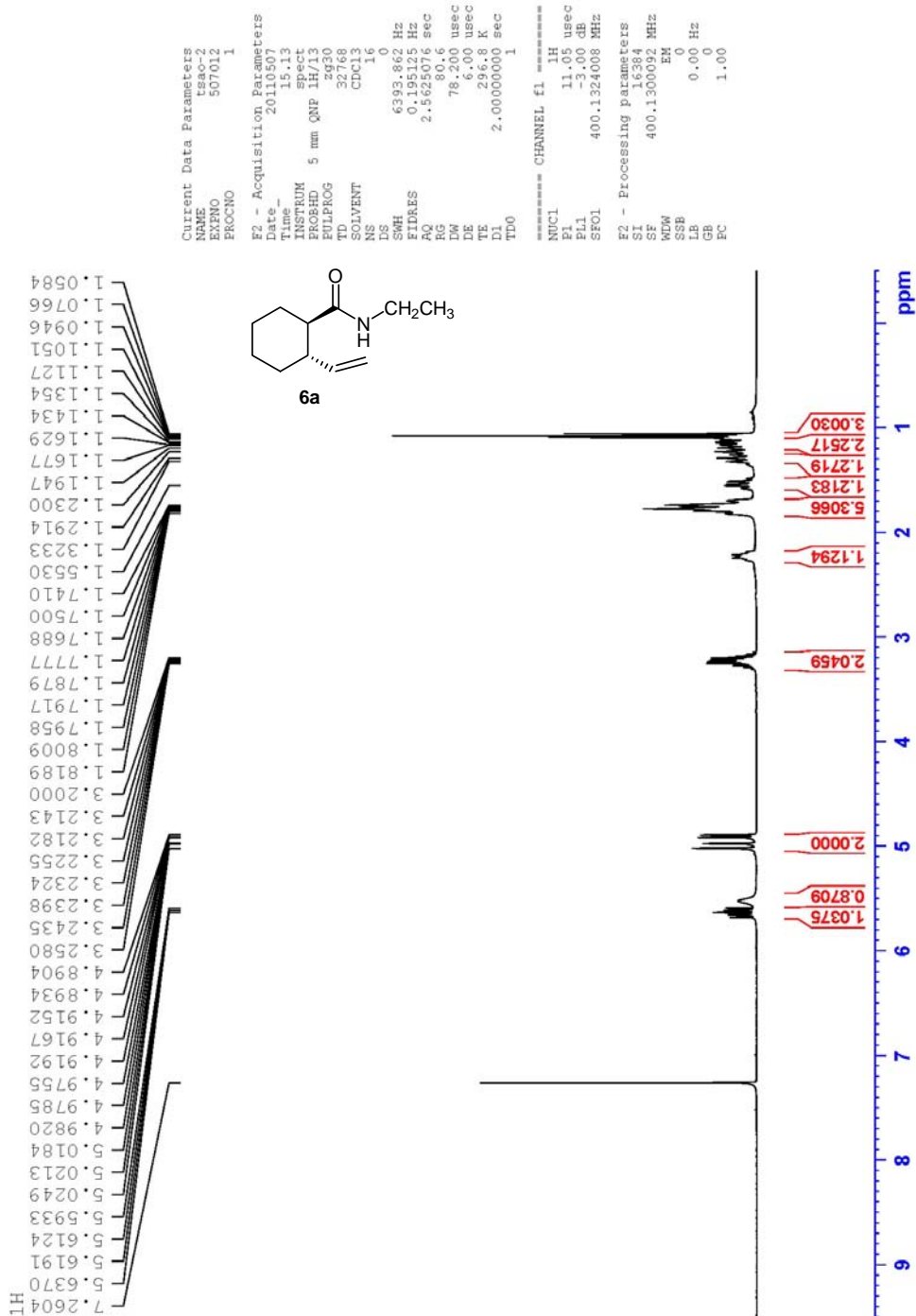
F2 - Acquisition Parameters  
Date\_ 20110619  
Time 11.09  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 340  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2845556 sec  
RG 2050  
DW 19.600 usec  
DE 7.00 usec  
TE 298.16 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999996 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

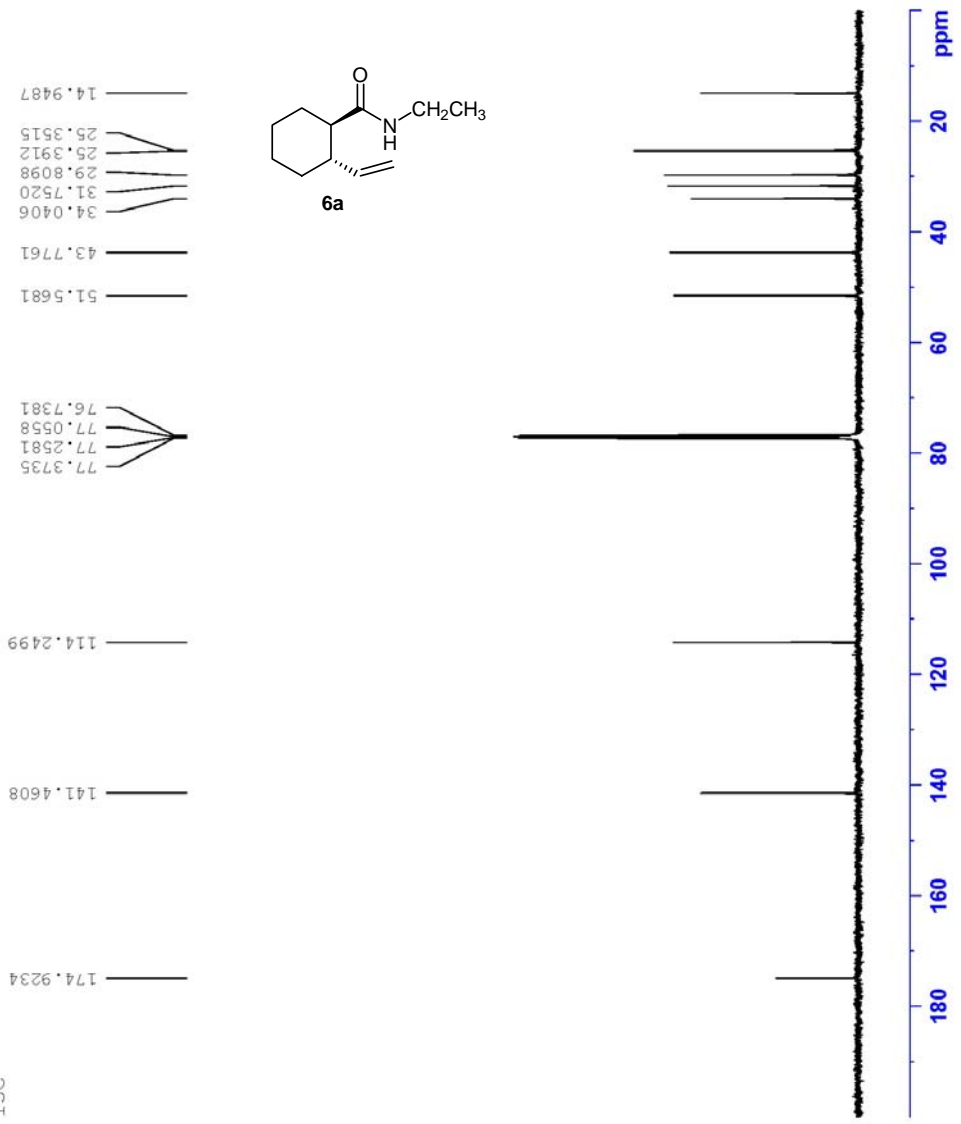
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.00

# 21) Compound 6a



13C



Current Data Parameters  
NAME tsao-2  
EXPNO 507013  
PROCNO 1

F2 - Acquisition Parameters

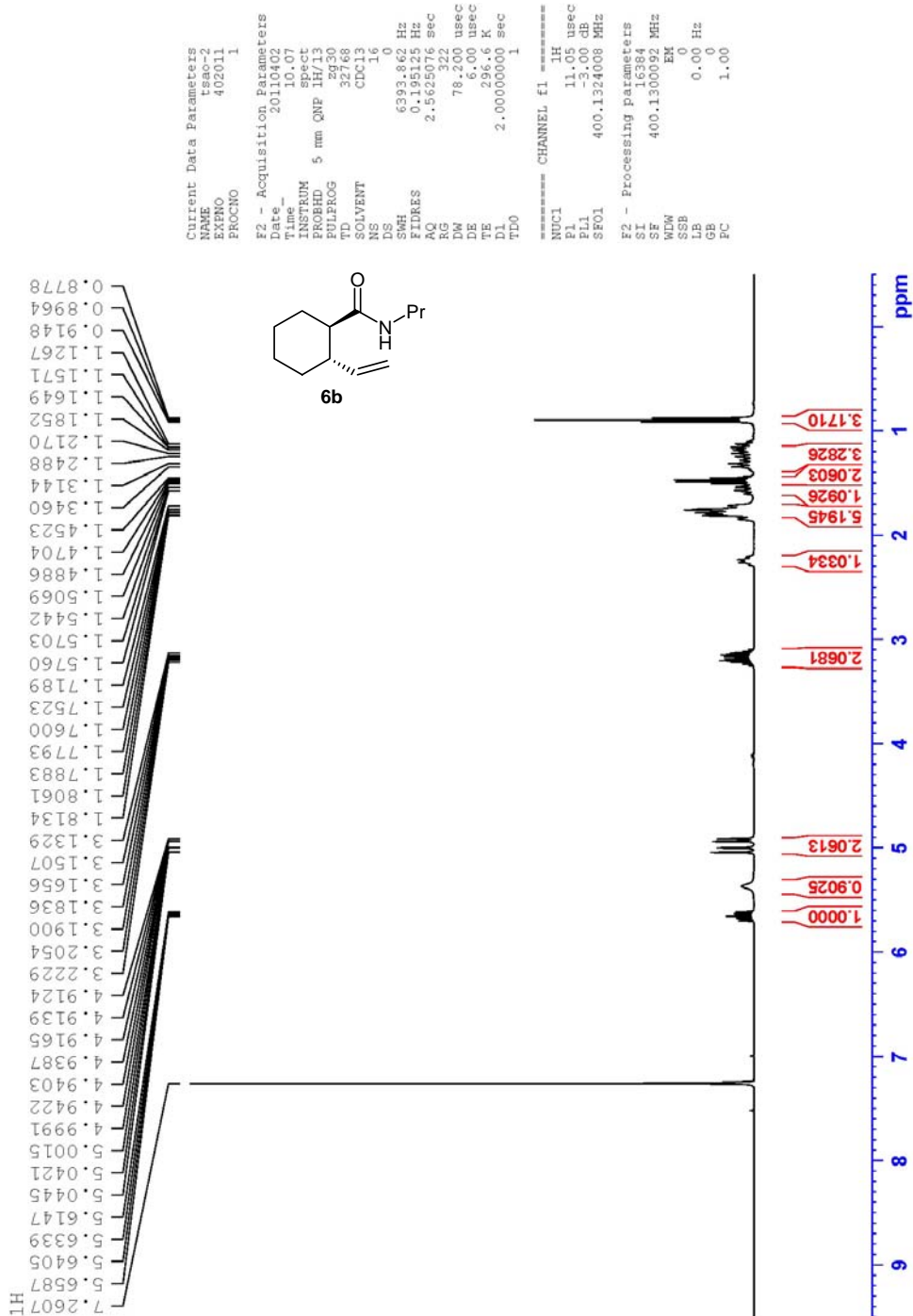
Date\_ 20110507  
Time 15.18  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 514  
DS 4  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2845556 sec  
RG 2050  
DM 19.600 usec  
DE 7.00 usec  
TE 297.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PL1 0.00 dB  
SFO1 100.628425 MHz

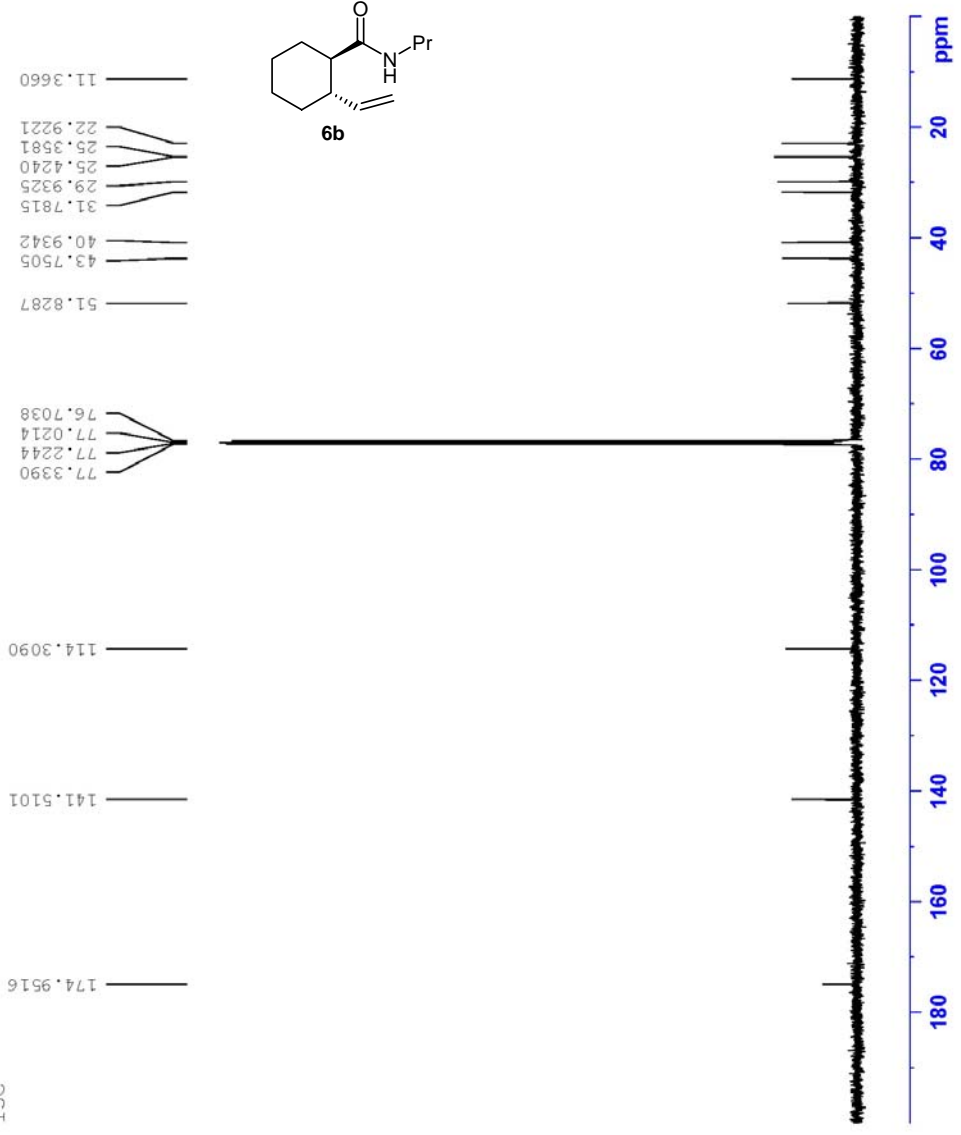
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
SW 6553.600 Hz  
SEB 0  
LB 2.00 Hz  
GB 0  
PC 1.00

## 22) Compound 6b



13C



Current Data Parameters  
NAME tssco-2  
SERNO 402012  
PROCNO 1

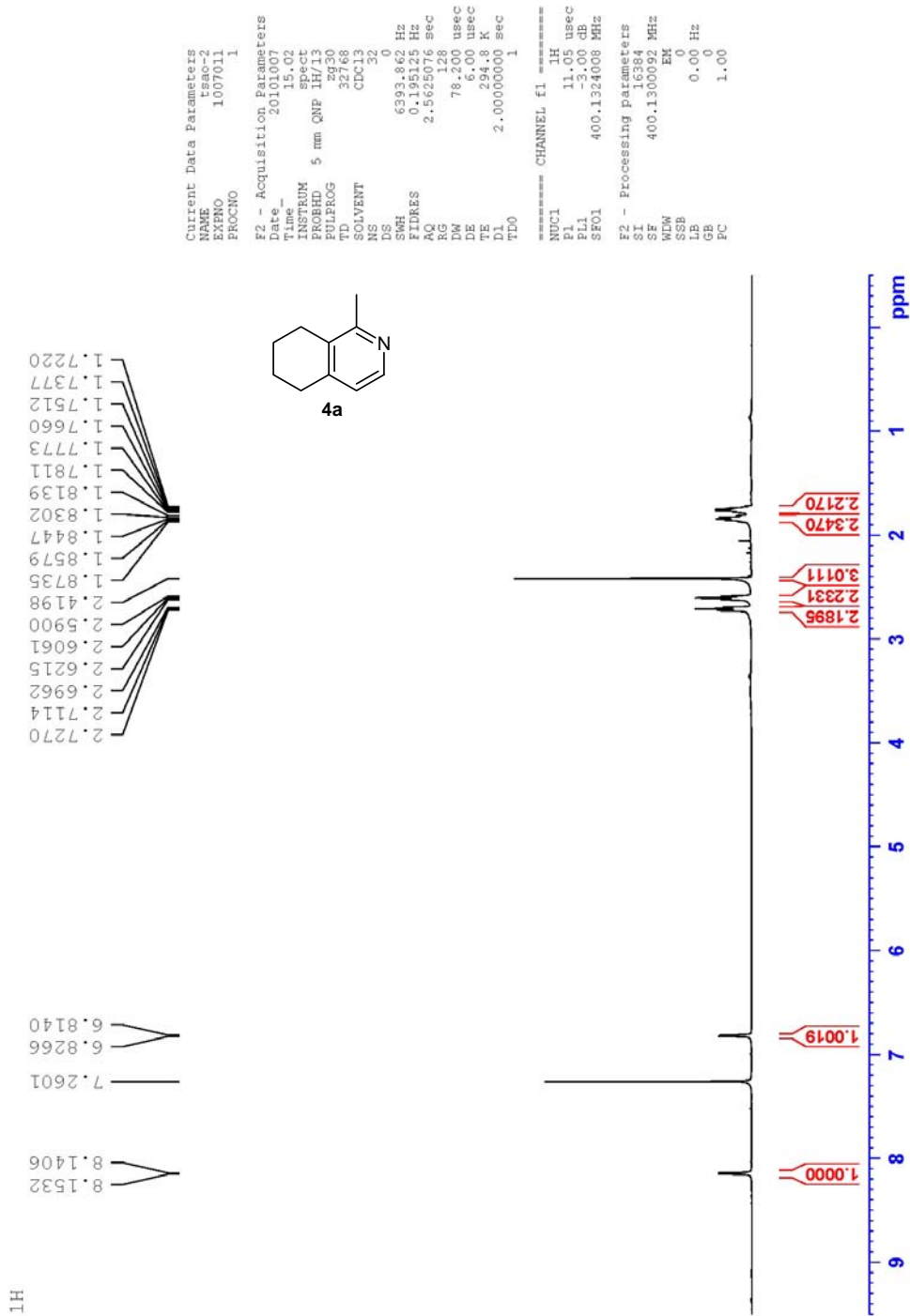
F2 - Acquisition Parameters  
Date\_ 20110402  
Time\_ 10.20  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CPC13  
NS 244  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2845556 sec  
RG 655.36  
DM 19.600  
DE 7.00 usec  
TE 287.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL F1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

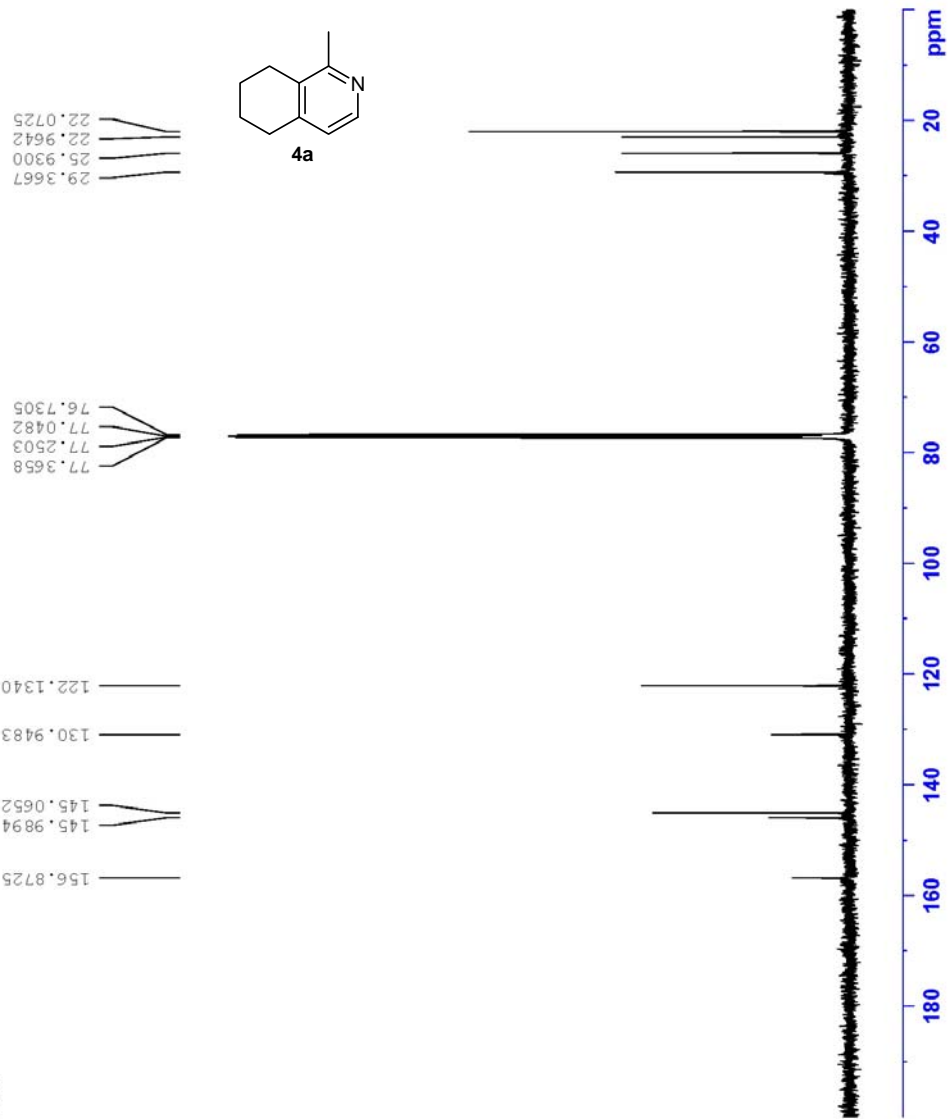
===== CHANNEL F2 =====  
CDEPRG2 waltz16  
NUC2 1H  
P2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.00

### 23) Compound 4a



13C



```
Current Data Parameters
NAME      tss0-2
EXPNO    1007012
PROCNO   1

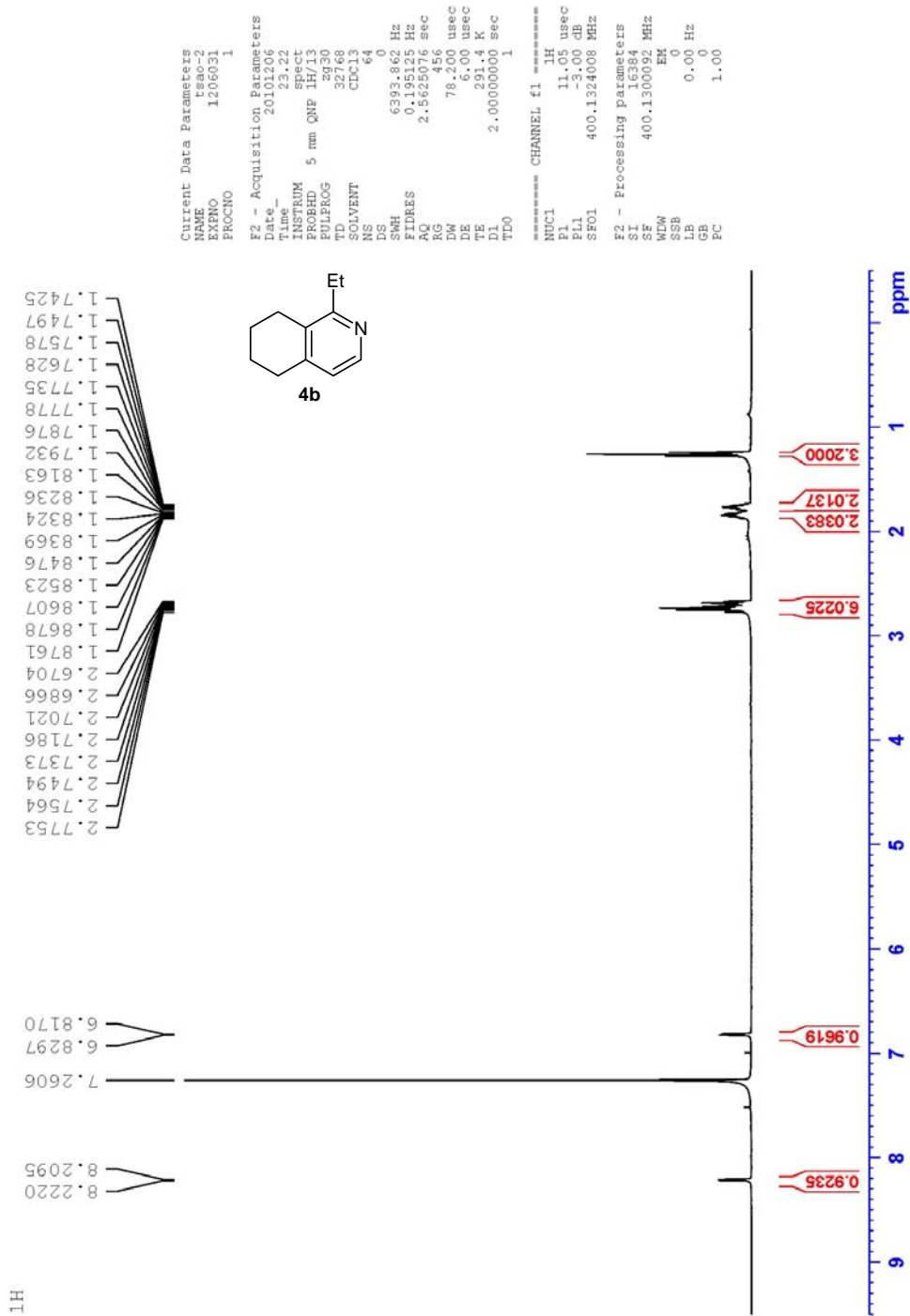
F2 - Acquisition Parameters
Date_    20101007
Time     15.11
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       300
DS       4
SWH      25510.203 Hz
FIDRES   0.389255 Hz
AQ       1.2884556 sec
RG       2050
DW       19.600 usec
DE       7.00 usec
TE       295.2 K
DL       2.0000000 sec
dL1      0.0300000 sec
DELTA    1.8999998 sec
TD0      1

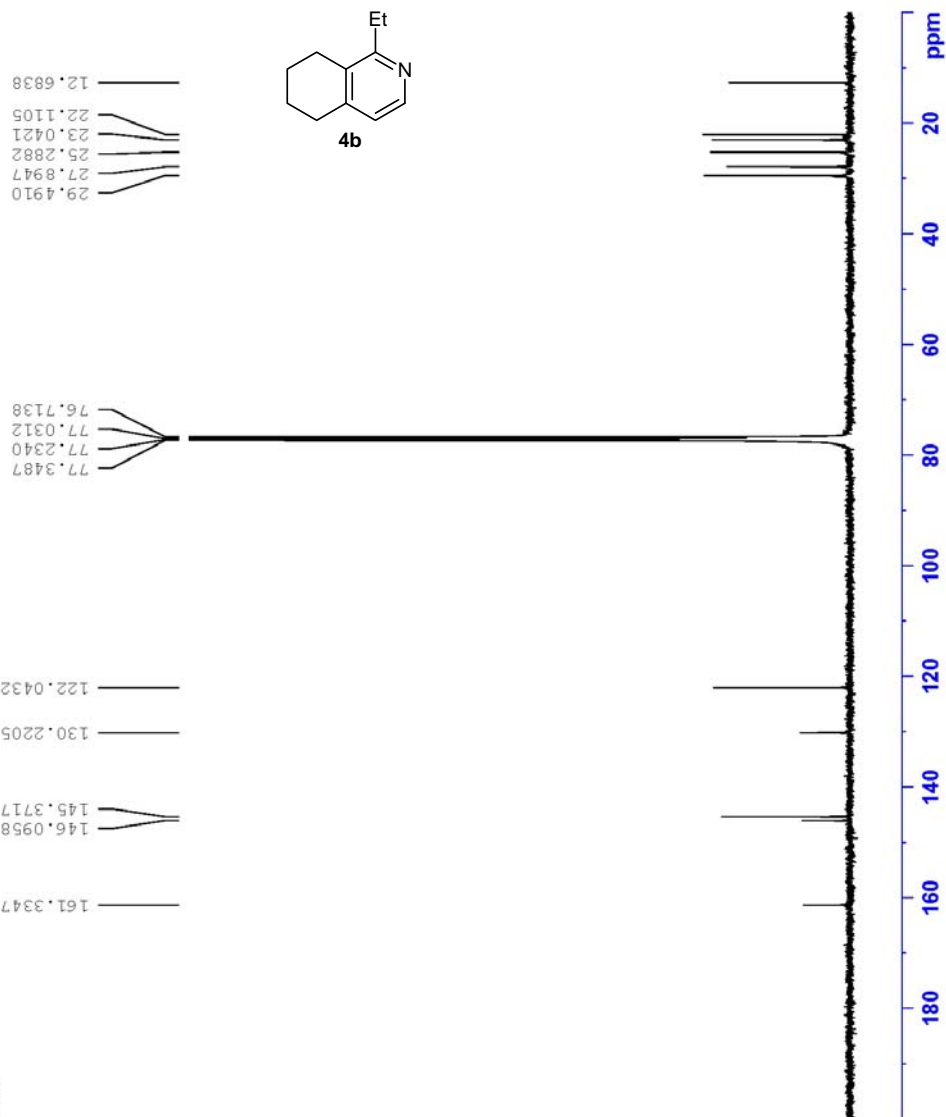
===== CHANNEL f1 =====
NUC1     13C
P1       8.80 usec
PL1      0.0 dB
SFO1     100.6248425 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    90.00 usec
PL2      -3.00 dB
PL12     14.00 dB
PL13     17.00 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       2.00 Hz
GB       0
PC       1.00
```

## 24) Compound 4b





```

Current Data Parameters
NAME      F5ao-2
EXPNO    1206032
PROCNO   1

F2 - Acquisition Parameters
Date_    20101206
Time     23.30
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        11247
DS        0
SWH       25510.203 Hz
FIDRES    0.389255 Hz
AQ        1.284556 sec
RG         1620
DW         19.500 usec
DE         2.01 k
TE         300.2 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TDO       1

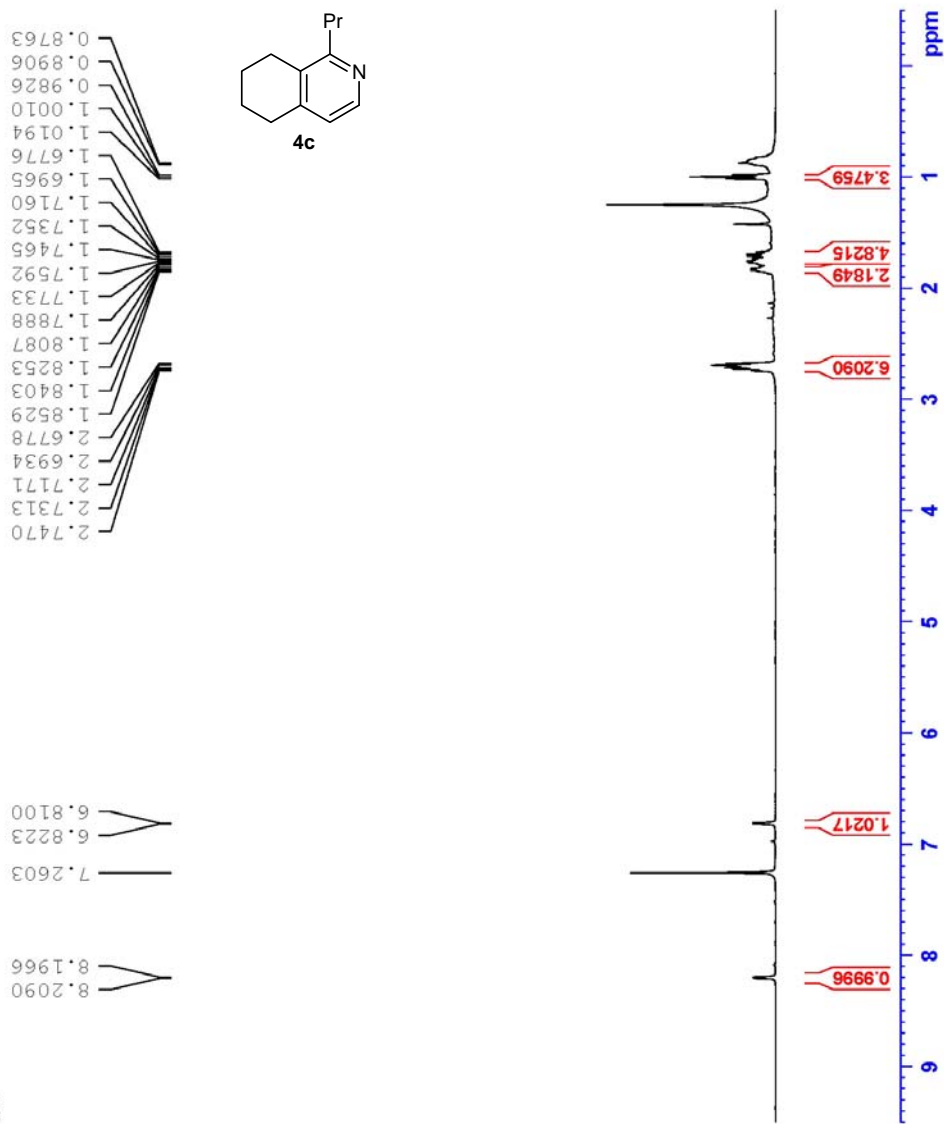
===== CHANNEL f1 =====
NUC1       13C
P1         9.80 usec
PL1        0.00 dB
SFO1       100.6248425 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       13C
P2         90.10 usec
PL2        -3.00 dB
SFO2       100.6248425 MHz
=====
PL12       14.00 dB
PL13       17.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         2.00 Hz
GB         0
FC         1.00
  
```

# 25) Compound 4c

1H



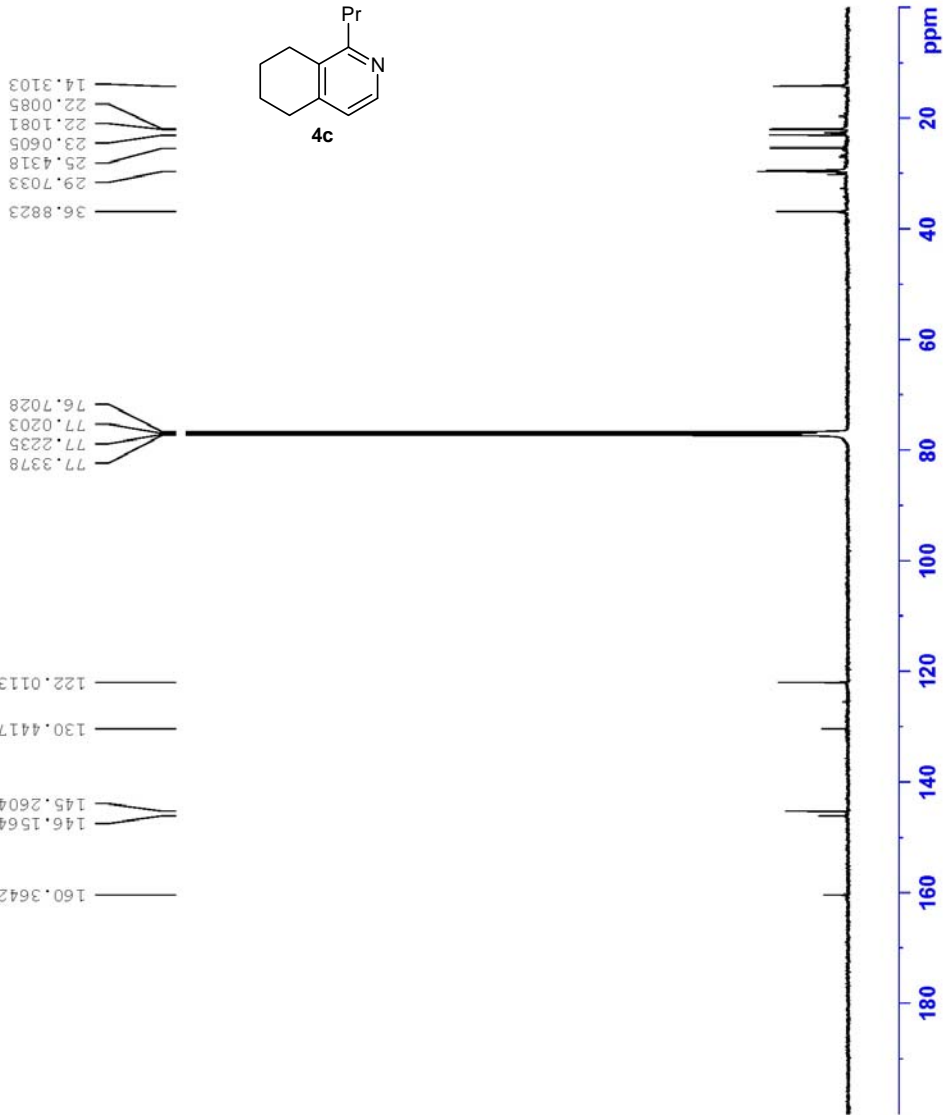
```

Current Data Parameters
NAME      tsgo-2
EXPNO    426021
PROCNO   1

F2 - Acquisition Parameters
Date_    20110426
Time     20.24
INSTRUM spect
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD        32768
SOLVENT  CDCl3
NS        48
DS        0
SWH       6393.862 Hz
FIDRES    0.195125 Hz
AQ         2.5625076 sec
RG         78.161 usec
DE         6.00 usec
TE         293.1 K
D1         2.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1        11.05 usec
PL1       -3.00 dB
SFO1      400.1324008 MHz

F2 - Processing parameters
SI         16384
SF         400.1300052 MHz
WDW        EM
SSB        0
GB         0.00 Hz
PC         1.00
  
```



```

Current Data Parameters
NAME      tsao-2
EXNO     426032
PROCNO   1

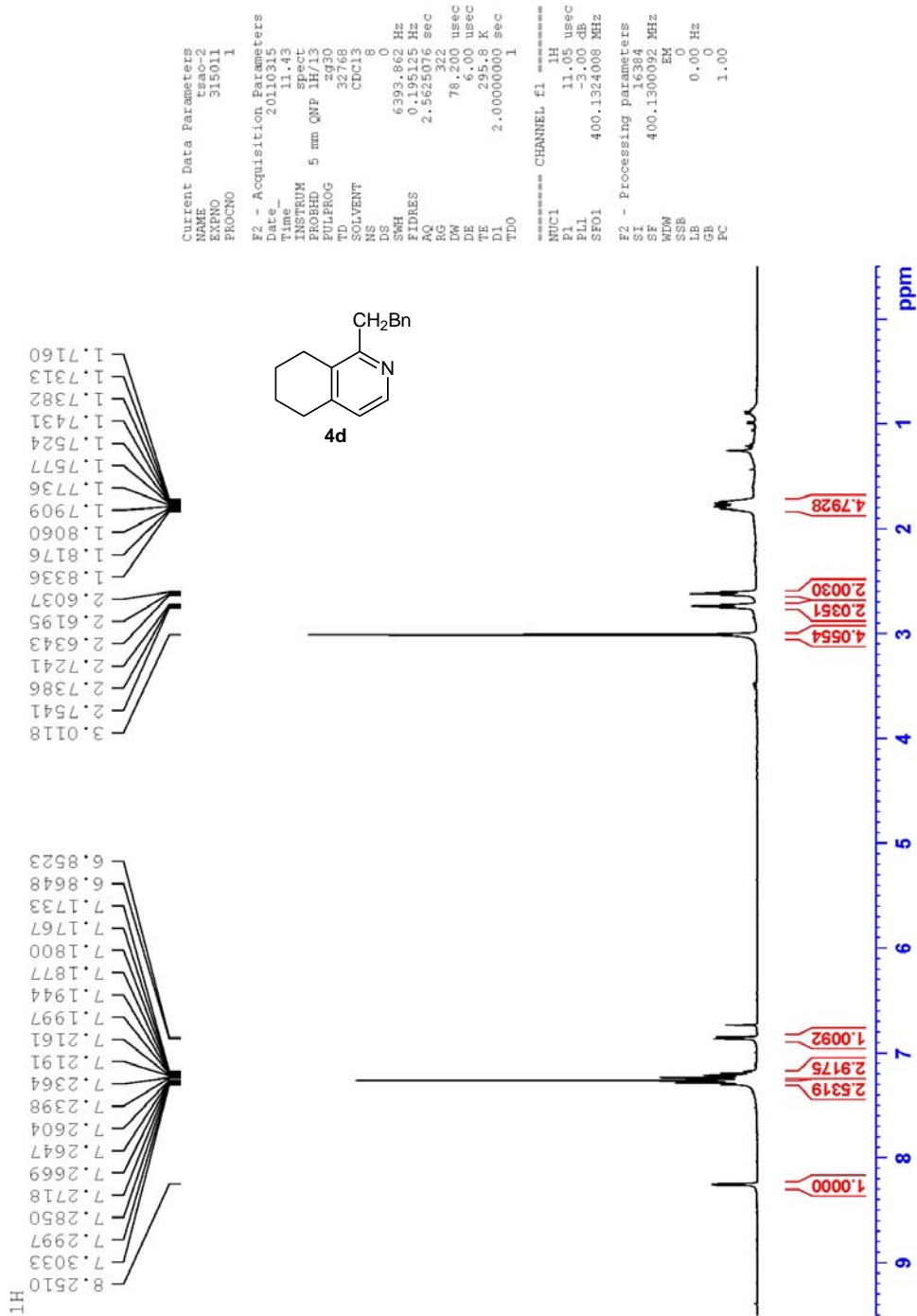
F2 - Acquisition Parameters
Date_    20110426
Time     22.57
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       10899
DS       4
SWH      25510.703 Hz
FIDRES   0.389255 Hz
AQ       1.28845556 sec
RG       1820
DM       19.600 usec
DE       7.00 usec
TE       295.8 K
D1       2.00000000 sec
d11      0.03000000 sec
DELTA    1.89999998 sec
TDO      1

===== CHANNEL f1 =====
NUC1     13C
P1       9.80 usec
PL1      0.00 dB
SFO1     100.628425 MHz

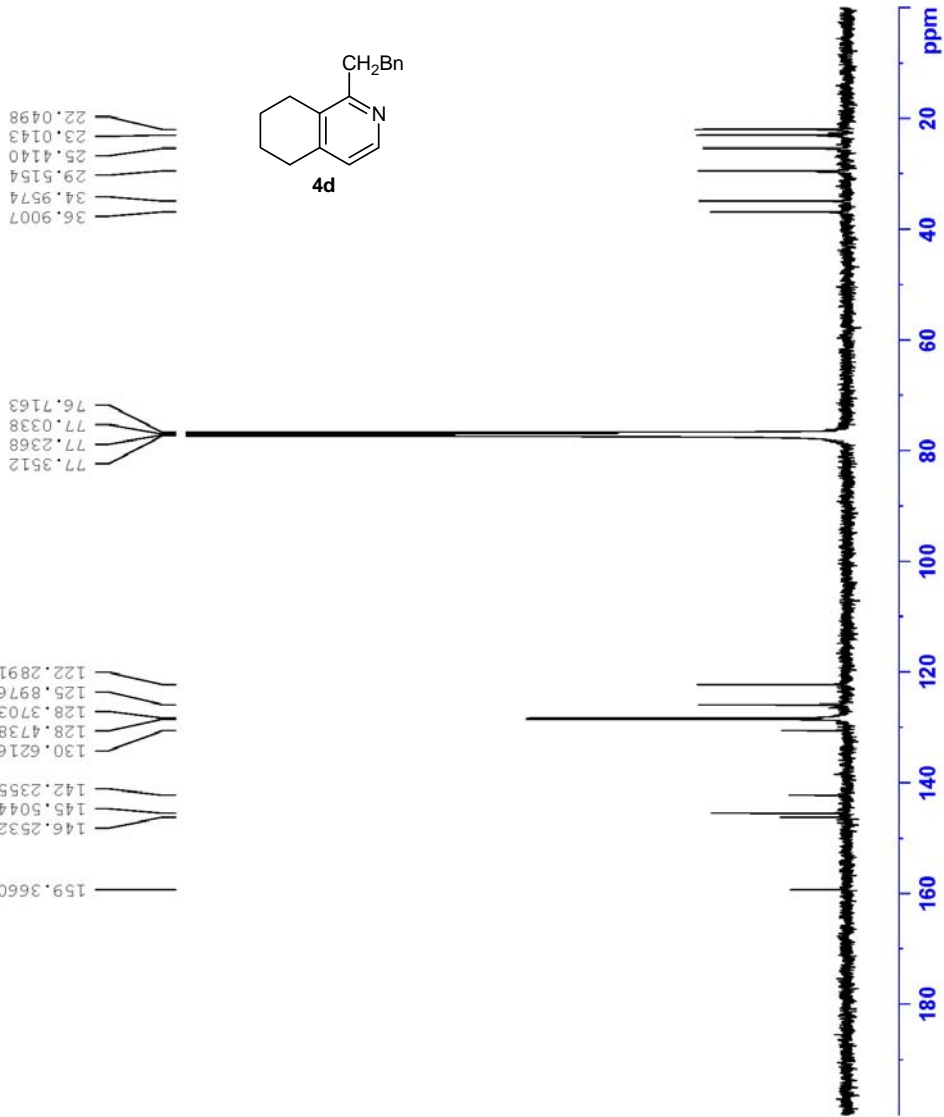
===== CHANNEL f2 =====
CDEPRG2  waltz16
NUC2     1H
PCPD2    90.00 usec
PL2      -3.00 dB
PL12     14.00 dB
PL13     17.00 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI       32768
SF       100.6127690 MHz
WDW      EM
SSB      0
LB       2.00 Hz
GB       0
PC       1.00
    
```

# 26) Compound 4d



13C



```
Current Data Parameters
NAME      tsso-2
EXPNO    123012
PROCNO   1

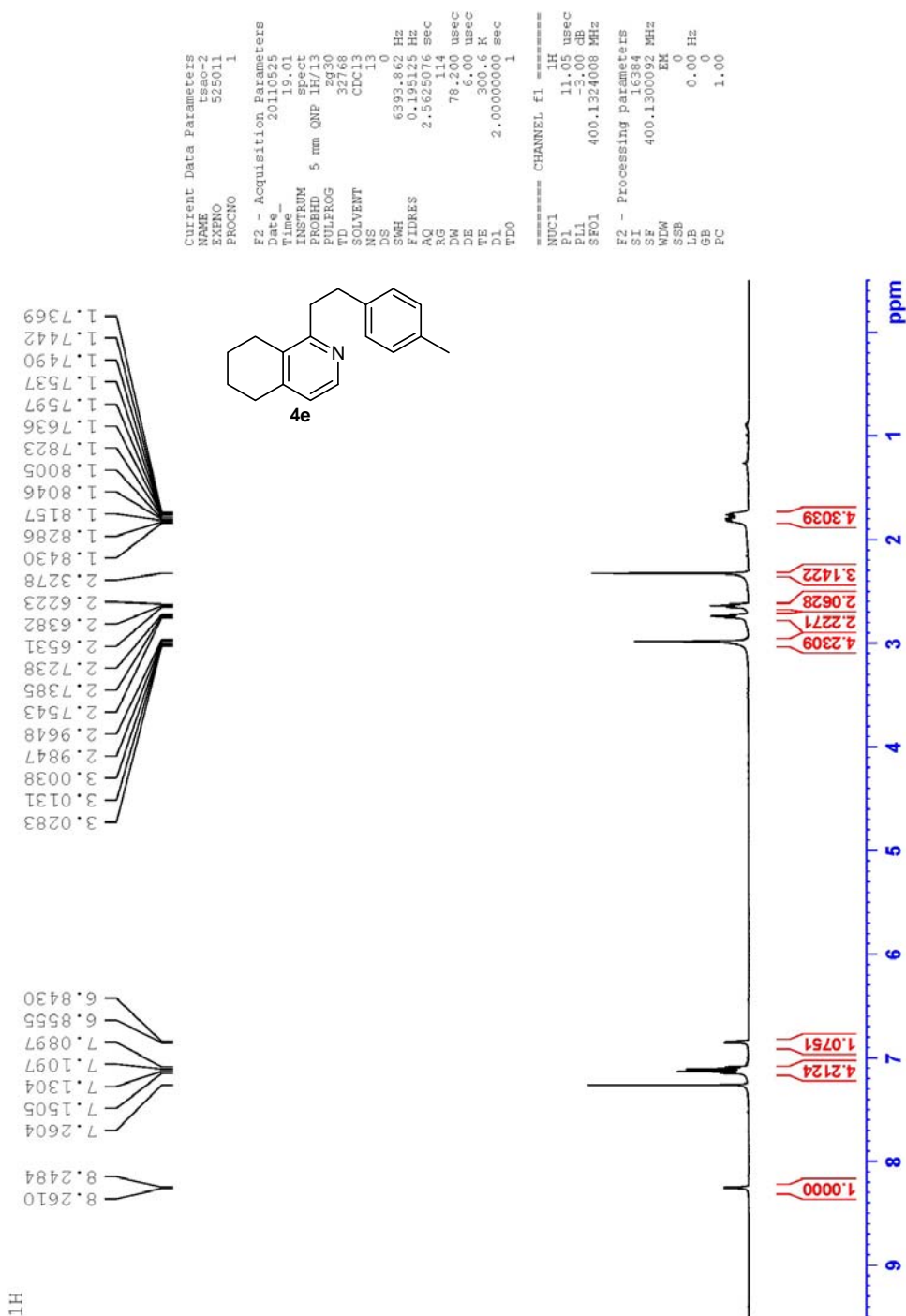
F2 - Acquisition Parameters
Date_    2010123
Time     23.20
INSTRUM  spect
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        11436
DS        4
SWH       25510.203 Hz
FIDRES   0.389255 Hz
AQ        1.2884556 sec
RG        2050
DW        19.600 usec
DE        7.00 usec
TE        292.6 K
DL        2.0000000 sec
d11       0.0300000 sec
DELTA    1.8999998 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        8.80 usec
PL1       0.0 dB
SFO1     100.6248425 MHz

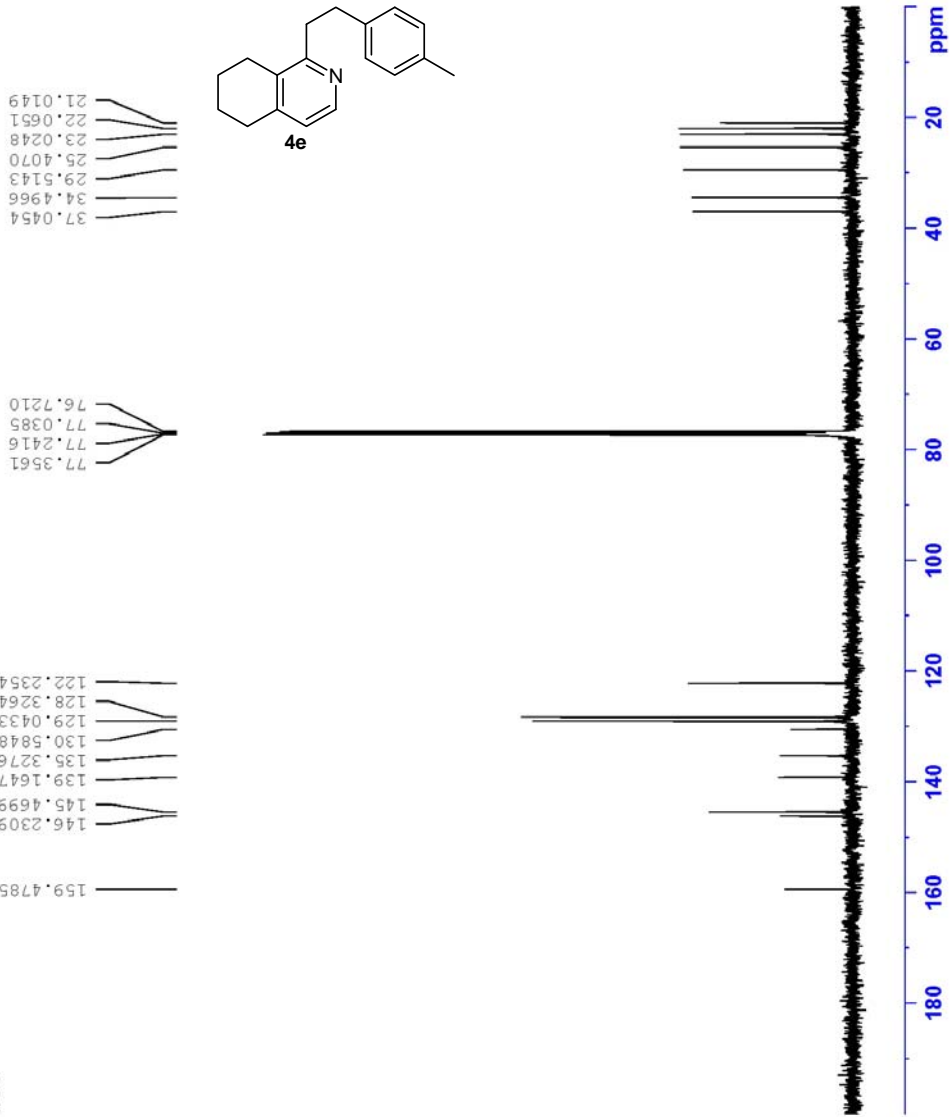
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    90.00 usec
PL2      -3.00 dB
PL12     14.00 dB
PL13     17.00 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        2.00 Hz
GB        0
PC        1.00
```

# 27) Compound 4e



13C



Current Data Parameters  
NAME ES80-2  
EXPNO 525012  
PROCNO 1

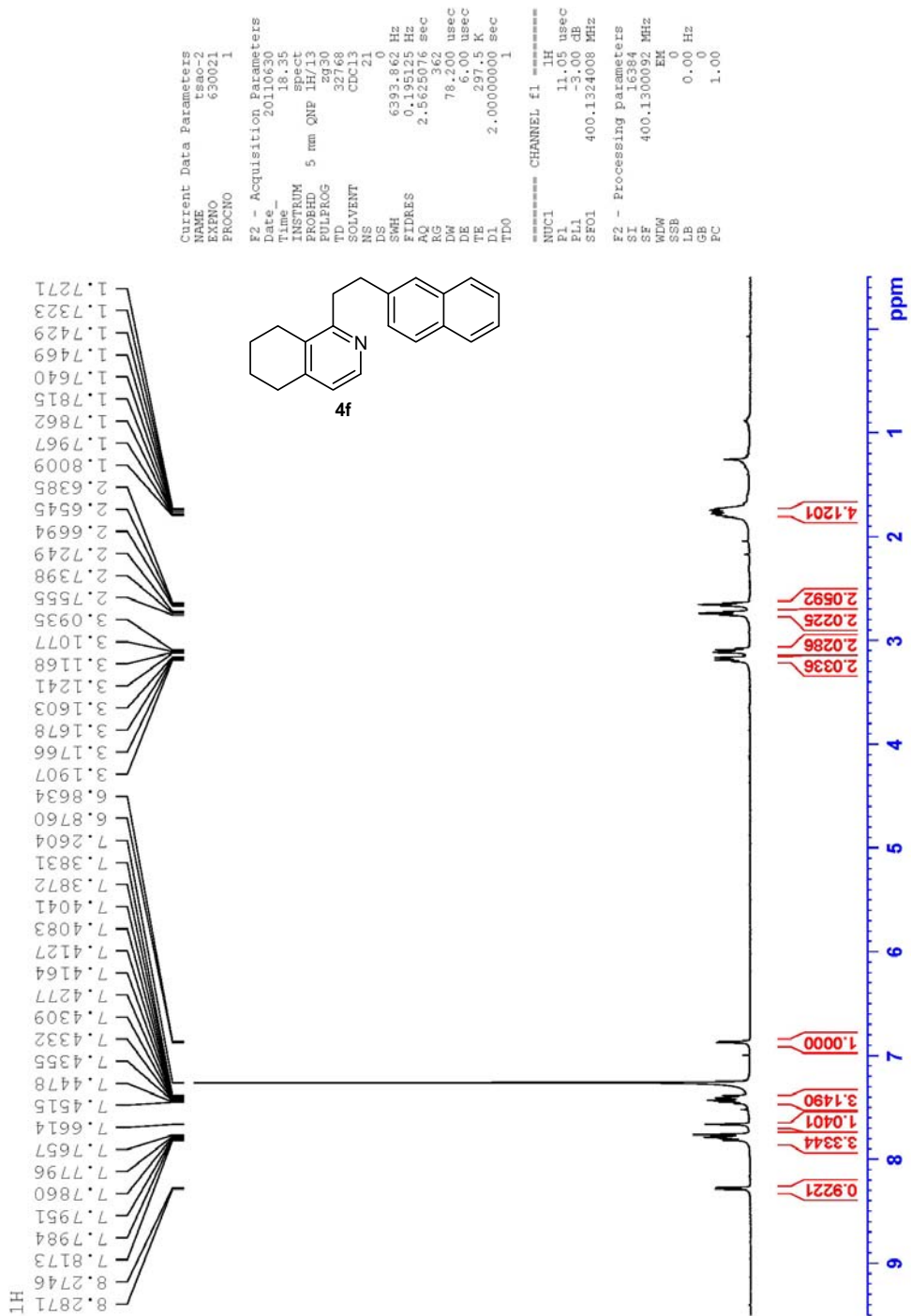
F2 - Acquisition Parameters  
Date\_ 20110525  
Time\_ 19.07  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2845556 sec  
RG 19.2050  
DM 6.00000000  
DE 19.60000000  
TE 301.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL F1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6284825 MHz

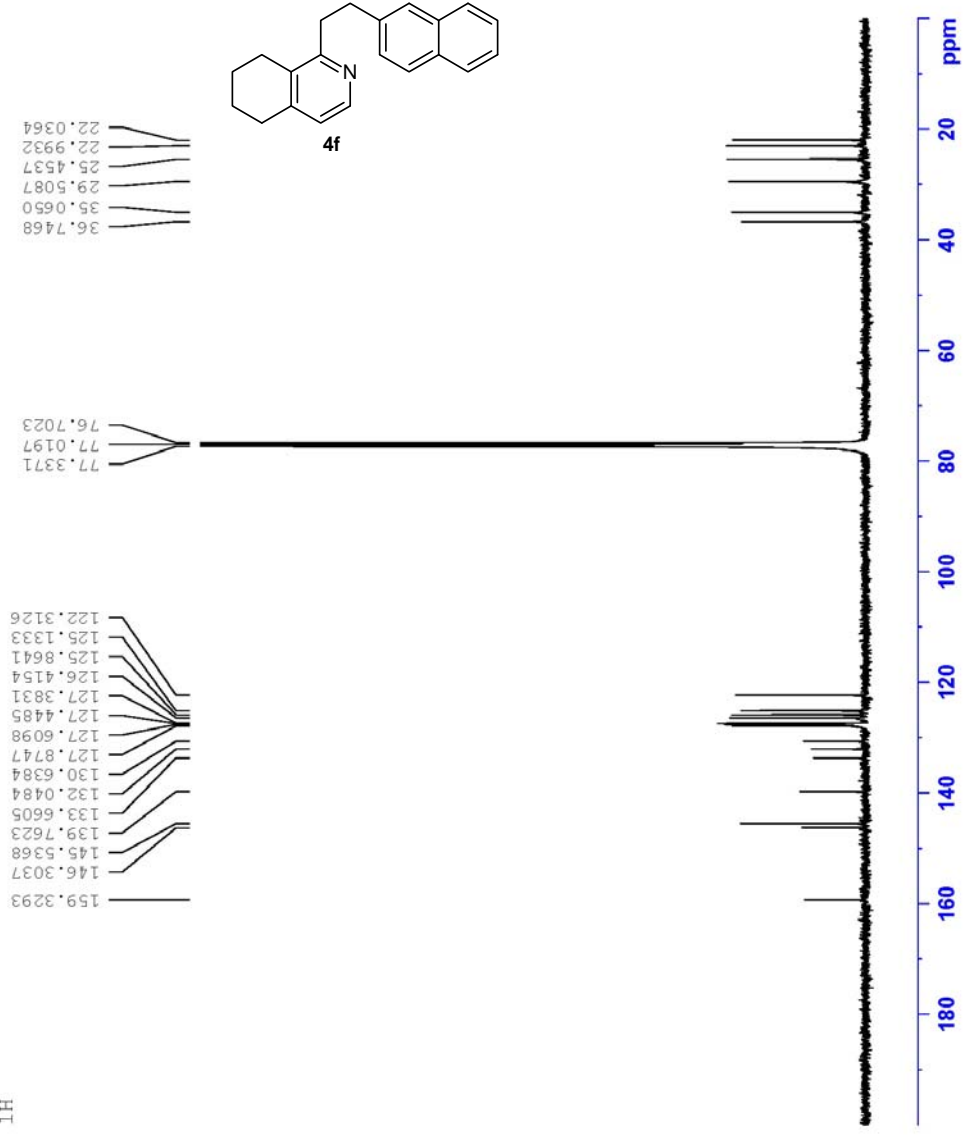
===== CHANNEL F2 =====  
CPDPRG2 waltz16  
NUC2 1H  
P2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
FC 1.00

28) Compound 4f



<sup>1</sup>H



Current Data Parameters  
NAME 1800-2  
F2PRG 701012  
PROCNO 1

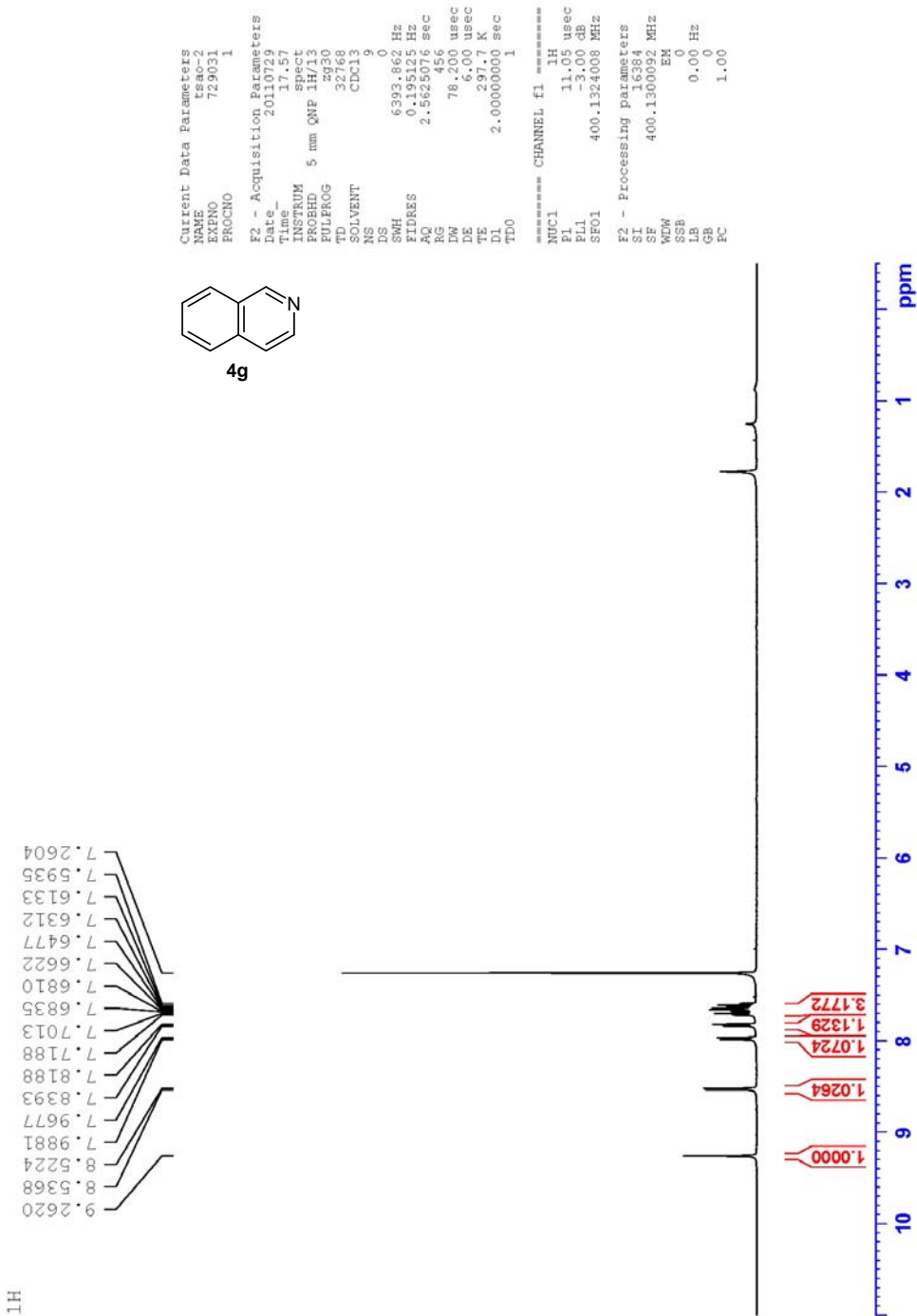
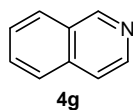
F2 - Acquisition Parameters  
Date\_ 20110701  
Time\_ 22.49  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 11848  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.284556 sec  
RG 256  
SFO1 100.6248425 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.00

F2 - Processing Parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.00

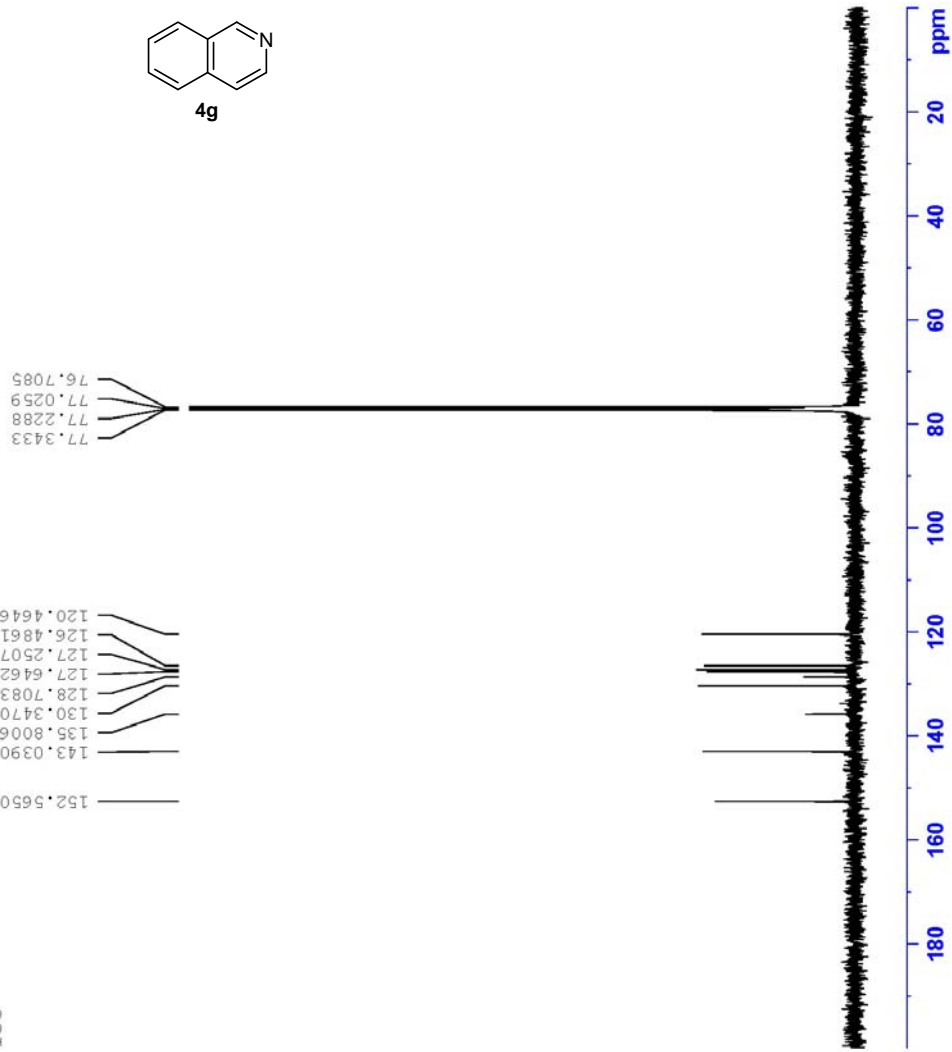
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

# 29) Compound 4g



13C



Current Data Parameters  
NAME tsa02  
EXPNO 729053  
PROCNO 1

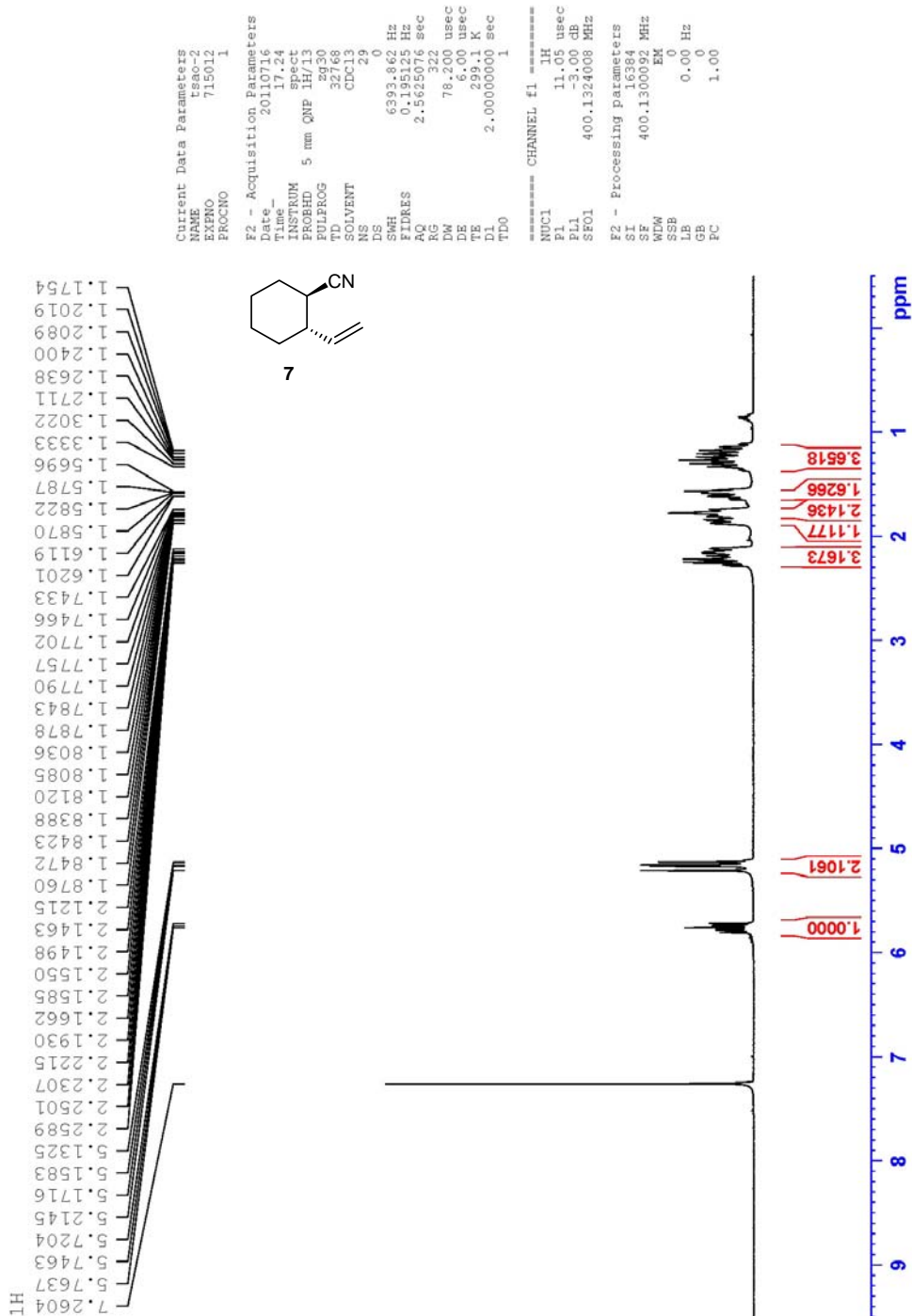
F2 - Acquisition Parameters  
Date\_ 20110729  
Time\_ 19.35  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 543  
DS 0  
SWH 25510.203 Hz  
FIDRES 0.389255 Hz  
AQ 1.2849556 sec  
RG 180  
DE 19.600 usec  
TE 297.9 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.80 usec  
PL1 0.00 dB  
SFO1 100.6248425 MHz

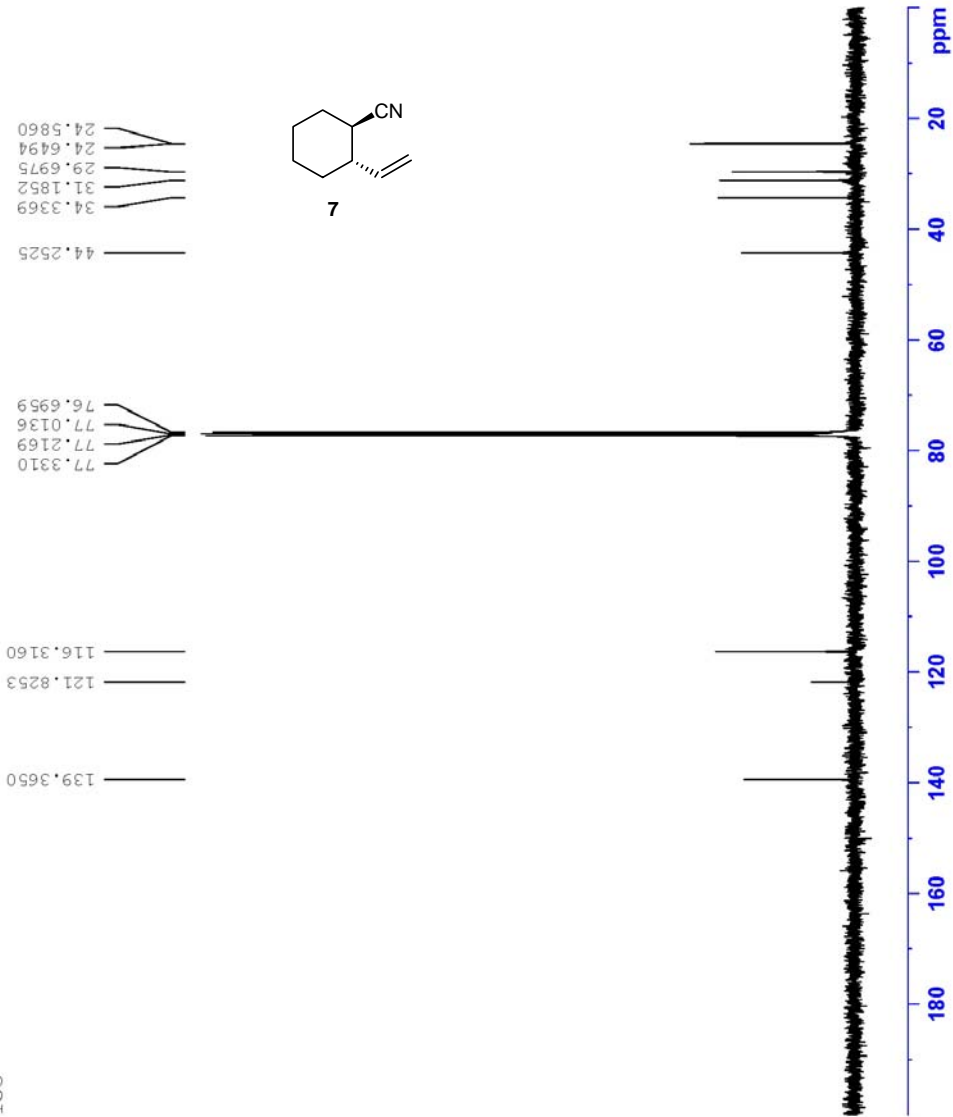
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -3.00 dB  
PL12 14.00 dB  
PL13 17.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127690 MHz  
WDW EM  
SSE 0  
LB 2.00 Hz  
GB 0  
FC 1.00

### 30) Compound 7



13C



B)

Tsao-I-264  
Pulse Sequence: NOESY

Tsao-I-264  
exp3 NOESY

SAMPLE	FLAGS	n
date Mar 7 2011	hs	
solvent CDCl3	sspu1	y
sample undefined	PF0r1g	y
ACQUISITION	hsglv1	5154
sv 8000.0	SPECIAL	
at 0.128	temp	not used
np 2048	gain	30
fb 4000	spin	0
ss 32	F2 PROCESSING	
d1 1.000	gf	0.053
nt 32	gfs	not used
2D ACQUISITION	fn	2048
sv1 8000.0	gf1 PROCESSING	
nl 450	gf1	0.030
tn TRANSMITTER	H1	not used
	pfoc1	1p
sfrq 598.836	fn1	2048
tor 500.0	DISPLAY	
tpwr 60	sp	-128.1
pw 12.500	wp	5523.4
mix NOESY	cp1	-114.2
	wp1	5597.8
presaturation	rf1	488.5
satmode	rfp	0
satpwr 0	rf11	489.2
satdly 0	rfp1	0
sattra 0	PLOT	
dn DECOUPLER	wc	145.0
	sc	0
de	wc2	145.0
	sc2	0
	vs	5068
	th	5
	a1	cdc ph

