

# **Supporting Information**

**for**

## **Aryl nitrile oxide cycloaddition reactions in the presence of pinacol boronic acid ester**

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\* Corresponding author

**<sup>1</sup>H and <sup>13</sup>C NMR spectra, 2D spectra where required,  
and mass spectra for all compounds**



Name Sarah Harding  
WBS R-366-9-3  
SLH052-starting material  
CSIRO Av400X\_1H CDCl3 C:\har97c 3

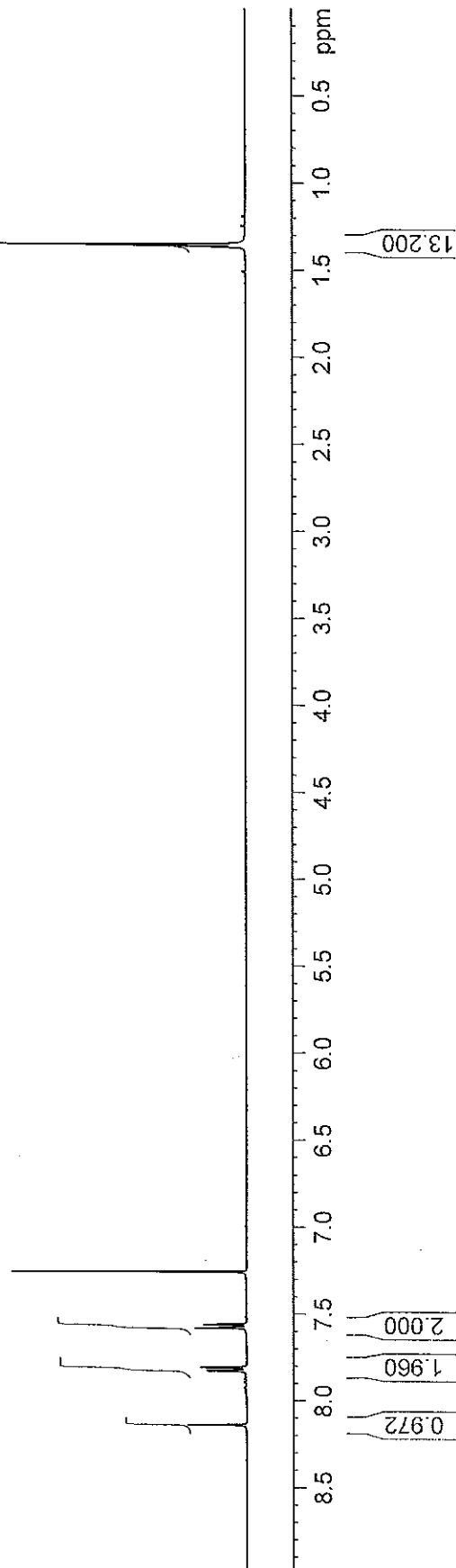
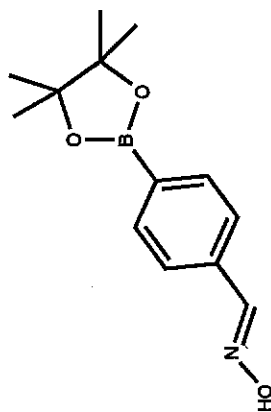


Current Data Parameters  
NAME HardingX40120  
EXNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111025  
Time\_ 15.03  
INSTRUM Av400X  
PROBHD 5 mm PATEO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6393.862 Hz  
FIDRES 0.195125 Hz  
AQ 2.5625076 sec  
RG 184.42  
DW 78.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 17.00 usec  
PLW1 20.00000000 W  
SFO1 400.1328009 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1300103 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





Name Sarah Harding  
WBS R-00366-09-003  
SLH-boronate  
CSIRO AV400X\_13C CDCI3 C:\har97c 6



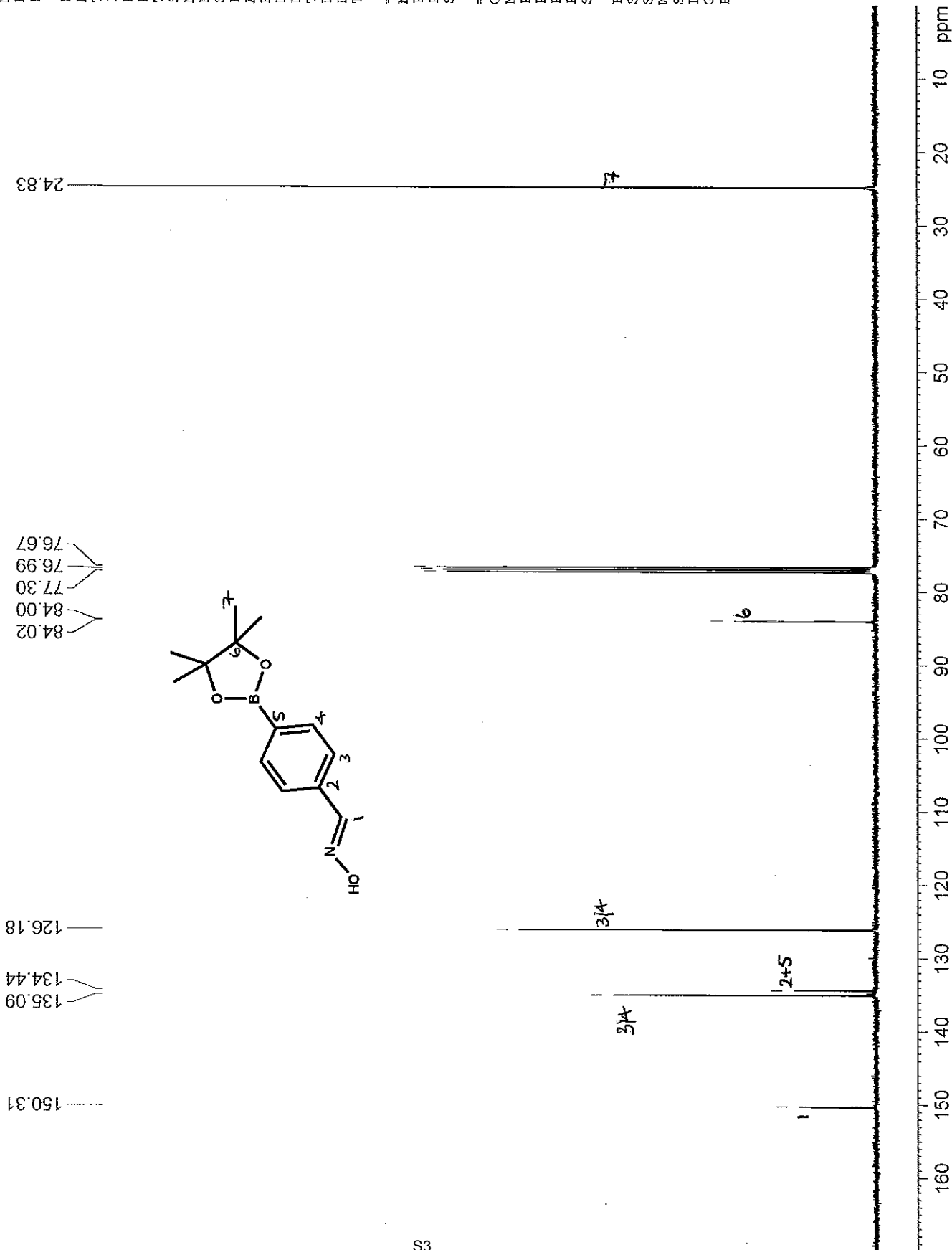
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NAME HardingX40198  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111205  
Time 12.34  
INSTRUM AV400X  
PROBHD 5 mm PATBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 750  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.42  
DW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 67.0000000 W  
SFO1 100.6249425 MHz

===== CHANNEL f2 =====  
CPDPRG2 bi\_waltz65\_256  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.0000000 W  
PLW12 0.71358001 W  
PLW13 0.57800001 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127734 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



```
Current Data Parameters
NAME      HardingX40198
EXPNO     14
PROCNO    1
```

```

E2 - Acquisition Parameters
Date-      2011:205
Time-      19:04

```

| NAME    | UNIT              |
|---------|-------------------|
| ASTRUM  | R400X             |
| PROBAC  | 5 mm EX-80 BE-    |
| PULPROG | hmbocypg12nd      |
| ID      | 4096              |
| SOLVENT | CDCI <sub>3</sub> |
| NS      | b                 |
| CS      | 16                |
| SK      | 79.1, 396         |
| FIDRES  | 1.10751 Hz        |
| QAQ     | 0.521263 sec      |
| RG      | -18.42            |
| MZ      | 101.267           |
| DE      | 6.50              |
| DEC     | sec               |

| TE     | 297.1 K     |
|--------|-------------|
| CNST6  | 160.0000000 |
| CNST7  | 10.0000000  |
| CNST13 | 8.0000000   |
| CNST20 | 0.5931140   |
| D0     | 0.0000000   |
| D1     | 1.5000000   |
| D6     | 0.6525000   |
| D16    | 0.0002000   |
| IND    | 0.00002360  |

```
===== CHANNEL 4: =====
NUC1
P1      17.00 usec
P2      34.00 usec
```

PLW1 20.0000000 W  
SF01 400.1322007 MHz

| CHANNEL | F2 | F3      | 13C  |
|---------|----|---------|------|
| NUC2    |    |         |      |
| P3      |    | 10.00   | usec |
| P24     |    | 2000.00 | usec |

```
PLW2      67.0000000 W
SFO2      100.6233333 MHz
SSNAM7    C=P60comp.4
SFO17      0.500
```

SP0FEST 0 ME 10.2370047 N

===== GRADIENT CHANNEL =====

SMSQ10.100  
SMSQ10.100  
SMSQ10.100  
SMSQ10.100

|        |            |
|--------|------------|
| SPNAM5 | SMSQ10.100 |
| SP21   | 80.00      |
| SP23   | 15.00      |
| SP24   | 0.00       |

|      |        |         |         |
|------|--------|---------|---------|
| 5000 | 100.00 | 1000.00 | 1000.00 |
| 5000 | 5.00   | 5.00    | 5.00    |
| 5000 | 100.00 | 100.00  | 100.00  |

| E1 - Acquisition parameters |              |
|-----------------------------|--------------|
| ID                          | 512          |
| SEFO1                       | 100.6233 MHz |
| SEFO2                       | 43.235508 Hz |

```

AS          219.995 ppm
EPMODE      Echo-2Tc1ch2

```

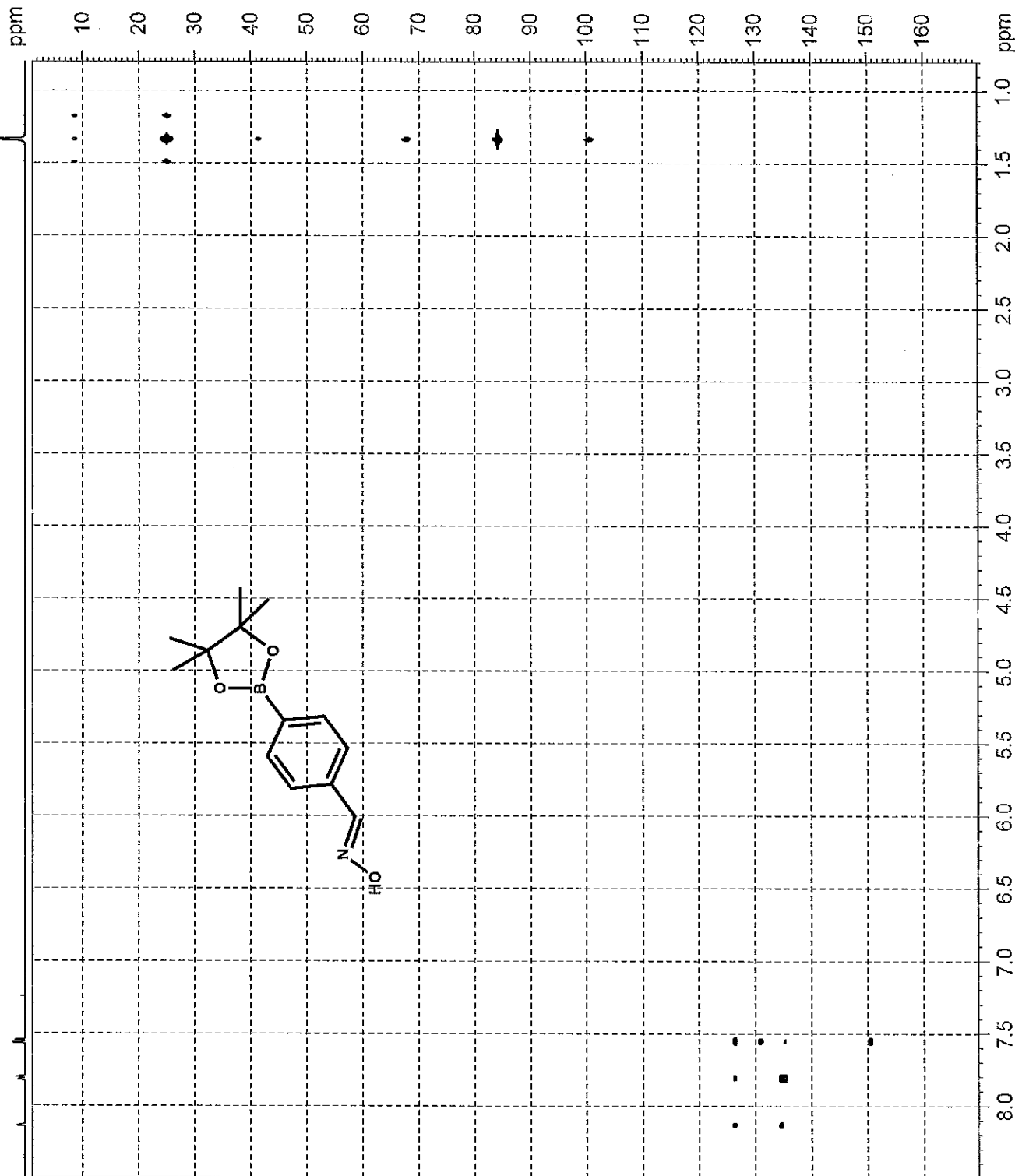
|                       |                 |
|-----------------------|-----------------|
| Processing parameters |                 |
| SI                    | 2048            |
| SF                    | 400.1360173 MHz |
| QW                    | OS:NE           |

[illegible]

Ob.: 2049  
F1 - processing parameters

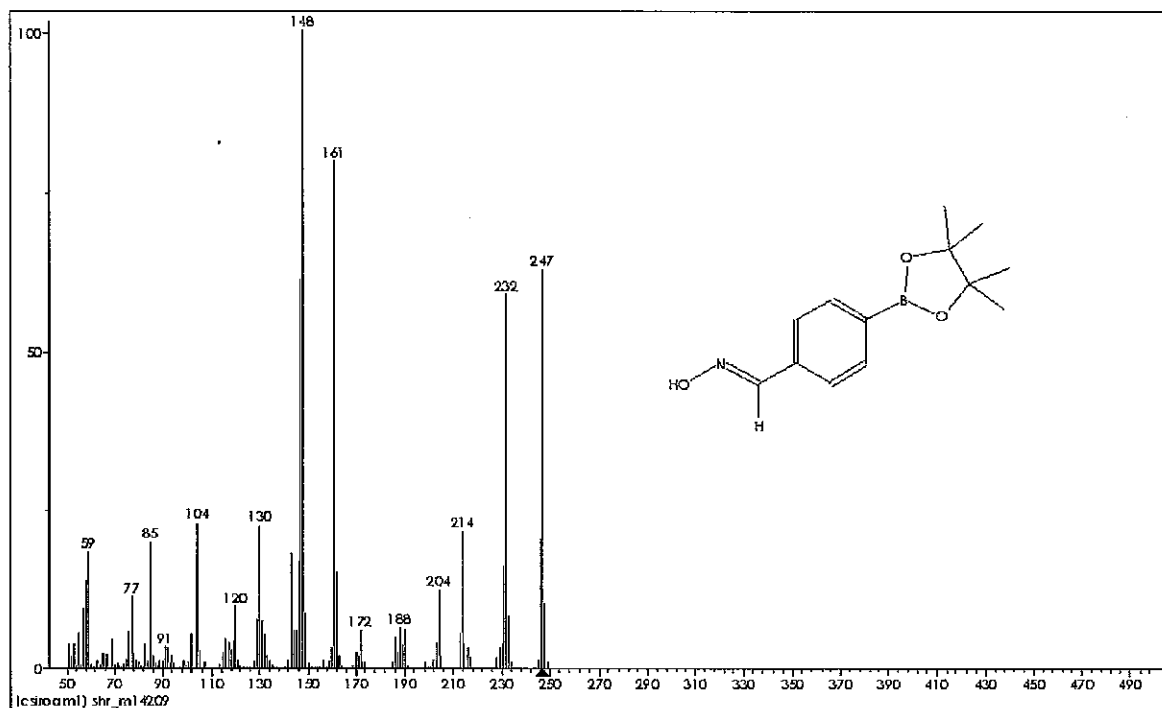
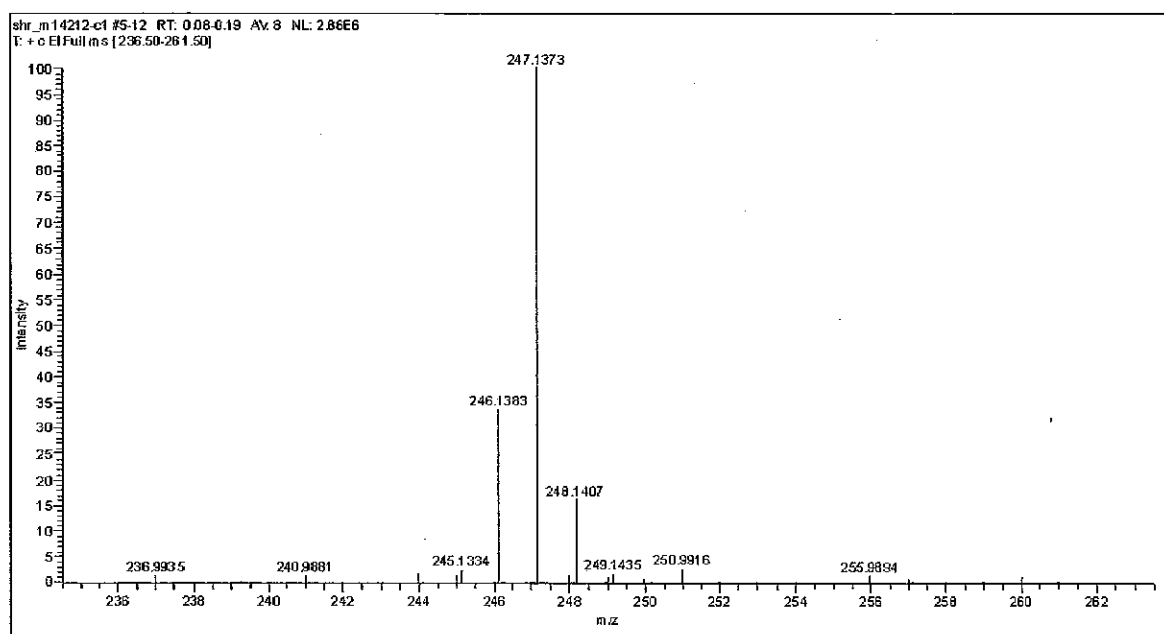
MC2  
SE  
NDW  
SEP

000  
000  
000





CSIRO

Low Resolution EI SpectrumHigh Resolution EI Spectrum

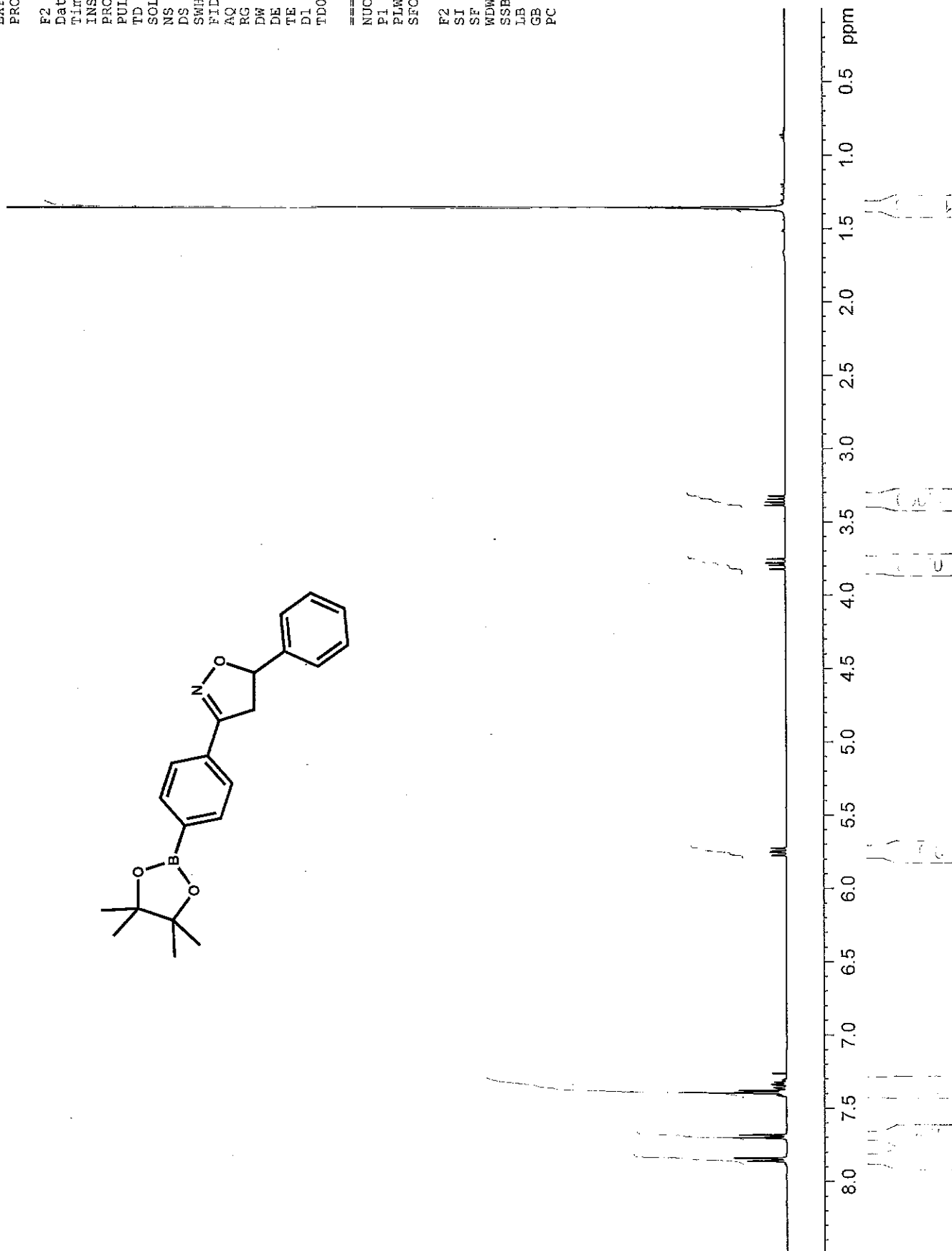
```

FF2 - Acquisition Parameters
Date_      20111130
Time_      16.09
INSTRUM    AV400X
PROBHD     5 mm PABO BB-
PULPROG    zg30
TD          32768
SOLVENT     CDC13
NS          32
DS          2
SWH         6393.862 Hz
FIDRES     0.195125 Hz
AQ         2.5625076 sec
RG         86.92
DW         78.200 usec
DE         6.50 usec
TE         297.1 K
D1         1.00000000 sec
TD0        1

```

```
===== CHANNEL f1 =====
NUC1      1H
P1         17.00 usec
PLW1       20.0000000 W
SF01       400.1328009 MHz
```

|                            |                |
|----------------------------|----------------|
| F2 - Processing parameters |                |
| SI                         | 65536          |
| SF                         | 400.130097 MHz |
| WDW                        | EM             |
| SSB                        | 0              |
| LB                         | 0.10 Hz        |
| GB                         | 0              |
| PC                         | 1.00           |





Name Sarah Harding  
WBS R-00366-09-003  
SLH077af1  
CSIRO Av400X\_13C CDC13 C:\har97c 27



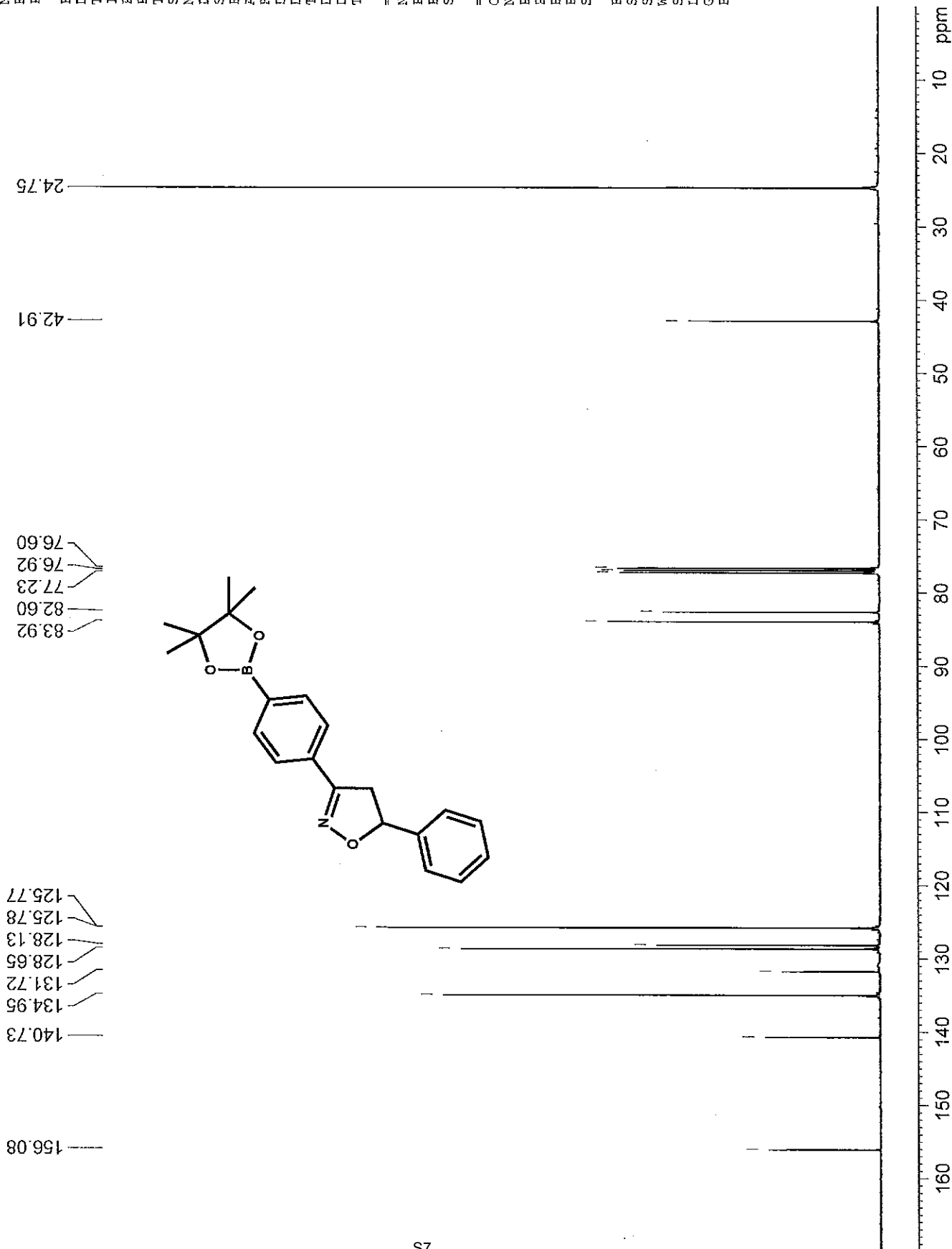
Current Data Parameters  
NAME HardingX40194  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111202  
Time 1.14  
INSTRUM Av400X  
PROBHD 5 mm PATBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 6000  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.42  
DW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 67.0000000 W  
SFO1 100.6248425 MHz

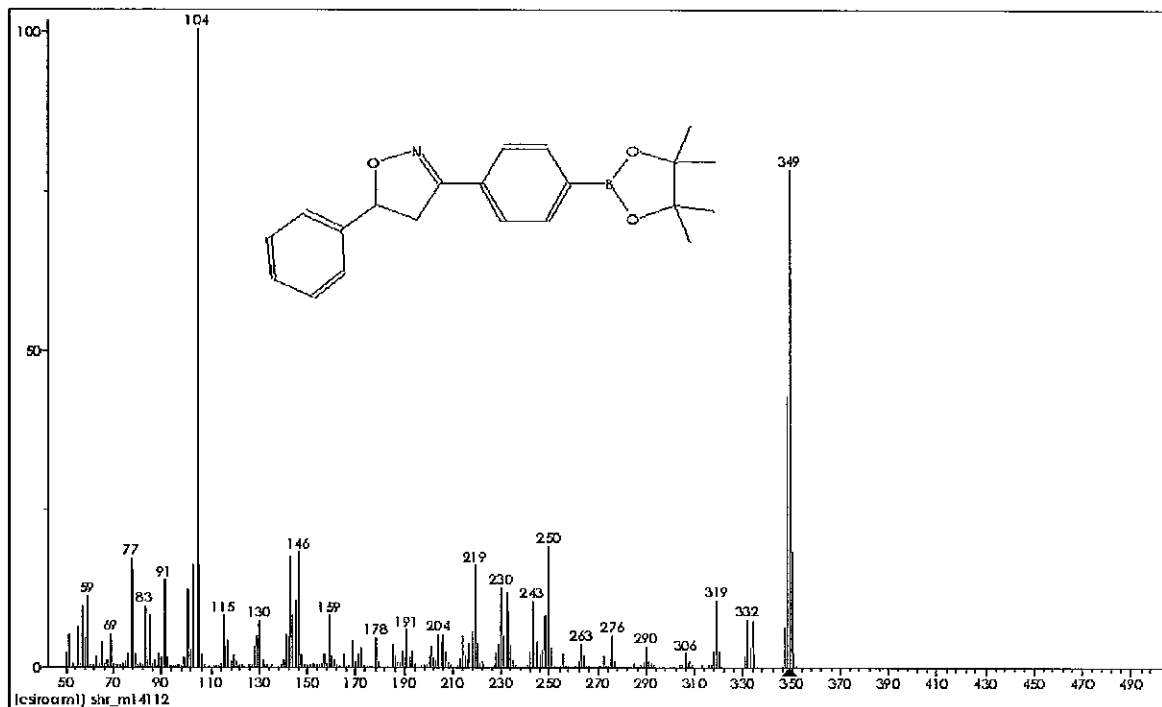
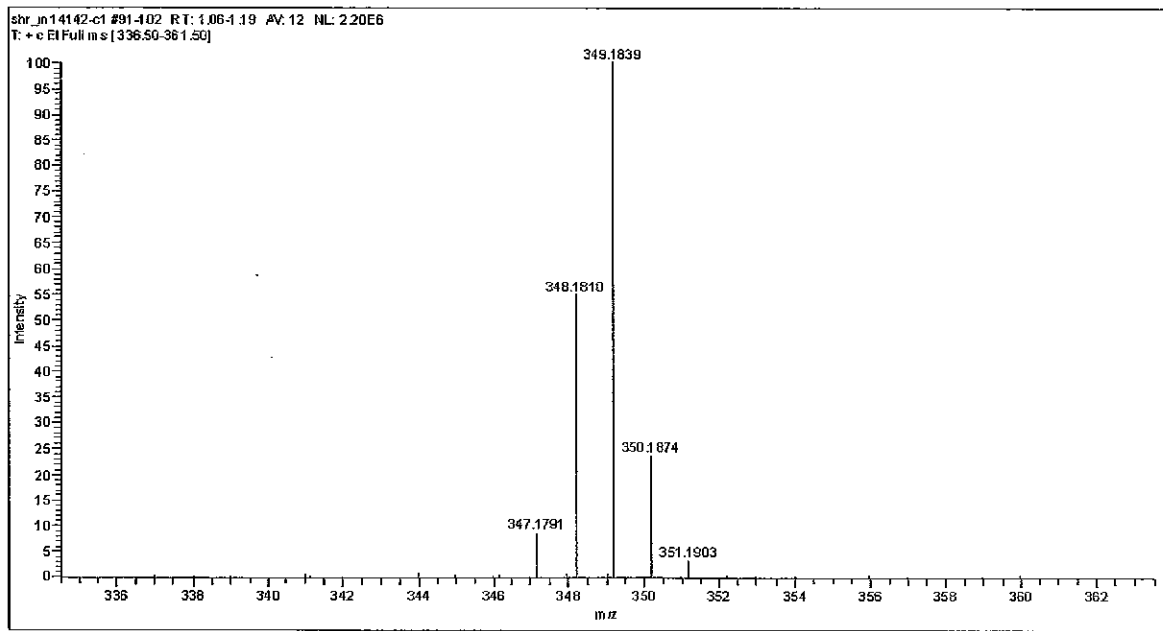
===== CHANNEL f2 =====  
CPDPRG2 bi\_waltz65\_1H  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.0000000 W  
PLW12 0.71358001 W  
PLW13 0.57800001 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127829 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





CSIRO

Low Resolution EI SpectrumHigh Resolution EI Spectrum





Name Sarah Harding  
WBS R-00366-09-003  
SLH077cf1  
CSIRO Av400X\_1H CDCl3 C:\har97c 26

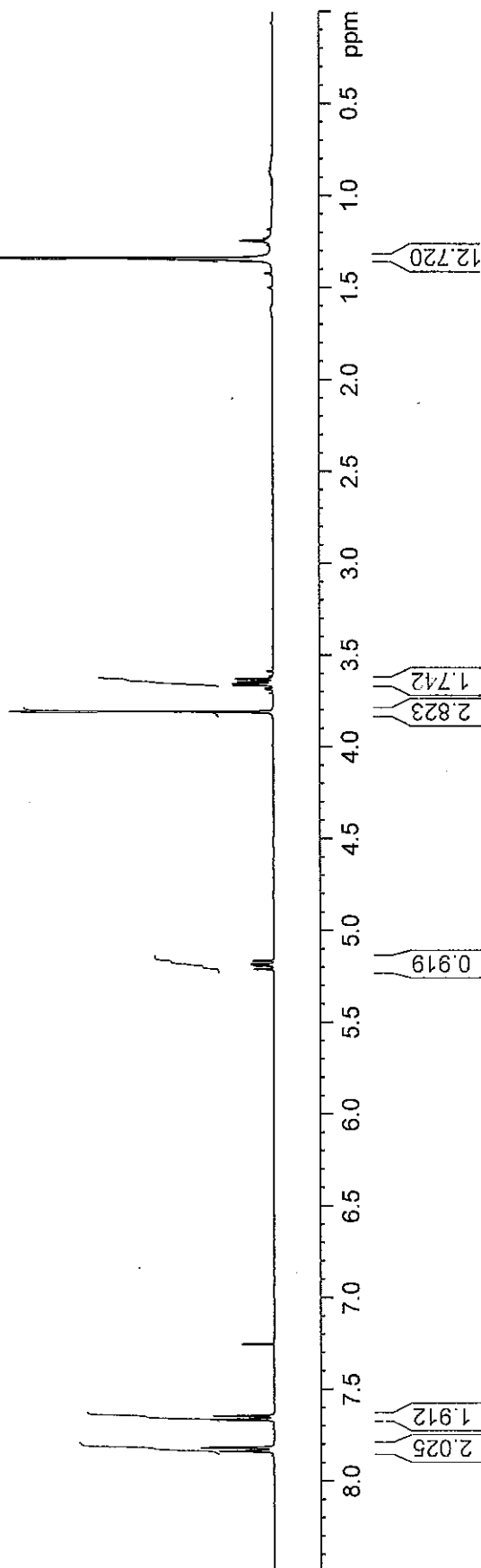
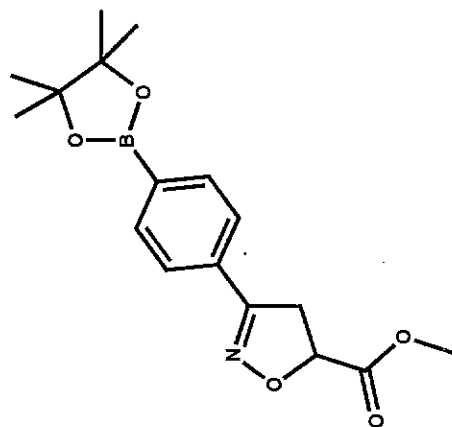


Current Data Parameters  
NAME HardingX40196  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111201  
Time\_ 14.50  
INSTRUM AV400X  
PROBHD 5 mm PABO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6393.862 Hz  
FIDRES 0.195125 Hz  
AQ 2.5625076 sec  
RG 119.37  
DW 78.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 17.00 usec  
PLW1 20.0000000 W  
SFO1 400.1328009 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1300127 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





Name Sarah Harding  
WBS R-00366-09-003  
SLH077cf1

CSTRO Av400X\_13C CDCI3 C:\har97c 26



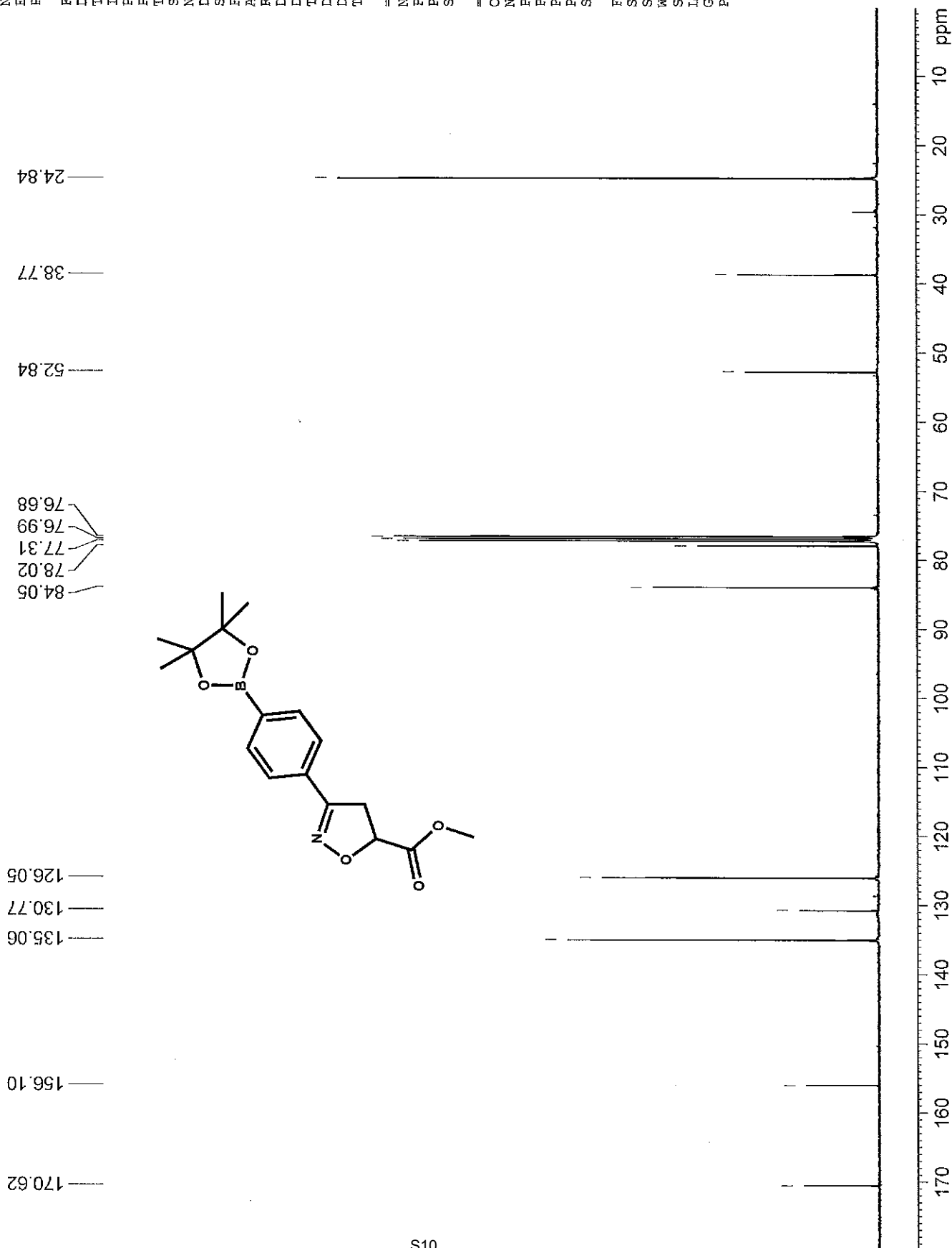
Current Data Parameters  
NAME HardingX40196  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111202  
Time 6.52  
INSTRUM Av400X  
PROBHD 5 mm PATBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 5000  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.42  
DW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 67.00000000 W  
SFO1 100.628425 MHz

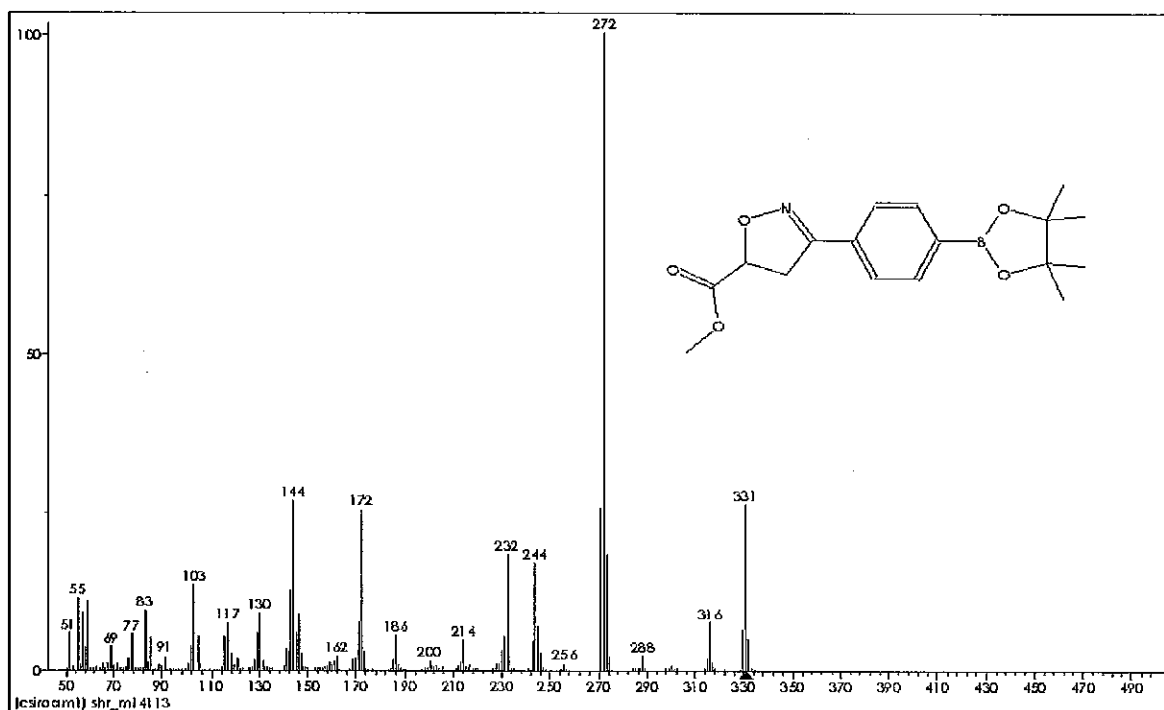
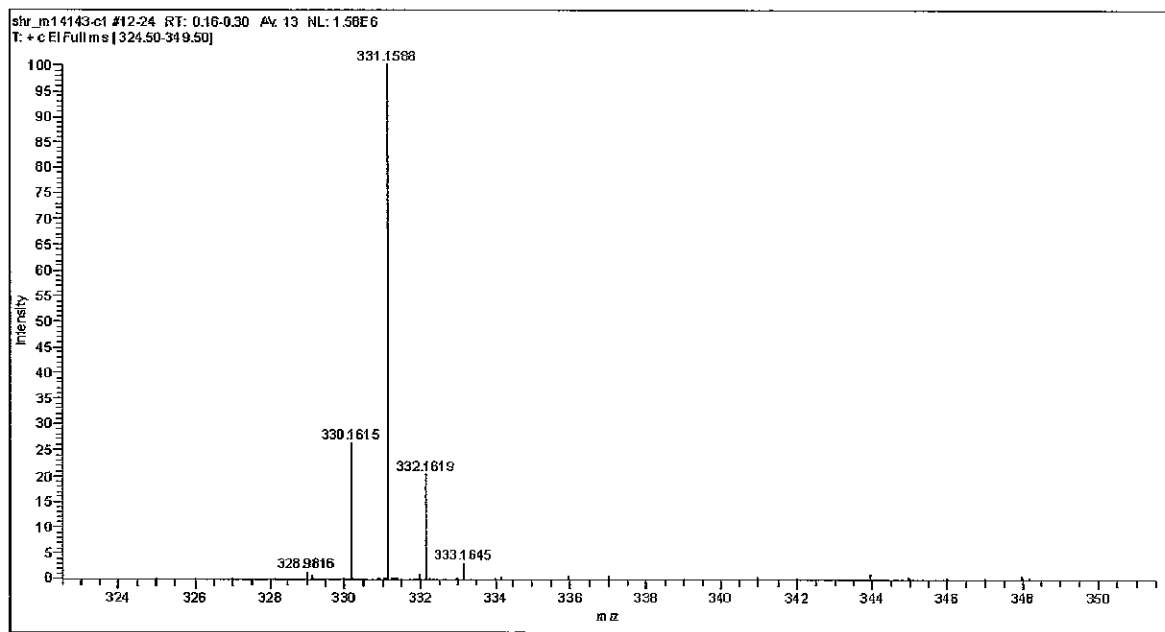
==== CHANNEL f2 =====  
CPDPRG2 bi\_waltz65\_256  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.00000000 W  
PLW12 0.71380001 W  
PLW13 0.57800001 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127734 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





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CSIRO Materials Science & Engineering  
S.HardingAccurate Mass Report  
SLH077cf1 (c)Low Resolution EI SpectrumHigh Resolution EI Spectrum



Name Sarah Harding  
WBS R-00366-09-003  
SLH078ef1  
CSIRO AV400X\_1H CDCl3 C:\har97c 26

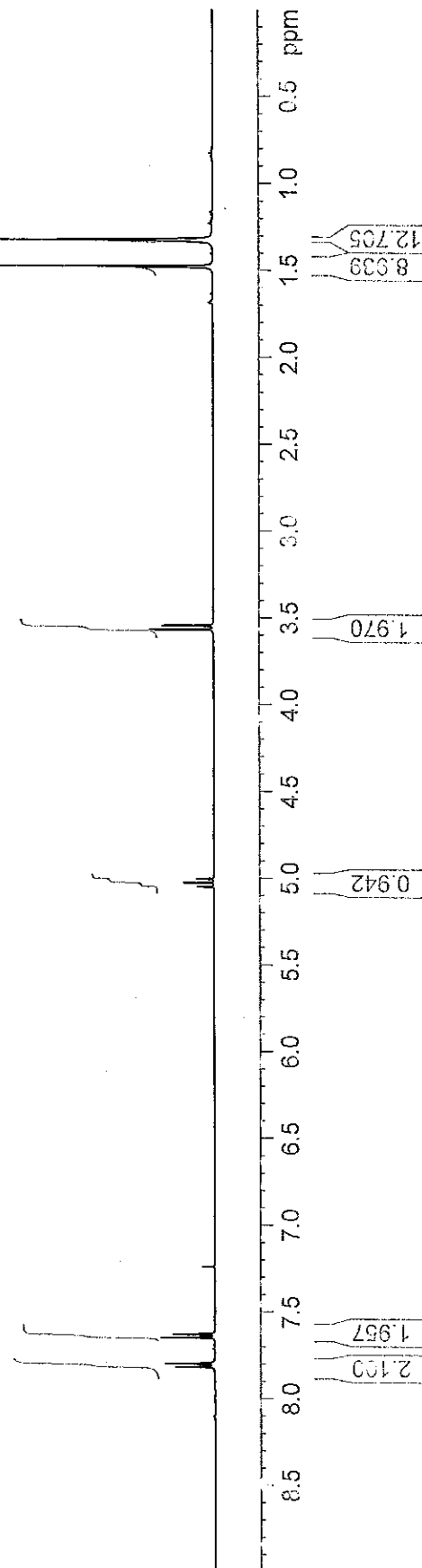
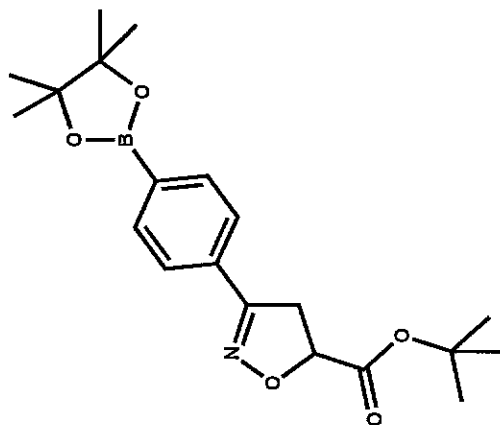
Current Data Parameters  
NAME HardingX40206  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111206  
Time 16.34

INSTRUM Av400X  
PROBHD 5 mm PATBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6393.862 Hz  
FIDRES 0.195125 Hz  
AQ 2.5625076 sec  
RG 75.1  
DW 78.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 17.00 usec  
PL1 20.0000000 W  
SFO1 400.1328009 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1300178 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





Name Sarah Harding  
WBS R-00366-09-003  
SLH078ef1  
CSIRO Av400X\_13C CDCI3 C:\har97c 26

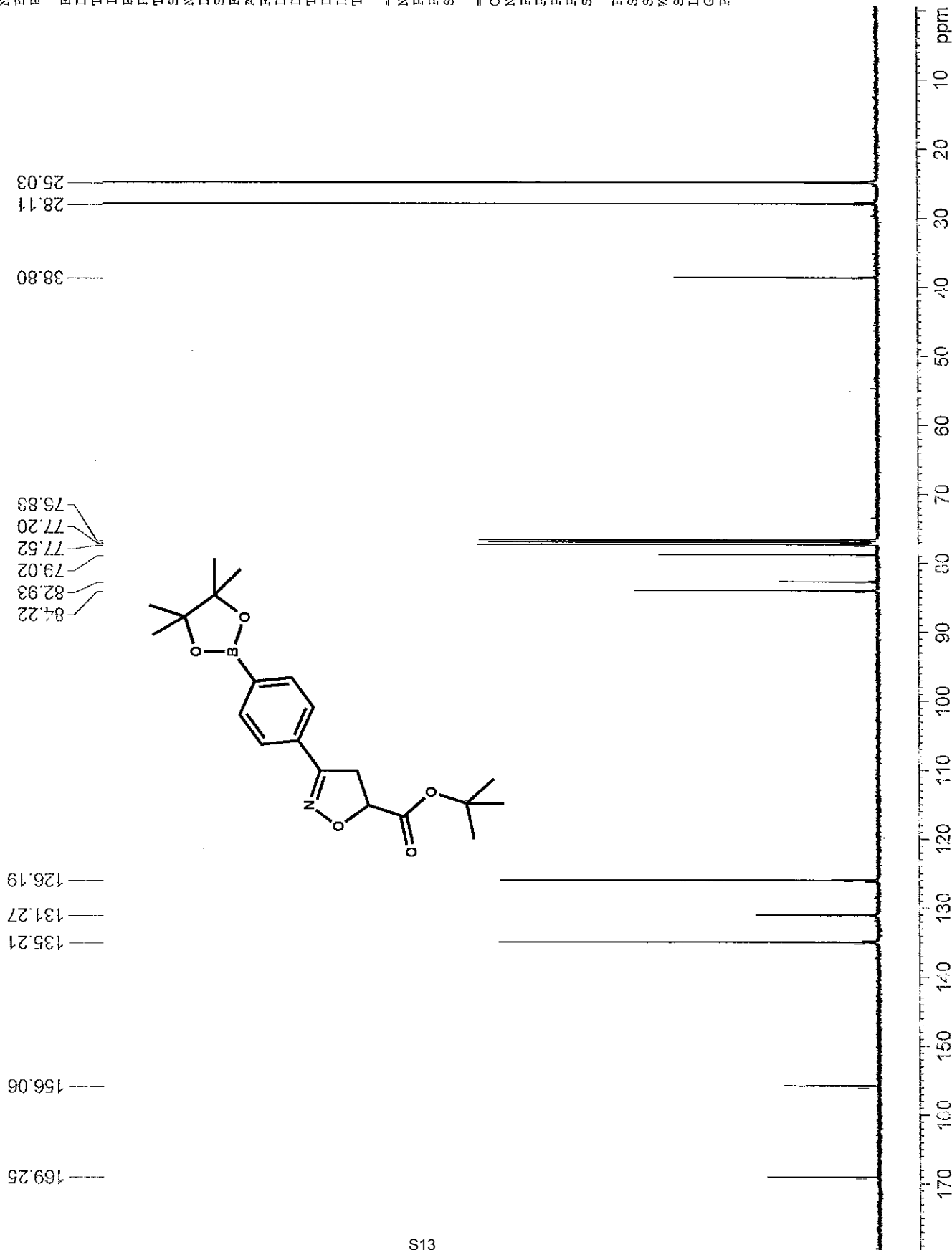
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EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111206  
Time\_ 17.18  
INSTRUM Av400X  
PROBHD 5 mm PAT30 BF-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 750  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.42  
DW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 67.00000000 W  
SFO1 100.6248425 MHz

===== CHANNEL f2 =====  
CPDPRG2 bi\_waltz85\_256  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.00000000 W  
PLW12 0.71358001 W  
PLW13 0.57800001 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127768 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



| Culture | Data Pathologies |
|---------|------------------|
| NAME    | HARDINGX40296    |
| EXNO    | 14               |
| PROGNO  |                  |

1972 - AQUASILION PAPERMAN  
2011-2017

Time 0.42  
INSTRUM ADVDEX  
PROBID 5 PM PATEO BR.

560b  
pirtivibazone  
Gilead  
Gilead

8  
51  
57  
58

| SPIN      | RES | RES | RES |
|-----------|-----|-----|-----|
| 4.195     | 390 | 42  |     |
| 1.170751  | 42  |     |     |
| 0.0271263 | sec |     |     |

|     |         |      |
|-----|---------|------|
| 169 | 163,422 | used |
| 167 | 104,667 | used |
| 165 | 6,50    | used |

```

102      297.0 K
103      140.0000000
104      110.0000000
105      297.0 K

```

CONST15  
CONST30  
0.598140  
3.000000  
10.000000

|     |               |     |
|-----|---------------|-----|
| EU  | 9,000,000,000 | SEC |
| 101 | 1,500,000,000 | SEC |
| 115 | 9,062,500,000 | SEC |

|     |               |
|-----|---------------|
| DLG | 0.002000 sec  |
| INI | 0.0007260 sec |

[illegible]

20.0000000 W

1986  
100.15207 MHz

|              |              |
|--------------|--------------|
| 13C          | 13C          |
| 10.00 usec   | 10.00 usec   |
| 2000.00 usec | 2000.00 usec |

67.0000000 Hz  
209.623333 MHz  
C06620000 4

005700 711 6 4:54:30655  
4:54:30655 2140655

... GRADIENT CLIMBER; ...  
... 10.735000000000000

GPNA241  
SMQ210.100  
GPNA213  
SMQ210.100  
GPNA241  
SMQ210.100

001 010 SMS  
 30 00  
 14 00  
 001 010 SMS  
 30 00  
 14 00

GP24  
3P25

FIGURE 1 Acquisition parameters

|       |              |
|-------|--------------|
| TD    | 512          |
| SFO1  | 100.6233 MHz |
| FTRES | 43.235908 Hz |

219.995 ppm  
Echo-Antiecho  
F1-MODE

## RF2 - Processing Parameters

7556  
7557  
7558  
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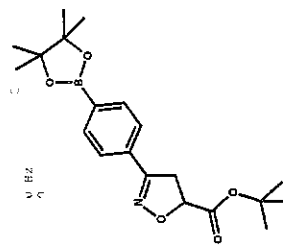
|    |      |
|----|------|
| LB | 0 Hz |
| GB | 0    |
| PC | 1.40 |

Processing parameters  
2046

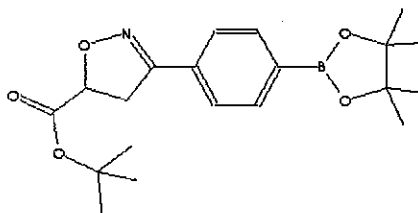
echo antiecho  
100.6127541 MHz

1. 122  
 2. 123  
 3. 124

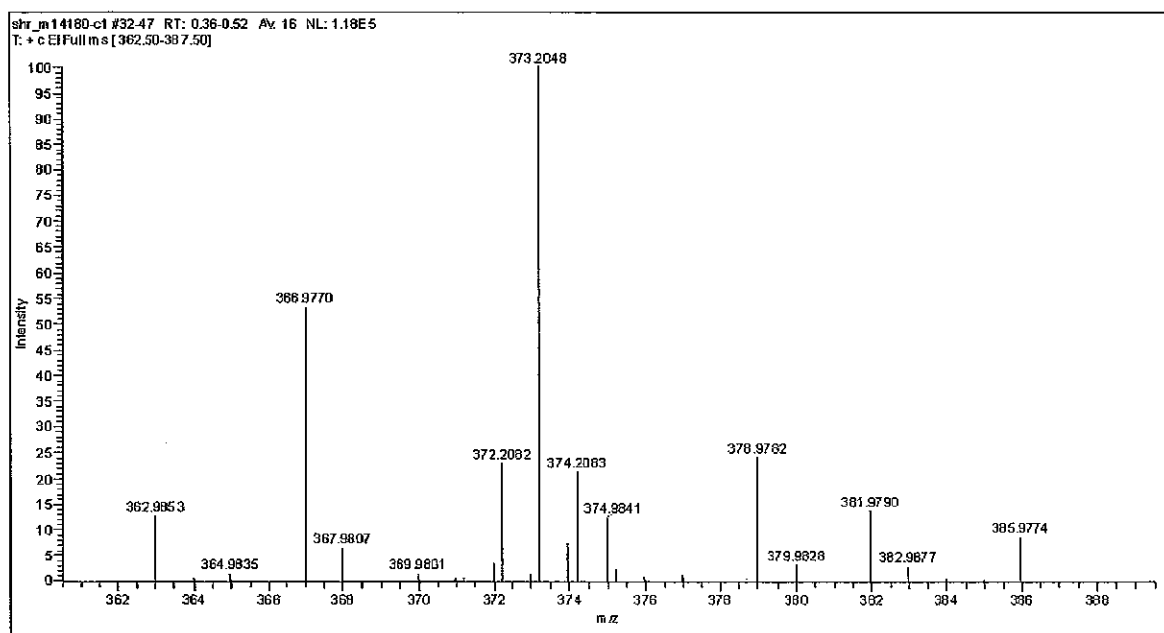
75

c1ccccc1ON#Cc1ccccc1c1ccoc1CC(=O)O

### Low Resolution EI Spectrum



### High Resolution EI Spectrum



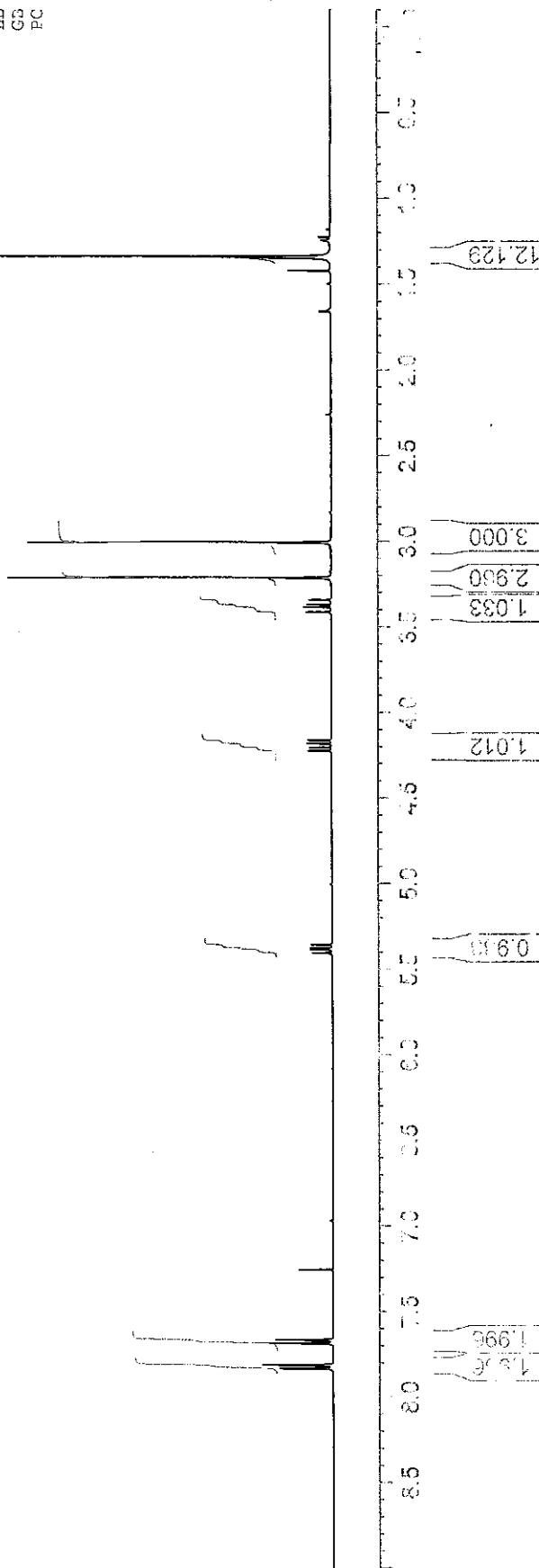
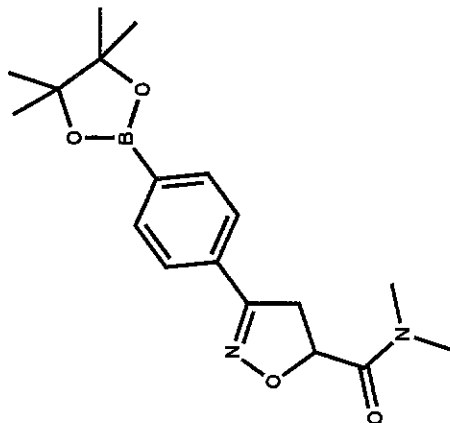
BRUKER

Current Data Parameters  
NAME HardingX40208  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111206  
Time\_ 18.15  
INSTRUM AV400X  
PROBHD 5 mm PATBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6393.862 Hz  
FIDRES 0.195125 Hz  
AQ 2.5625076 sec  
RG 132.48  
DW 78.200 usec  
DE 6.50 usec  
TE 297.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 17.00 usec  
PLW1 20.0000000 W  
SFO1 400.122809 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1300127 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00







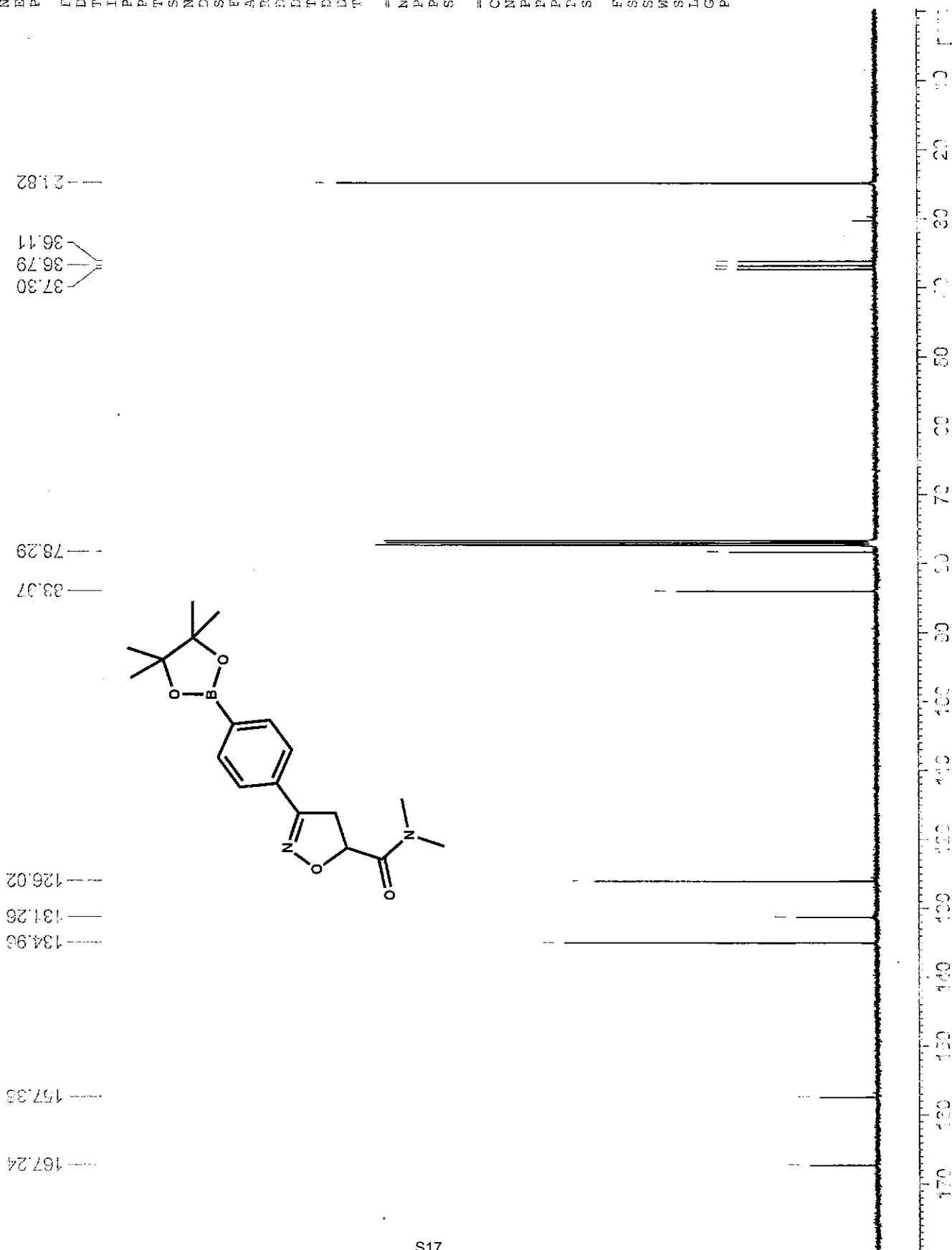
Current Data Parameters  
NAME HardingX40208  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111207  
Time\_ 3.42  
INSTRUM Av400X  
PROBHD 5 mm PATBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1000  
DS 4  
SWH 26011.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.12  
RW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 67.00000000 W  
SFO1 100.6248425 MHz

===== CHANNEL f2 =====  
CPDPRG2 bi\_waltz65\_256  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.00000000 W  
PLW12 0.71358001 W  
PLW13 0.57800001 W  
SFO2 400.1316095 MHz

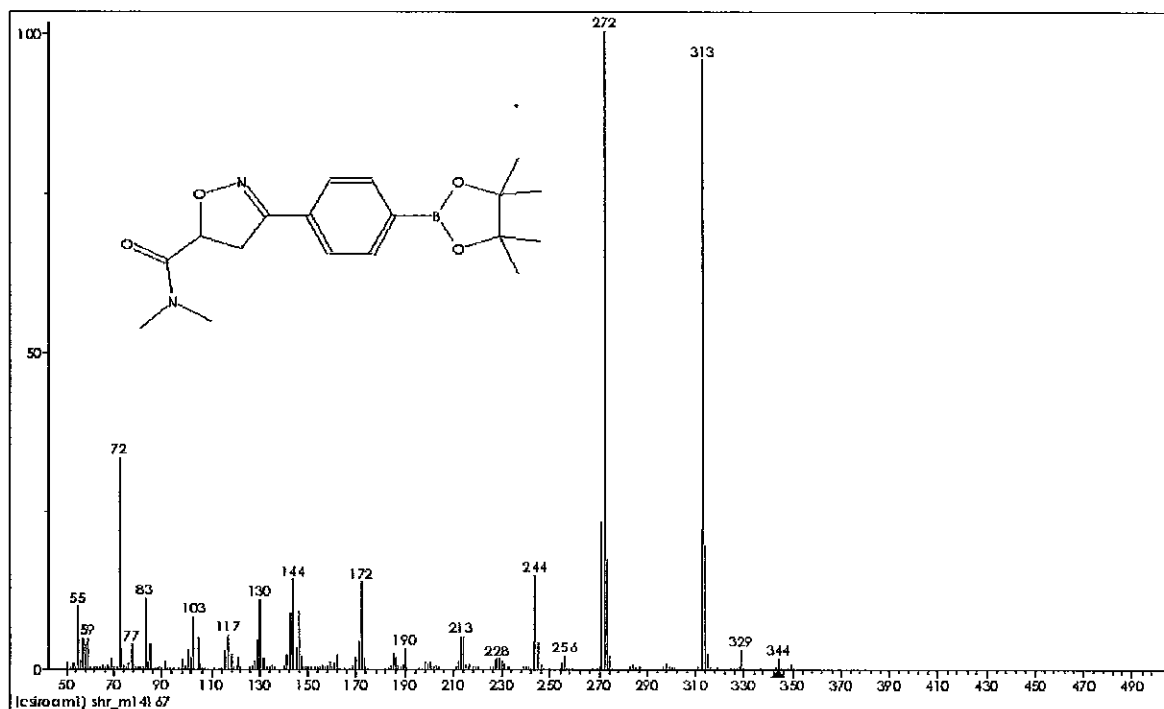
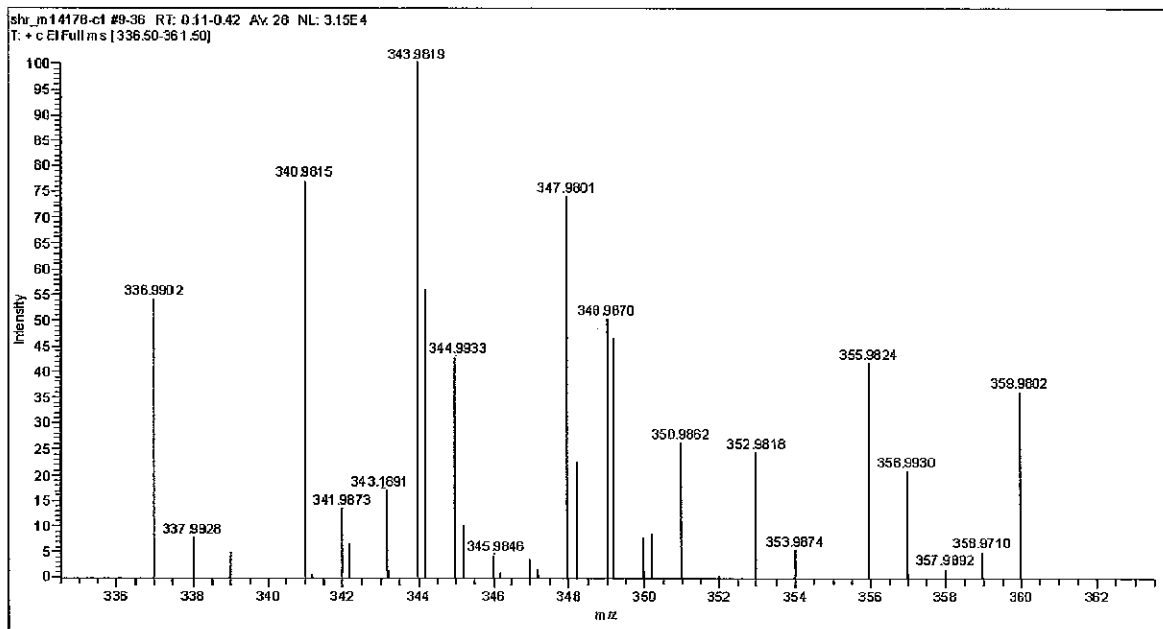
F2 - Processing parameters  
SI 32768  
SF 100.6127758 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







CSIRO

Low Resolution EI SpectrumHigh Resolution EI Spectrum

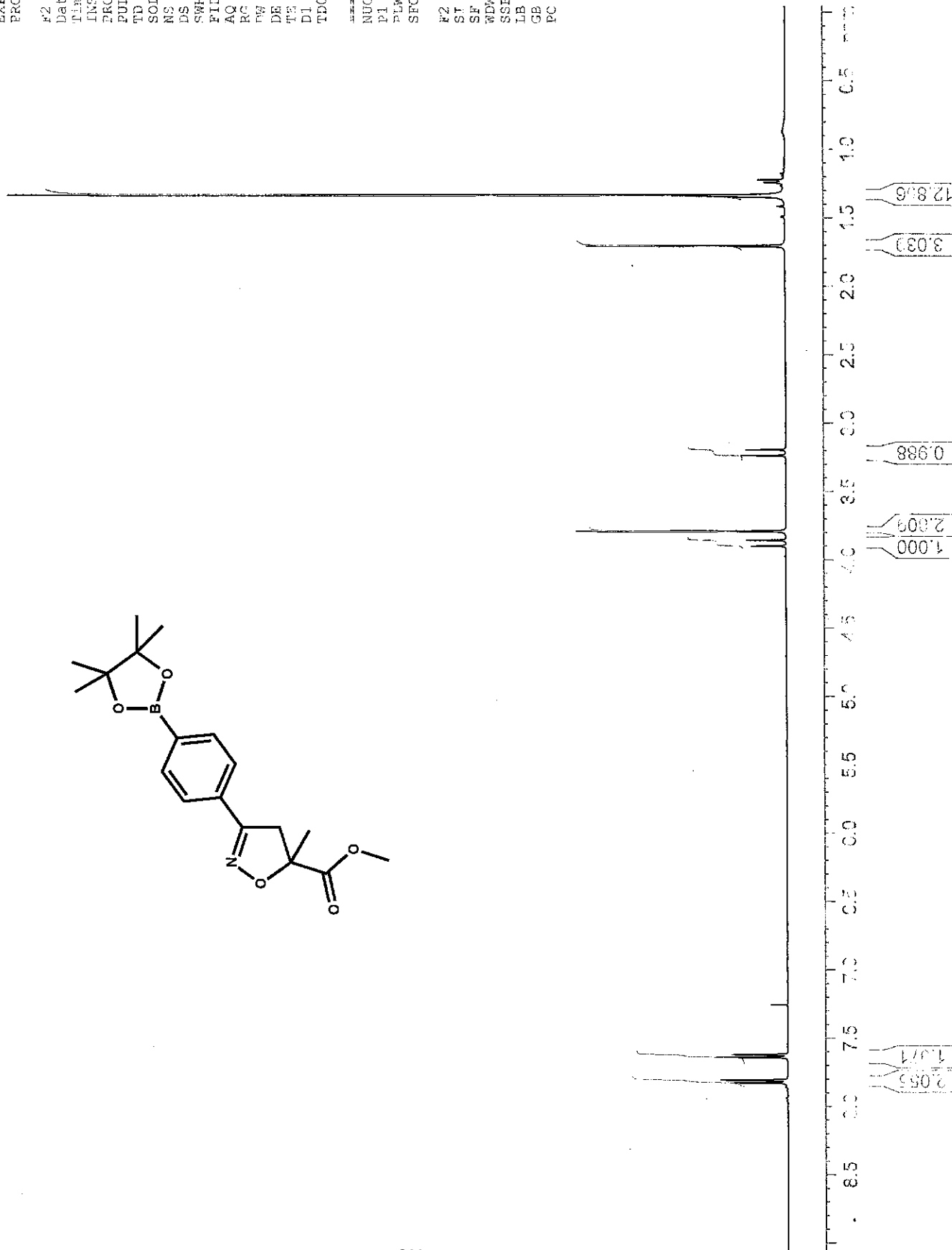
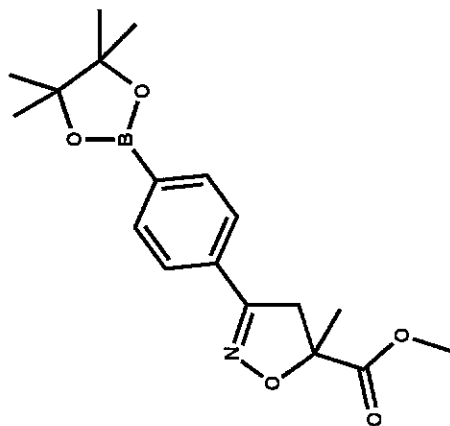


Current Data Parameters  
NAME HardingX10209  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111206  
Time\_ 15.21  
INSTRUM AV400X  
PROBHD 5 mm PABO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6393.862 Hz  
FIDRES 0.195125 Hz  
AQ 2.5625076 sec  
RG 60.07  
RW 78.200 usec  
DE 6.50 usec  
TE 297.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 <sup>1</sup>H  
P1 17.00 usec  
PL1 20.0000000 W  
SFO 400.132809 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1302127 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME HardingX40209  
EXPNO 1  
PROCNO 1

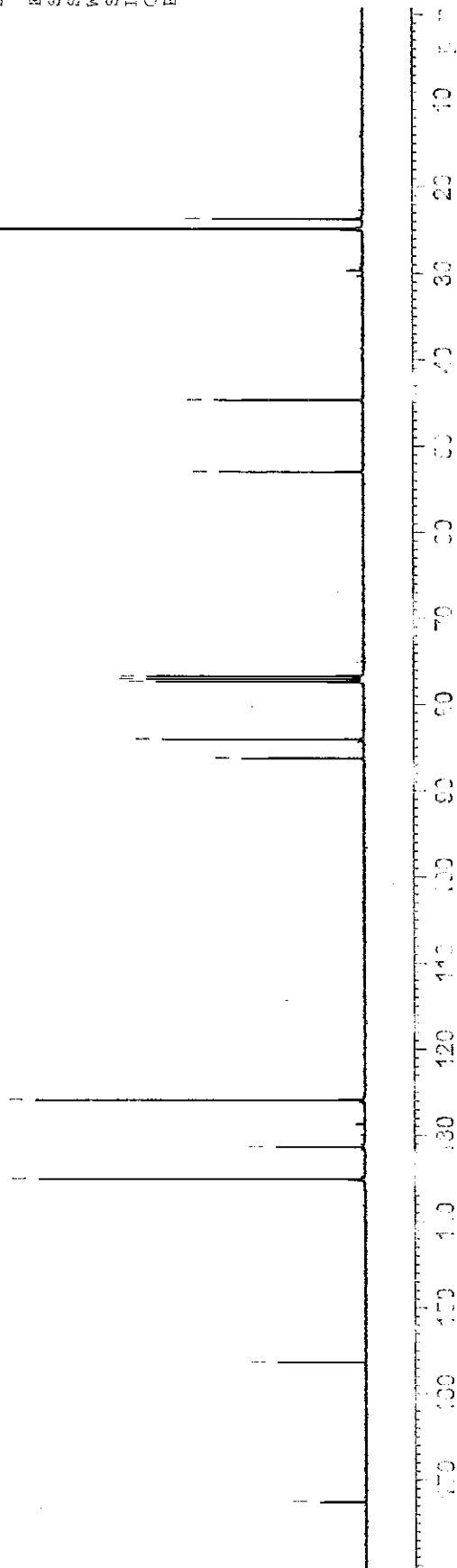
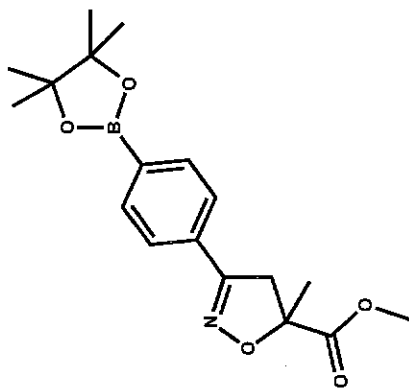
F2 - Acquisition Parameters  
Date\_ 20111206  
Time\_ 19.42  
INSTRUM AV400X  
PROBHD 5 mm F400 EL-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1000  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.42  
DW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 67.0000000 W  
SFO1 100.6248425 MHz

===== CHANNEL f2 =====  
CPDPRG2 biwaltz65\_256  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.0000000 W  
PLW12 0.71358001 W  
PLW13 0.57800001 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127749 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

172.62  
156.30  
135.00  
131.30  
126.86  
86.22  
84.01  
77.32  
77.00  
76.68  
52.97  
14.65  
24.82  
23.64



Name Sarah Harding  
 WBS R-00366-09-003  
 SLH078df1  
 CSIRO AV400X\_cosy CDC13 C:\har97c 32



Current Data Parameters  
 NAME: HardingX10210  
 EXPNO: 12  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_ Time: 20110620 19:53  
 INSTRUM: AV400X  
 PROBRG: 5 mm 1H/13C BBI  
 PULPROG: zgpg30  
 TD: 65536  
 SOLVENT: CDCl3  
 NS: 16  
 DS: 4  
 SWH: 4007.632 Hz  
 FIDRES: 0.1347508 Hz  
 AQ: 0.13130471 sec  
 RG: 327.5  
 DB: 104.000 usec  
 DE: 3.50 usec  
 TE: 296.2 K  
 D1: 0.00000000 sec  
 D11: 0.00000000 sec  
 D12: 0.00000000 sec  
 D16: 0.00000000 sec  
 LNO: 0.00000000 sec

===== CHANNEL f1 =====  
 NUC1: 13C  
 P1: 8.50 usec  
 PL1: 0.00 dB  
 FWH: 20.00000000 MHz  
 SFO1: 400.1322007 MHz

===== CHANNEL f2 =====  
 NUC2: 1H  
 P2: 12.54 usec  
 PL2: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO2: 400.1300178 MHz

===== CHANNEL f3 =====  
 NUC3: 1H  
 P3: 12.54 usec  
 PL3: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO3: 400.1300178 MHz

===== CHANNEL f4 =====  
 NUC4: 1H  
 P4: 12.54 usec  
 PL4: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO4: 400.1300178 MHz

===== CHANNEL f5 =====  
 NUC5: 1H  
 P5: 12.54 usec  
 PL5: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO5: 400.1300178 MHz

===== CHANNEL f6 =====  
 NUC6: 1H  
 P6: 12.54 usec  
 PL6: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO6: 400.1300178 MHz

===== CHANNEL f7 =====  
 NUC7: 1H  
 P7: 12.54 usec  
 PL7: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO7: 400.1300178 MHz

===== CHANNEL f8 =====  
 NUC8: 1H  
 P8: 12.54 usec  
 PL8: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO8: 400.1300178 MHz

===== CHANNEL f9 =====  
 NUC9: 1H  
 P9: 12.54 usec  
 PL9: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO9: 400.1300178 MHz

===== CHANNEL f10 =====  
 NUC10: 1H  
 P10: 12.54 usec  
 PL10: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO10: 400.1300178 MHz

===== CHANNEL f11 =====  
 NUC11: 1H  
 P11: 12.54 usec  
 PL11: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO11: 400.1300178 MHz

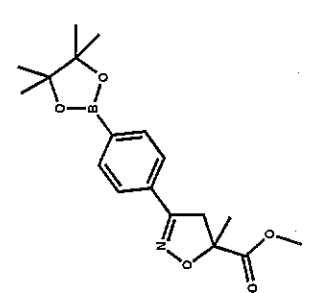
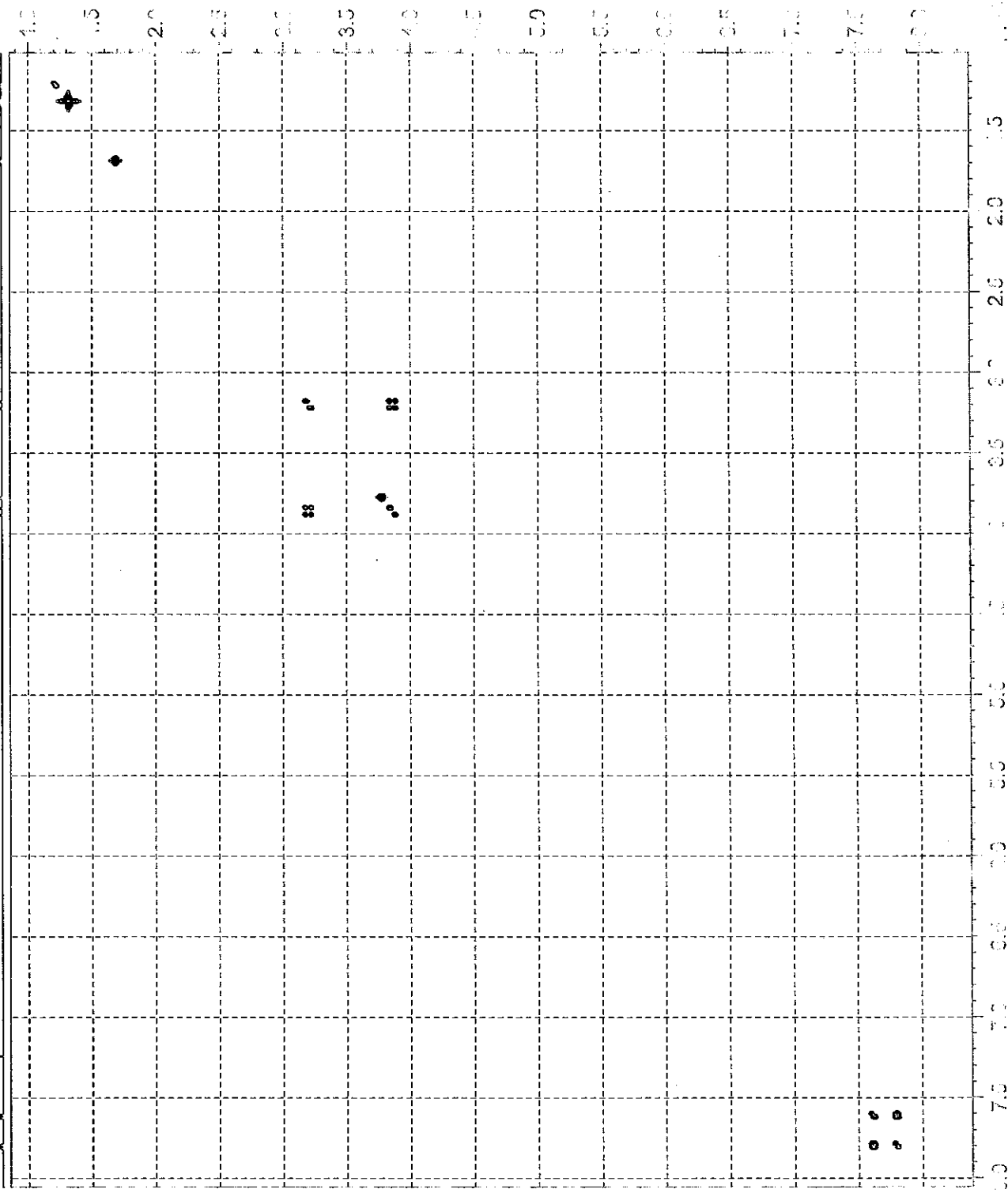
===== CHANNEL f12 =====  
 NUC12: 1H  
 P12: 12.54 usec  
 PL12: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO12: 400.1300178 MHz

===== CHANNEL f13 =====  
 NUC13: 1H  
 P13: 12.54 usec  
 PL13: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO13: 400.1300178 MHz

===== CHANNEL f14 =====  
 NUC14: 1H  
 P14: 12.54 usec  
 PL14: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO14: 400.1300178 MHz

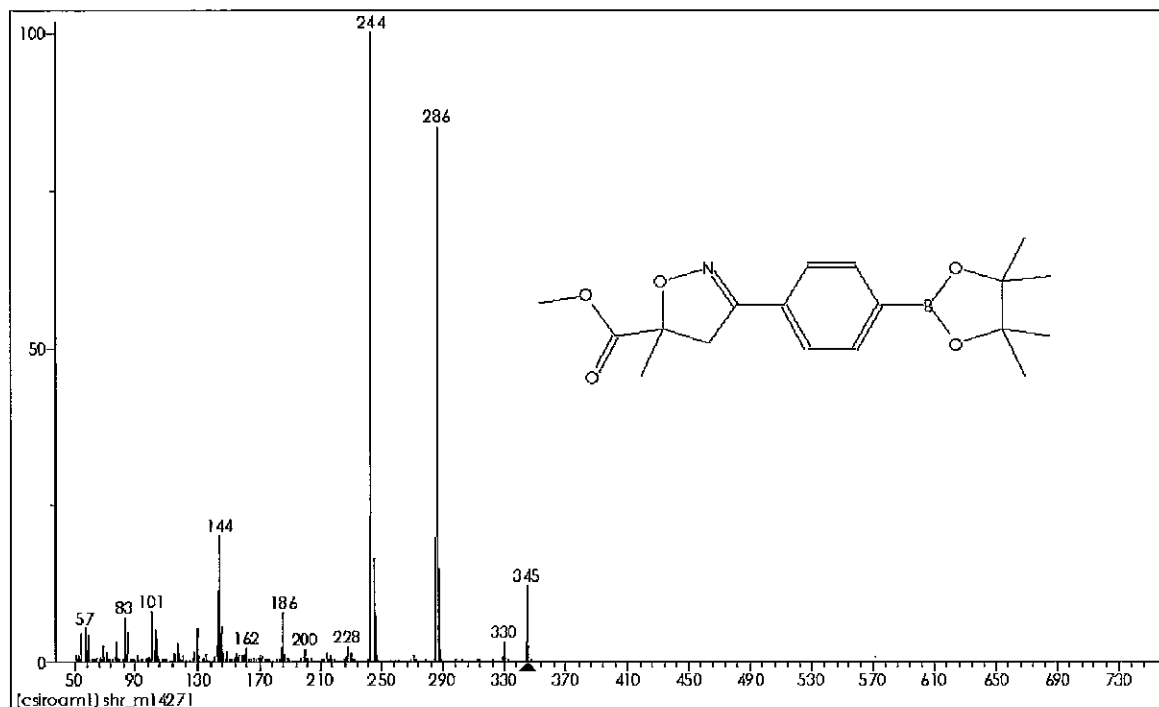
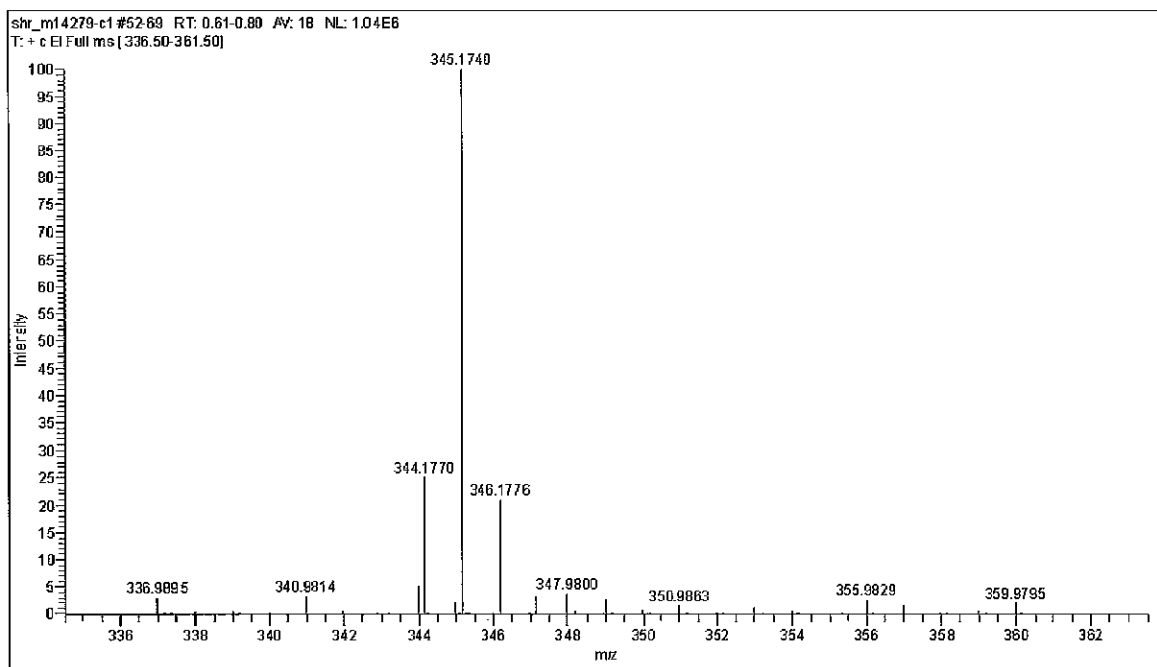
===== CHANNEL f15 =====  
 NUC15: 1H  
 P15: 12.54 usec  
 PL15: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO15: 400.1300178 MHz

===== CHANNEL f16 =====  
 NUC16: 1H  
 P16: 12.54 usec  
 PL16: 1.00 dB  
 FWH: 400.1300178 MHz  
 SFO16: 400.1300178 MHz





CSIRO

Low Resolution EI SpectrumHigh Resolution EI Spectrum

Name Sarah Harding  
WBS R-00366-09-003  
SLH079hfl

CSIRO AV400X\_1H CDCl3 C:\har97c 7

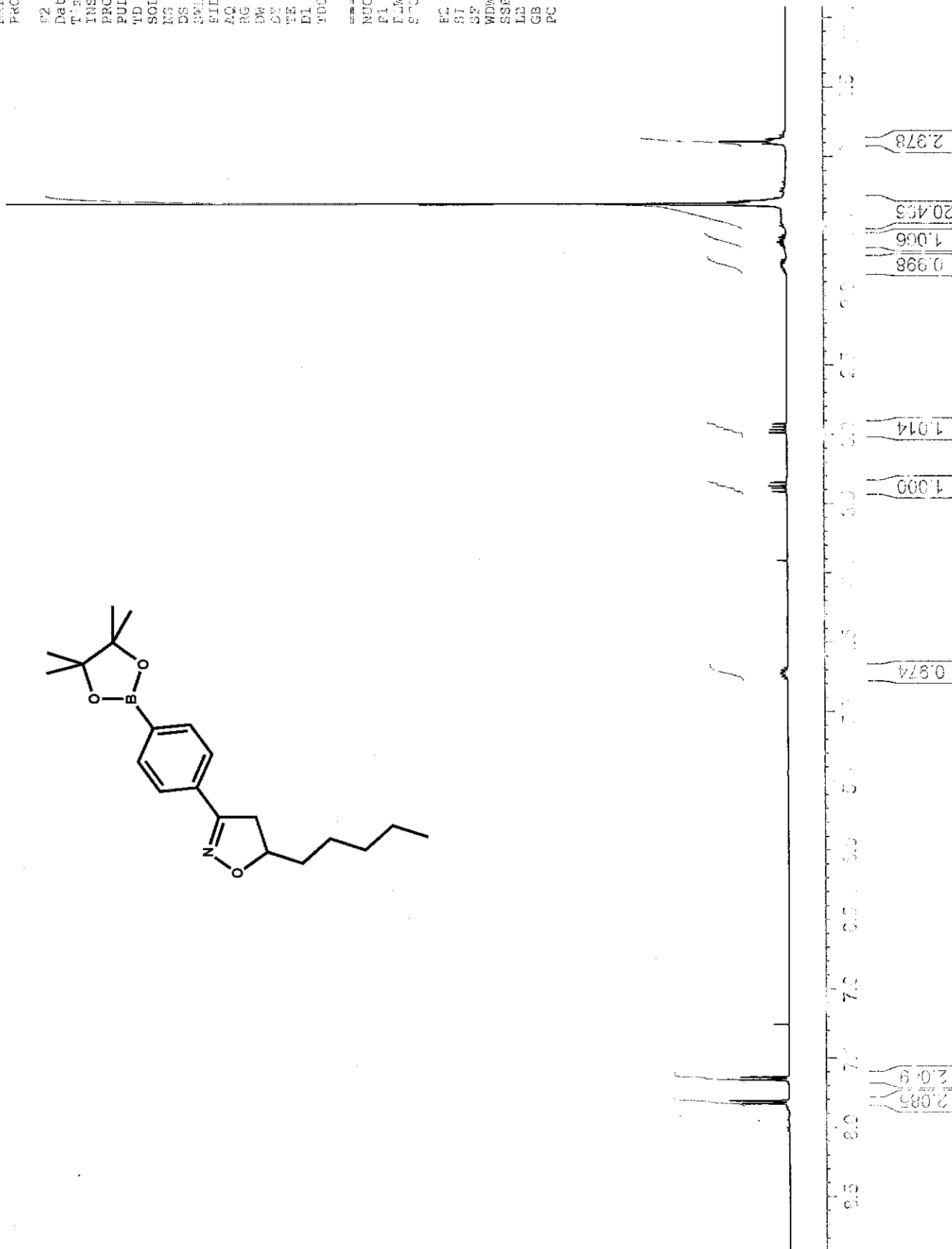
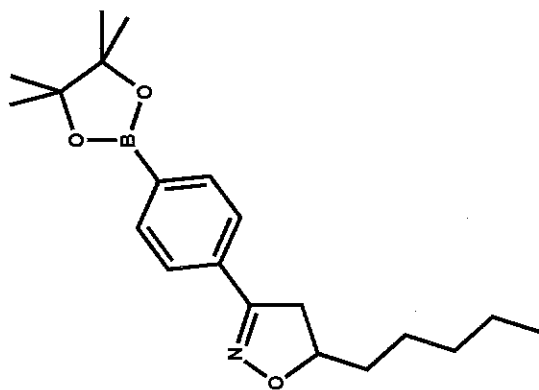
BRUKER

Current Data Parameters  
NAME HardingX40214  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111207  
Time 16.55  
INSTRUM AV400X  
PROBHD 5 mm 1H/13C BBO  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6393.062 Hz  
FIDRES 0.195125 Hz  
AQ 2.5625076 sec  
RG 68.07  
DM 78.200 usec  
DE 6.50 usec  
TE 297.0 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL F1 =====  
NUC1 1H  
P1 17.00 usec  
PL1 20.0000000 W  
SFO1 400.1326000 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1300137 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





BRUKER

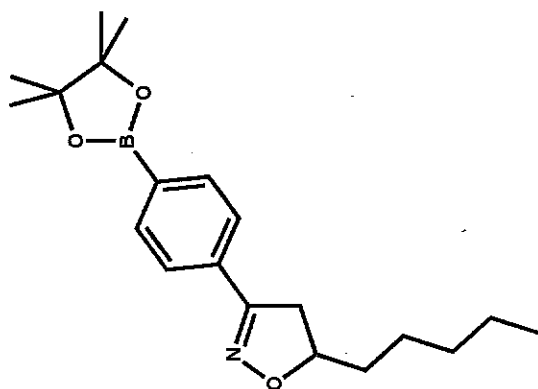
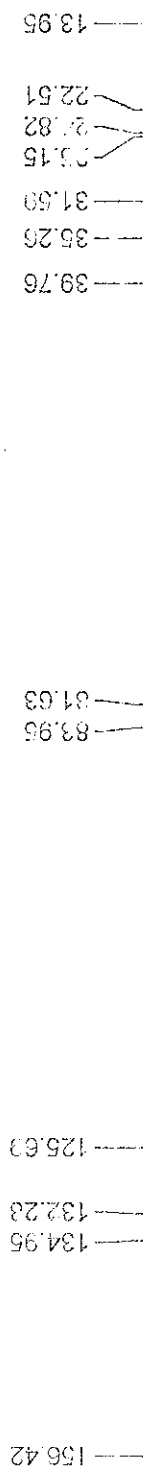
Current Data Parameters  
 NAME Hardin0014  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 2011207  
 Time 18.11  
 INSTRUM A100X  
 PROBHD 5 mm PABBO 9B-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 750  
 DS 4  
 SWH 26044.366 Hz  
 FIDRES 0.397364 Hz  
 AQ 1.2583412 sec  
 RG 184.42  
 DW 10.200 usec  
 DE 3.50 usec  
 TE 297.0 K  
 D1 1.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 67.00000000 W  
 SFO1 100.628425 MHz

===== CHANNEL f2 =====  
 CPDPRG2 bi\_waltz65 256  
 NUC2 1H  
 PCPD2 90.00 usec  
 PLW2 20.00000000 W  
 PLW12 0.71358001 W  
 PLW13 0.57800001 W  
 SFO2 400.131603 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127746 MHz  
 WDW EM  
 SSF 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Name Sarah Harding  
WBS R-00366-09-003  
SLH079ht1

CSIRO Av400X cosy CDC13 C:\har97c 7

BRUKER

Current Data Parameters  
NAME: R-00366-09-003  
EXPER: 1  
PROCNO: 1

F1 - Acquisition Parameters

Date: 20111207  
Time: 15.12  
INSTRUM: AV400X  
PROBHD: 5 mm PABBO 2B-  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: CDCl3  
NS: 1  
DS: 4  
SWH: 4907.672 Hz  
FIDRES: 0.213420 sec  
AQ: 194.73  
RG: 655.36  
DQ: 1.79 sec  
W2: 204.000 MHz  
F2: 296.7 K  
RG: 0.0000000 sec  
RG2: 2.0000000 sec  
RG3: 3.0000000 sec  
RG4: 0.0000000 sec  
RG5: 0.0000000 sec  
RG6: 0.0000000 sec

F2 - Processing Parameters

SI: 32768  
SF: 400.146179 MHz  
WDW: EM  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

F3 - Acquisition Parameters

SI: 32768  
SF: 400.146179 MHz  
WDW: EM  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

F4 - Processing Parameters

SI: 32768  
SF: 400.146179 MHz  
WDW: EM  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

F5 - Acquisition Parameters

SI: 32768  
SF: 400.146179 MHz  
WDW: EM  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

F6 - Processing Parameters

SI: 32768  
SF: 400.146179 MHz  
WDW: EM  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

F7 - Acquisition Parameters

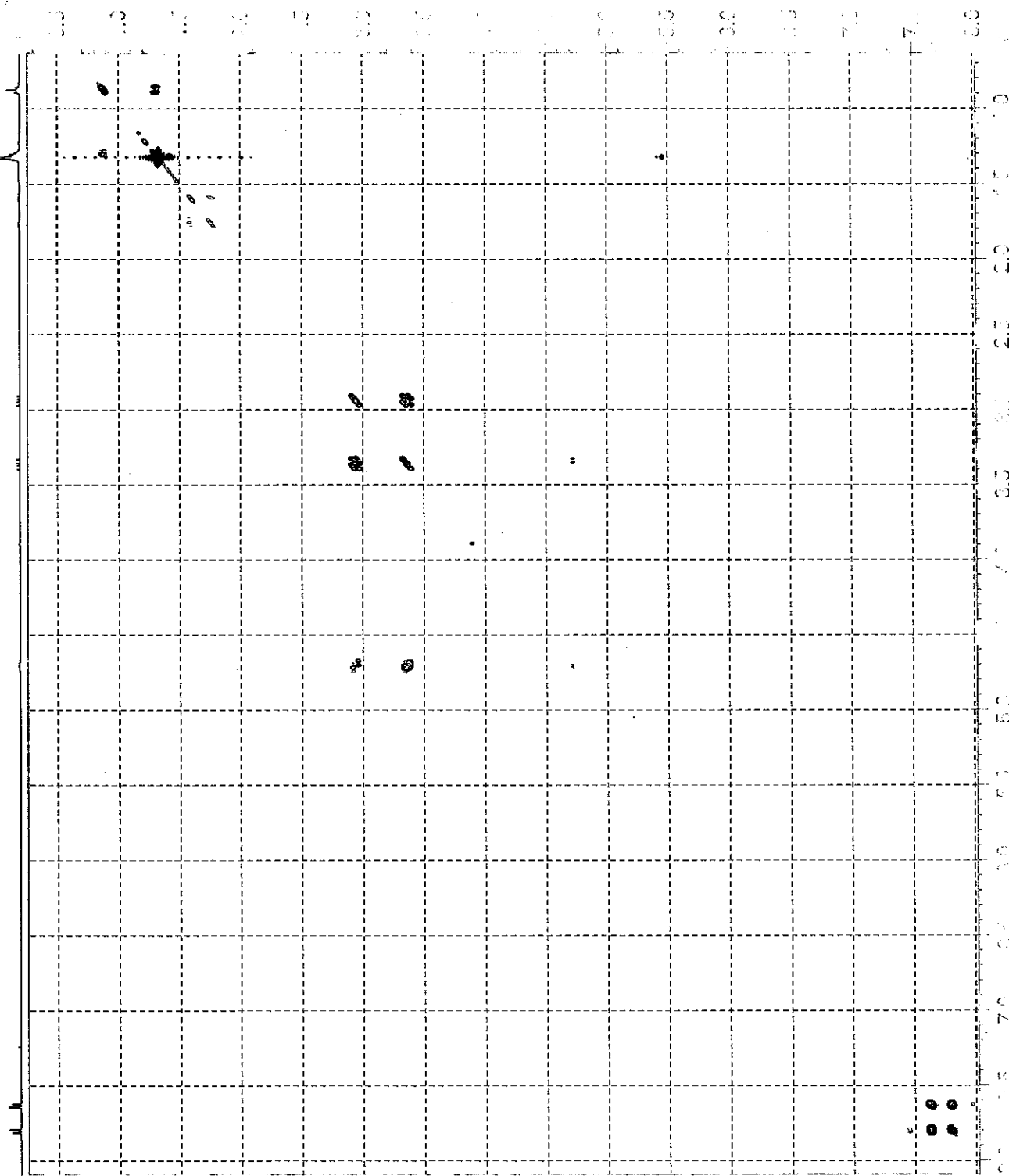
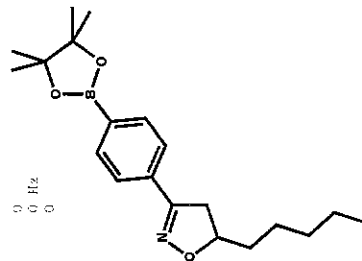
SI: 32768  
SF: 400.146179 MHz  
WDW: EM  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

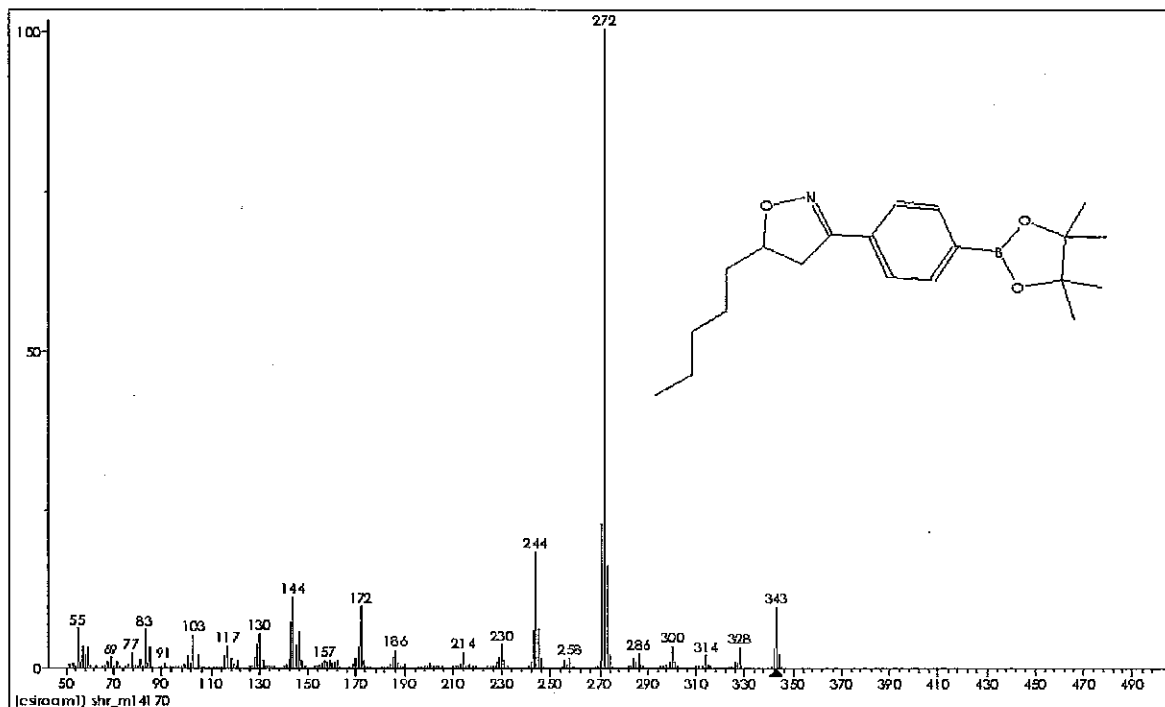
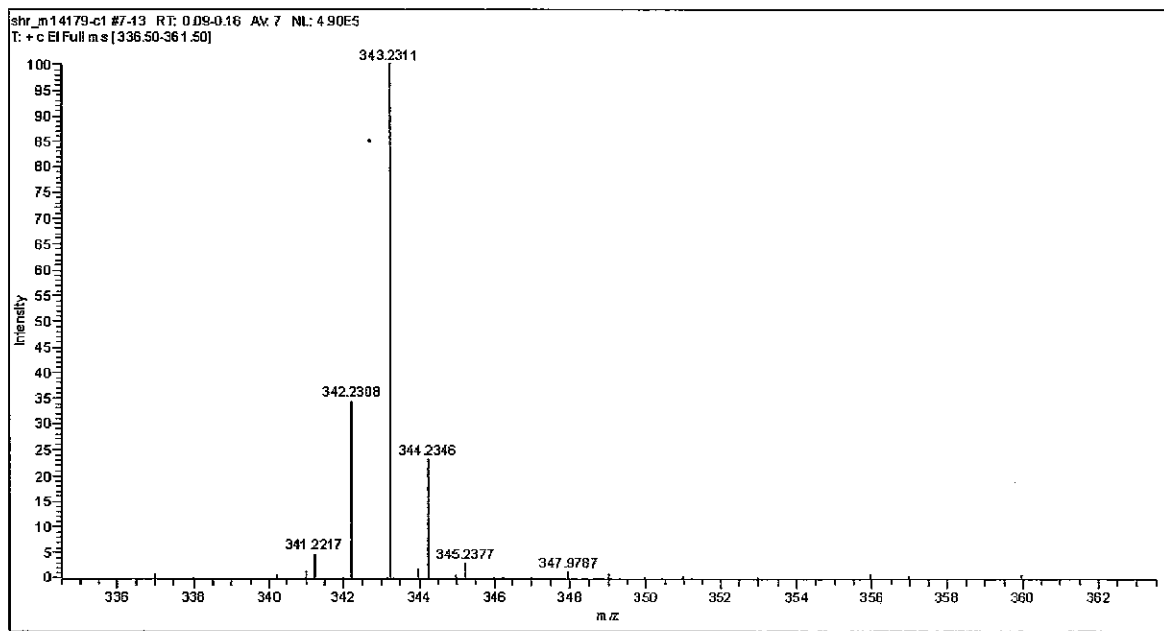
F8 - Processing Parameters

SI: 32768  
SF: 400.146179 MHz  
WDW: EM  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

F9 - Acquisition Parameters

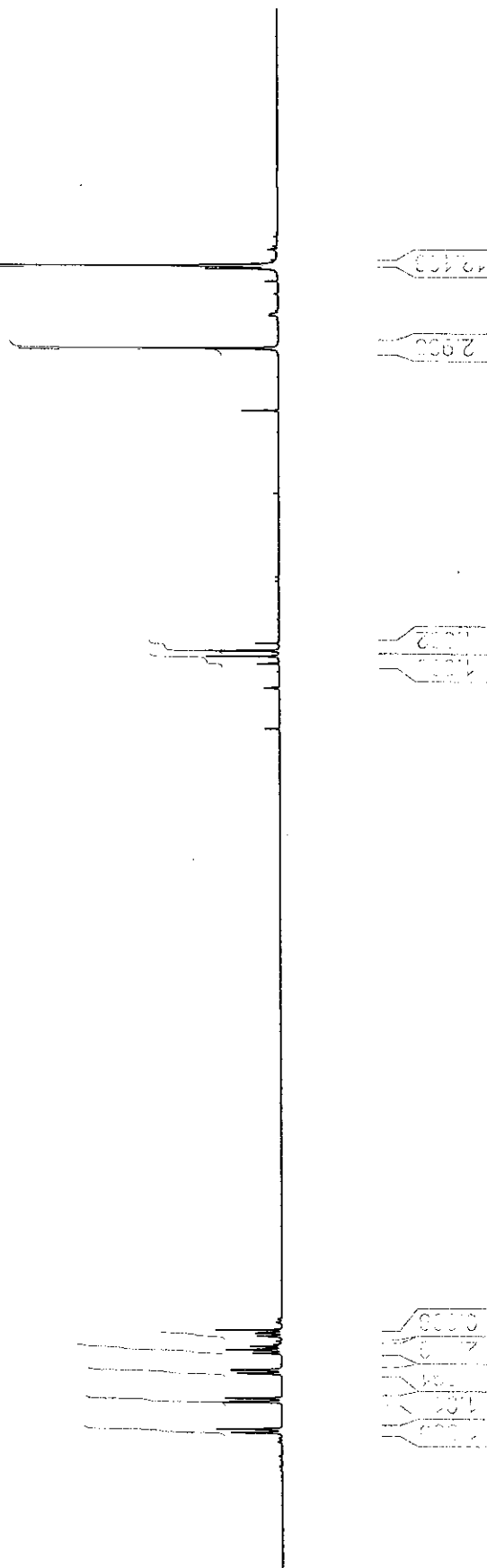
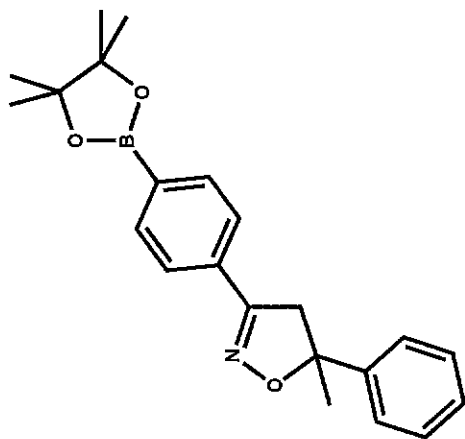
SI: 32768  
SF: 400.146179 MHz  
WDW: EM  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00



Low Resolution EI SpectrumHigh Resolution EI Spectrum

Name Sarah Harding  
WBS R-00366-09-003  
SLH084-2d-alpha-f1  
CSIRO AV400X\_1H CDCl3 C:\har97c 22

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Name Sarah Harding  
WBS R-00366-09-003  
SLH084-2d-alpha-f1  
CSIRO Av400X\_13C CDC13 C:\har97c 22



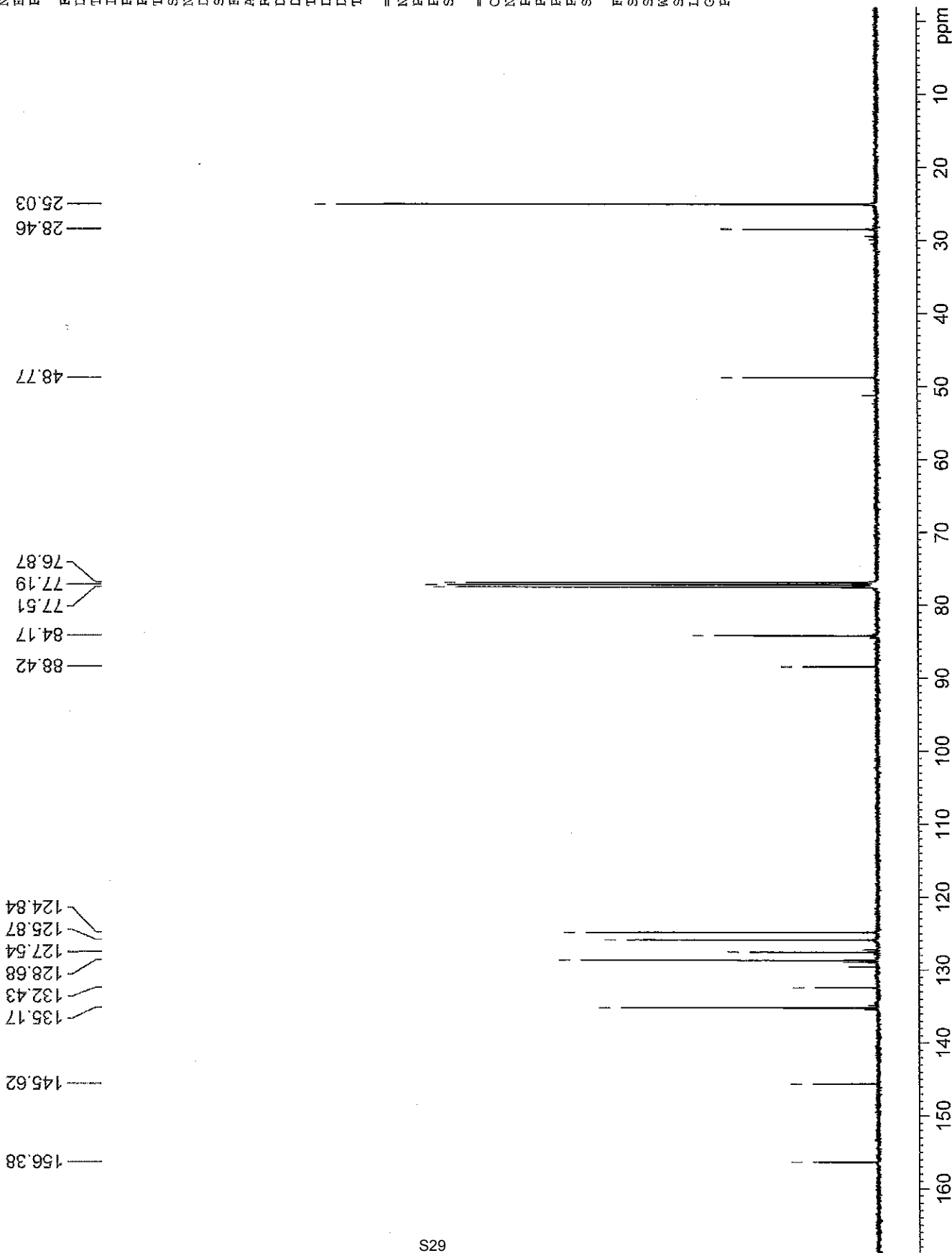
Current Data Parameters  
NAME HardingX40253  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111221  
Time\_ 3.29  
INSTRUM AV400X  
PROBHD 5 mm FATEO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1000  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.42  
DW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PL1 67.00000000 W  
SFO1 100.6248425 MHz

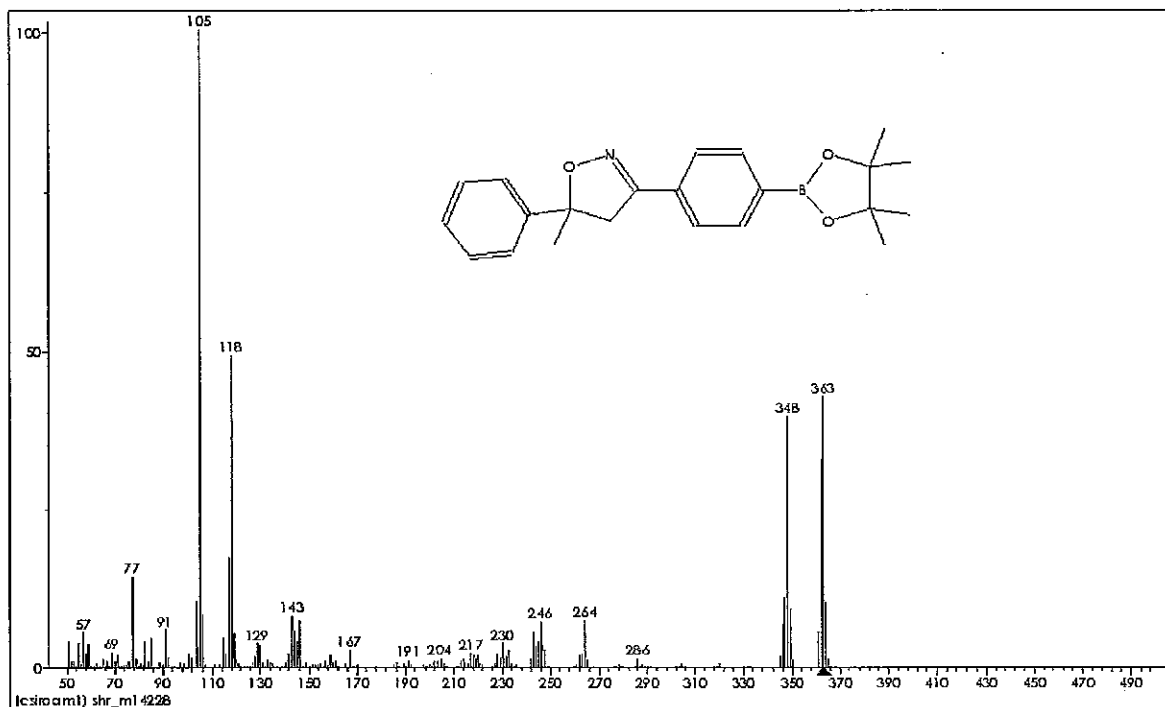
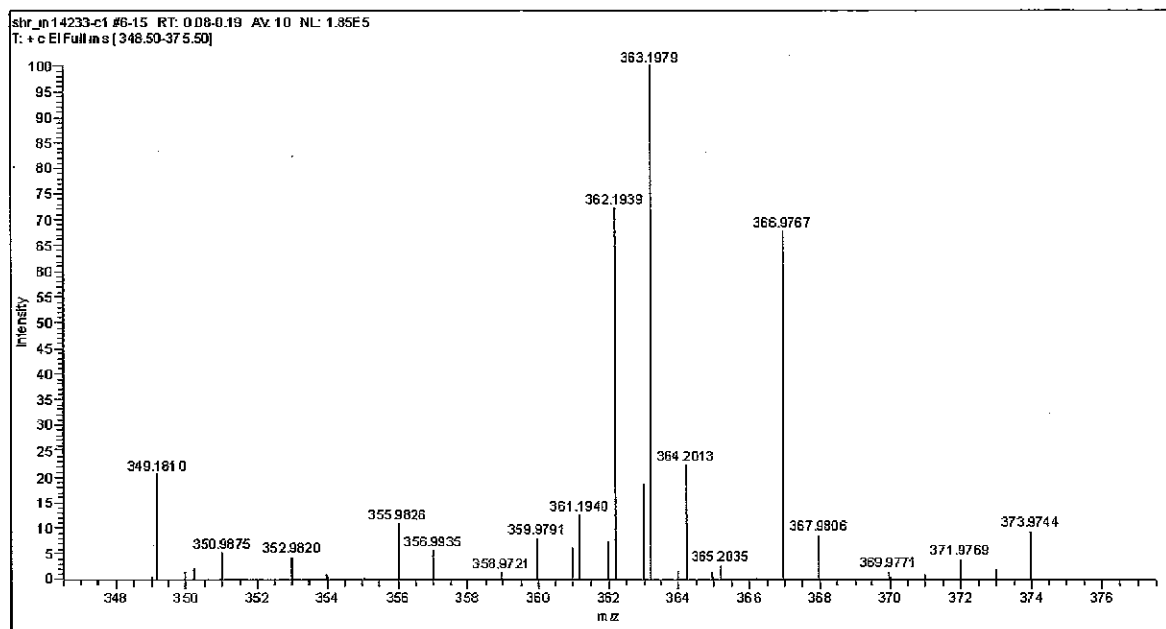
===== CHANNEL f2 =====  
CPDPRG2 bi\_waltz65\_256  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.00000000 W  
PLW12 0.71358001 W  
PLW13 0.57800001 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127541 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





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Low Resolution EI SpectrumHigh Resolution EI Spectrum

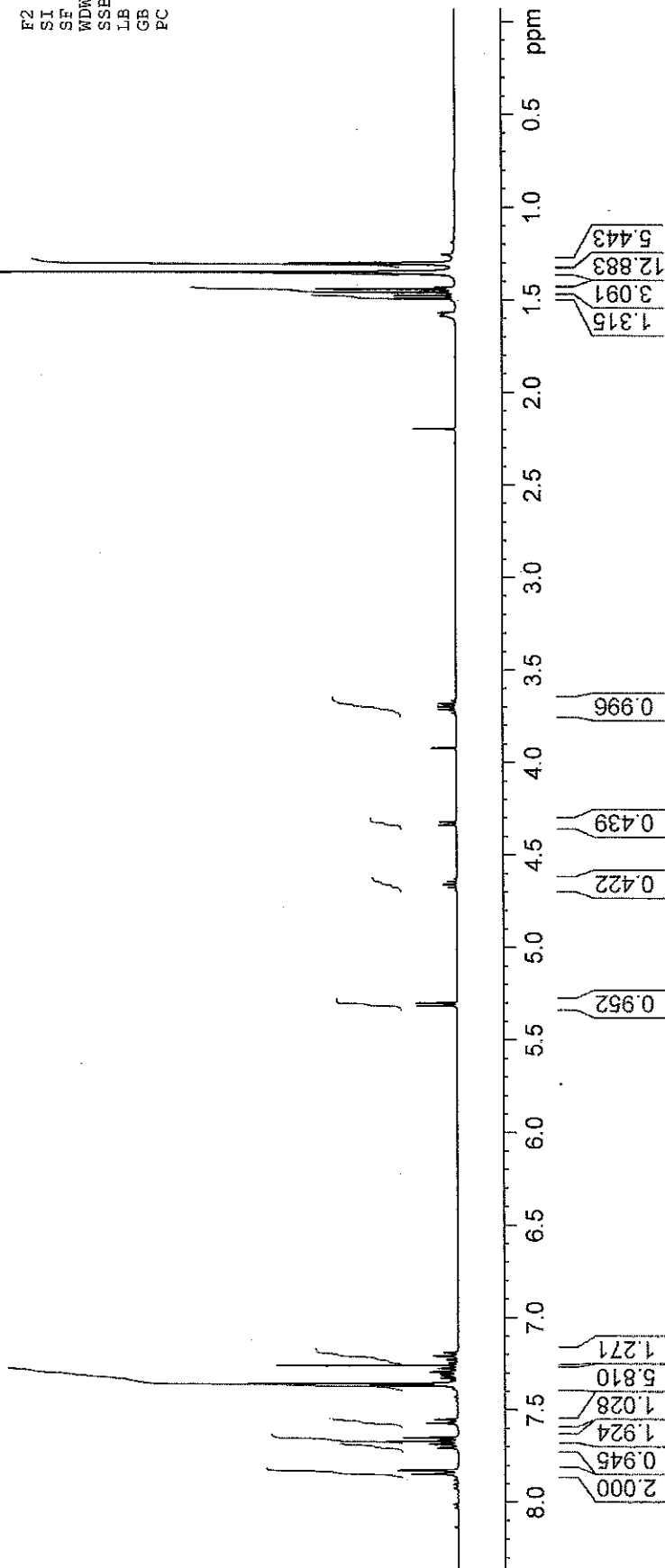
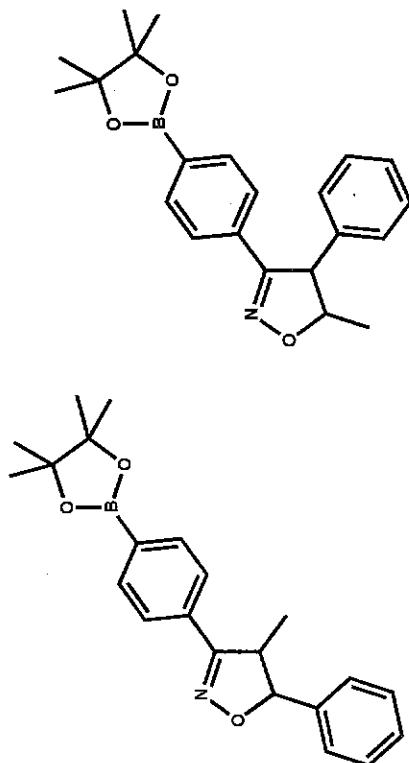


Current Data Parameters  
NAME HardingX40255  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111220  
Time 16.32  
INSTRUM AV400X  
PROBHD 5 mm PATBO BB-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6393.862 Hz  
FIDRES 0.195125 Hz  
AQ 2.5625076 sec  
RG 184.42  
DW 78.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 17.00 usec  
PLW1 20.0000000 W  
SFO1 400.1328009 MHz

F2 - Processing parameters  
SI 65536  
SF 400.1300101 MHz  
WDW EM  
SSB 0  
LB 0.10 Hz  
GB 0  
PC 1.00





Name Sarah Harding  
WBS R-00366-09-003  
SLH084-2e-beta-f1  
CSIRO AV400X\_13C CDCI3 C:\har97c 19



Current Data Parameters  
NAME HardingX40255  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111221  
Time\_ 4.41  
INSTRUM Av400X  
PROBHD 5 mm PATBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1000  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.42  
DW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 67.00000000 W  
SFO1 100.6248425 MHz

==== CHANNEL f2 =====  
CPDPRG2 bi\_waltz65\_256  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.00000000 W  
PLW12 0.71358001 W  
PLW13 0.57800001 W  
SFO2 400.1316005 MHz

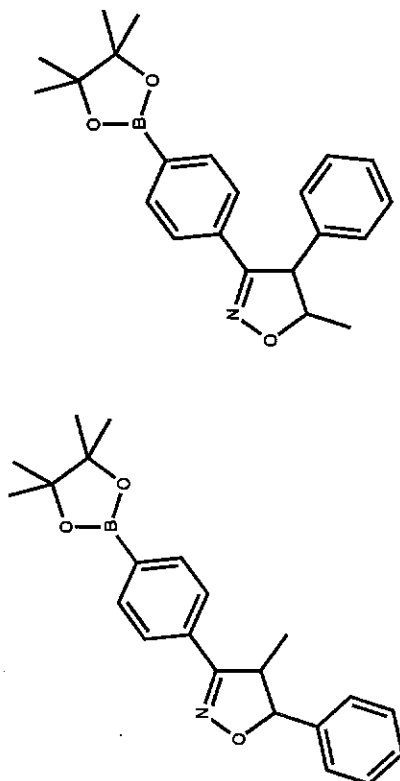
F2 - Processing parameters  
SI 32768  
SF 100.6127746 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

24.81  
24.75  
20.54  
18.17

61.01  
50.75

90.15  
86.95  
83.99  
83.88

160.16  
158.08  
140.76  
138.96  
135.09  
134.79  
131.49  
131.16  
130.37  
129.16  
128.72  
128.13  
127.57  
127.45  
126.32  
126.20  
125.37



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





Name Sarah Harding  
WBS R-00366-09-003  
SLH084-2e-beta-f1  
CSIRO AV400X\_cosy CDCI3 C:\har97c 19



Current Data Parameters  
NAME Harding40255  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20111222  
Time 14.42  
INSTRUM AV400X  
PROBHD 5 mm PABBO BB-  
PULPROG cosygpqf15 CSIRO  
TD 65536  
SOLVENT CDCl3  
NS 15  
DS 1  
SWH 4807.592 Hz  
FIDRES 2.347026 Hz  
AQ 0.2130226 sec  
RG 184.42  
RW 164.000 Hz  
DE 6.50 usec  
TE 297.0 K  
D0 0.0000300 sec  
D1 1.0000000 sec  
D13 0.0000000 sec  
D16 0.0002000 sec  
INVO 0.0002000 sec

===== CHANNEL f1 =====

NUC1 1H  
P0 8.50 usec  
F1 19.00 usec  
PL1 23.0000000  
SF01 400.1322007 MHz

===== GRADIENT CHANNEL =====

GENPML SMS10.100  
GF1 10.00 Hz  
F16 1000.00 usec

F1 - Acquisition Parameters

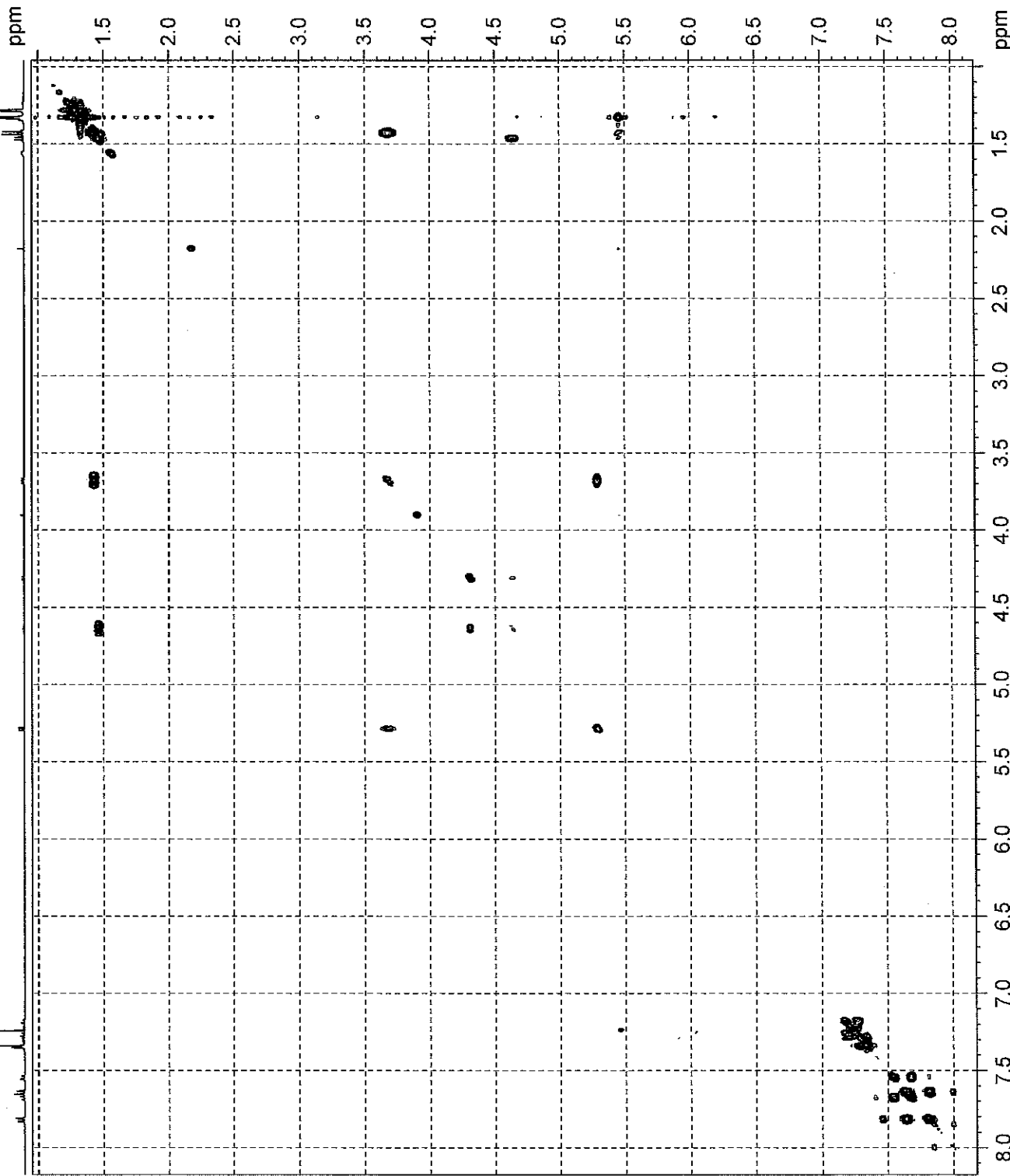
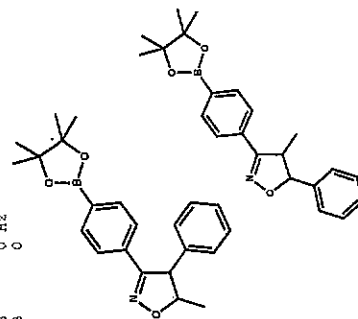
TD 65536  
SF01 400.1322 MHz  
FIDRES 9.56022 Hz  
SW 12.015 ppm  
FMA000 QF

F2 - Processing Parameters

SI 1024  
SF 400.1300178 MHz  
WDW SINE  
SSB 0 Hz  
LB 0  
GB 0  
PC 1.00

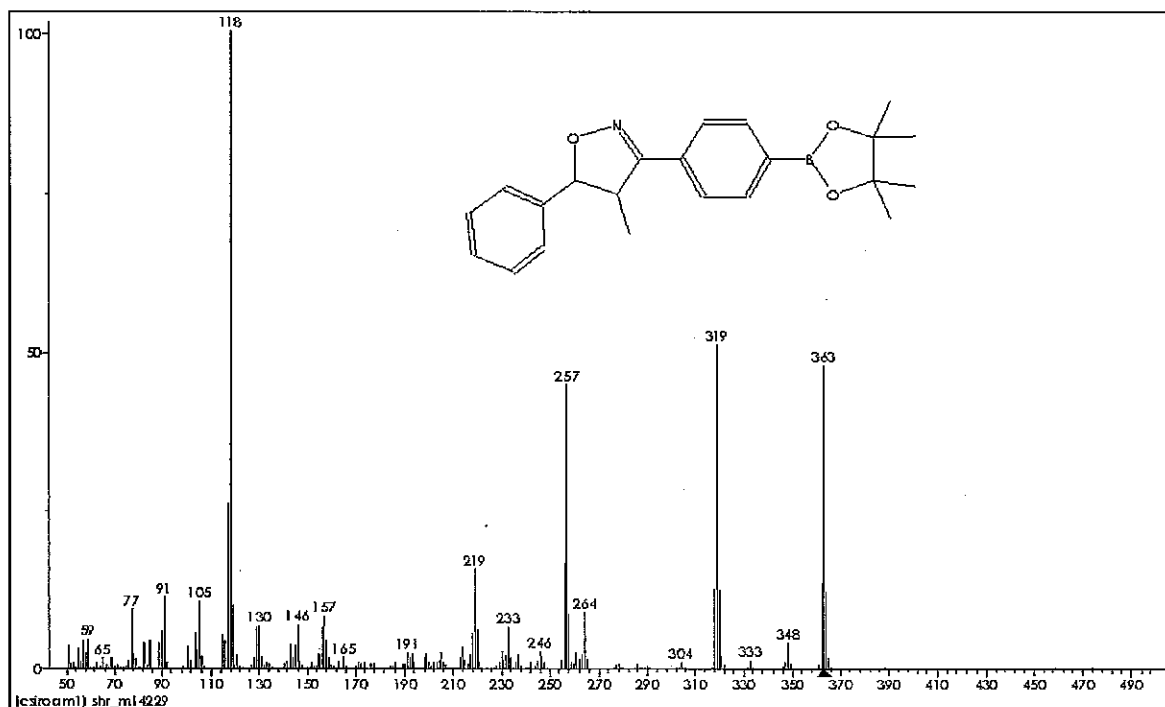
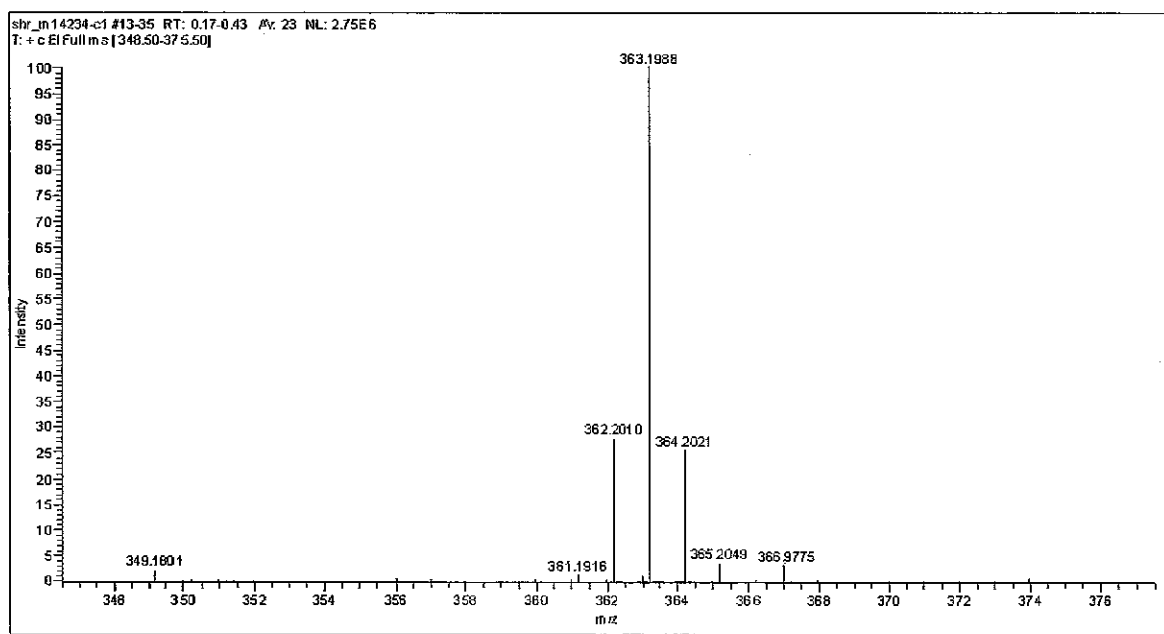
F1 - Processing Parameters

SI 1024  
SF 400.1300178 MHz  
WDW QF  
SSB 0 Hz  
LB 0  
GB 0



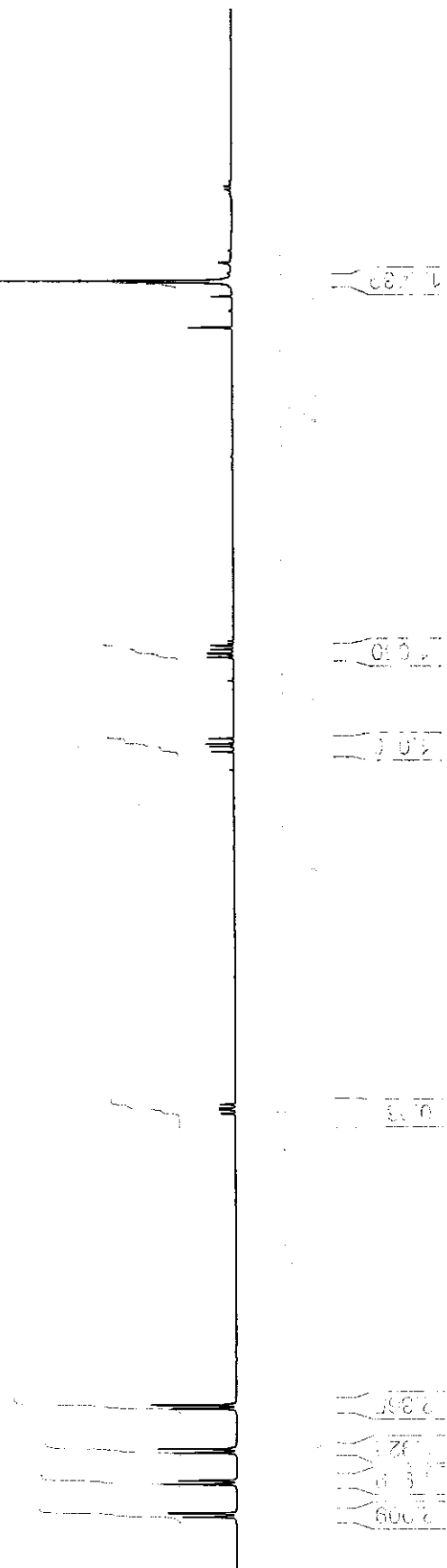
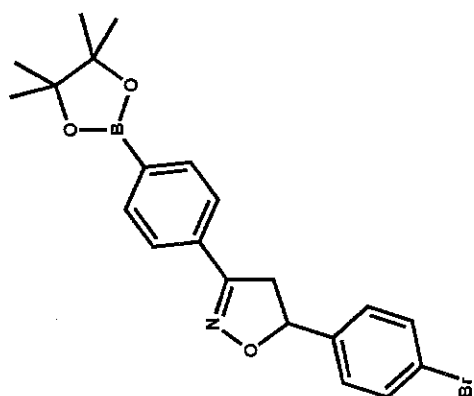


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Low Resolution EI SpectrumHigh Resolution EI Spectrum

Name Sarah Harding  
WBS R-00366-09-003  
SLH085-2f-f2  
CSIRO AV400X\_1H CDCl3 C:\har97c 6

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Name Sarah Harding  
WBS R-00366-09-003  
SLH085-2f-f2  
CSIRO Av400X\_13C CDCl3 C:\har97c 6



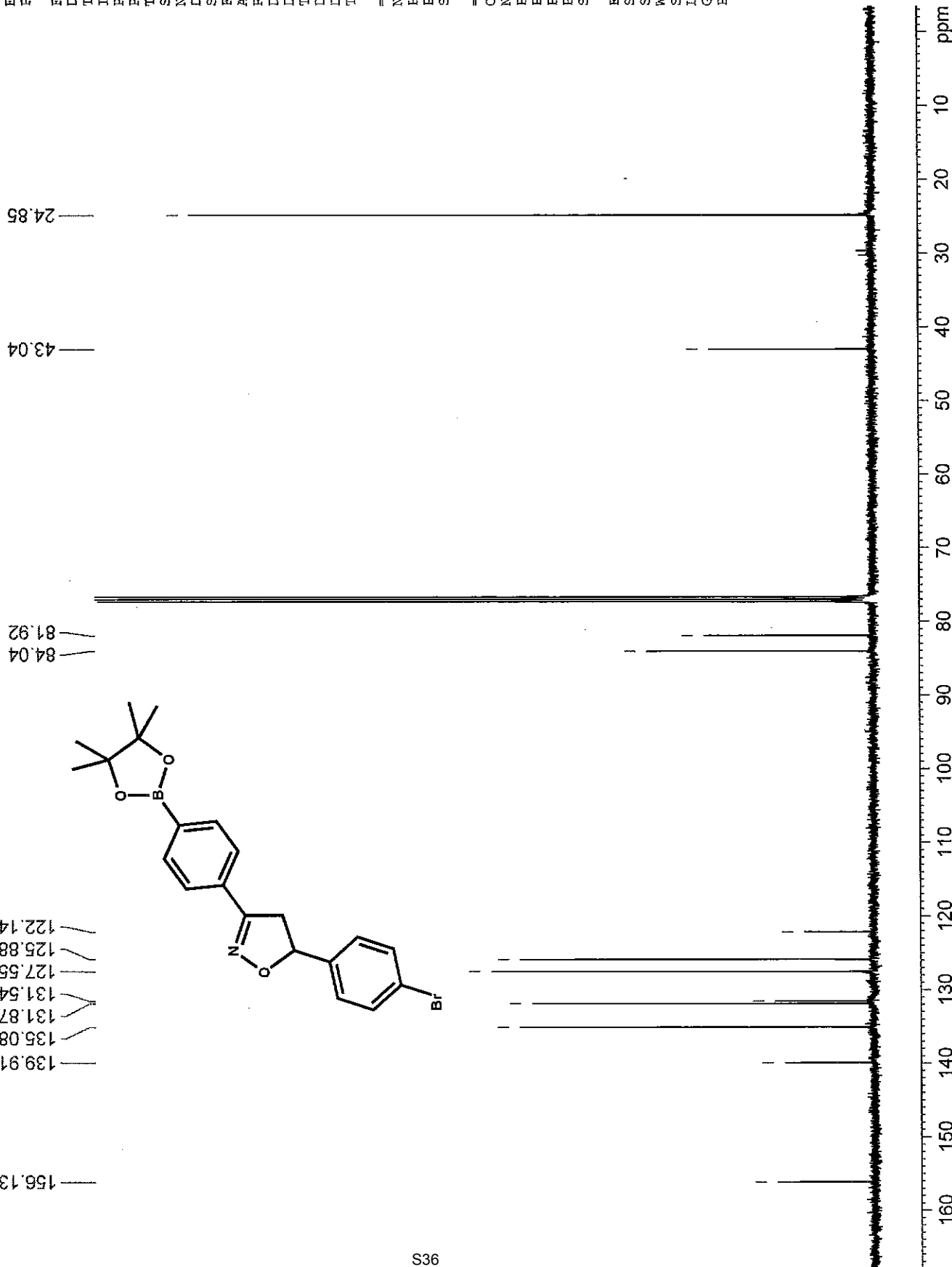
Current Data Parameters  
NAME HardingX40266  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20111222  
Time\_ 12.15  
INSTRUM AV400X  
PROBHD 5 mm PATEO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 500  
DS 4  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2583412 sec  
RG 184.42  
DW 19.200 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.00 usec  
PLW1 67.00000000 W  
SFO1 100.6248425 MHz

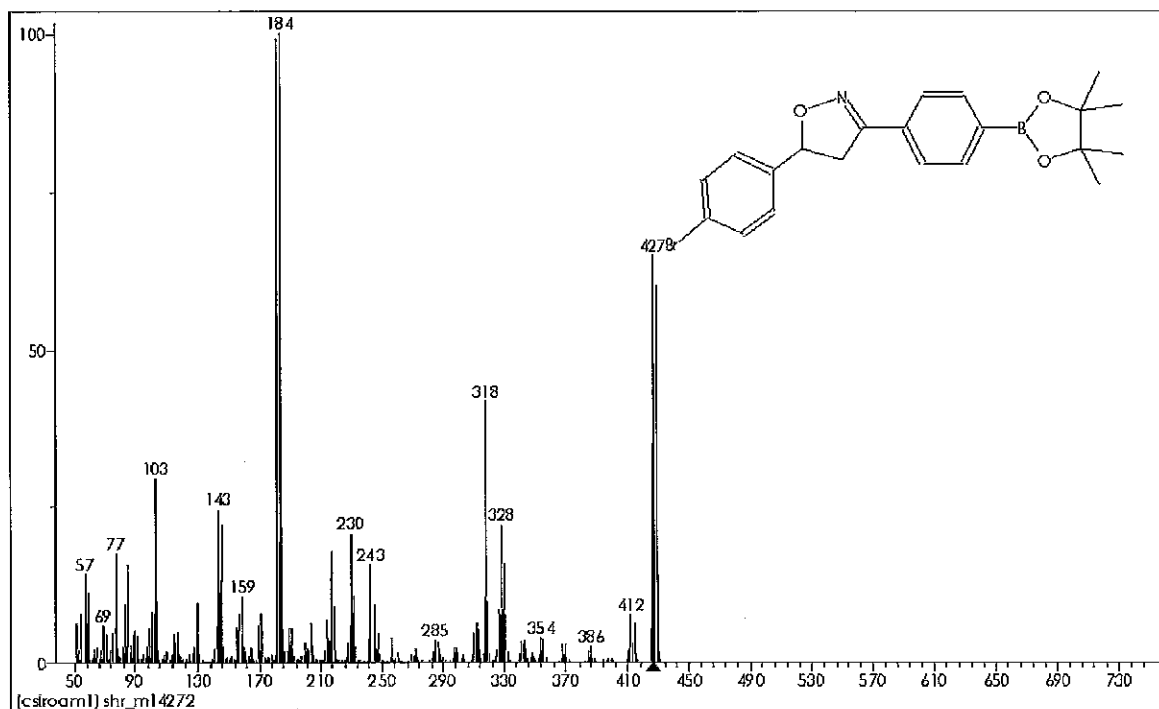
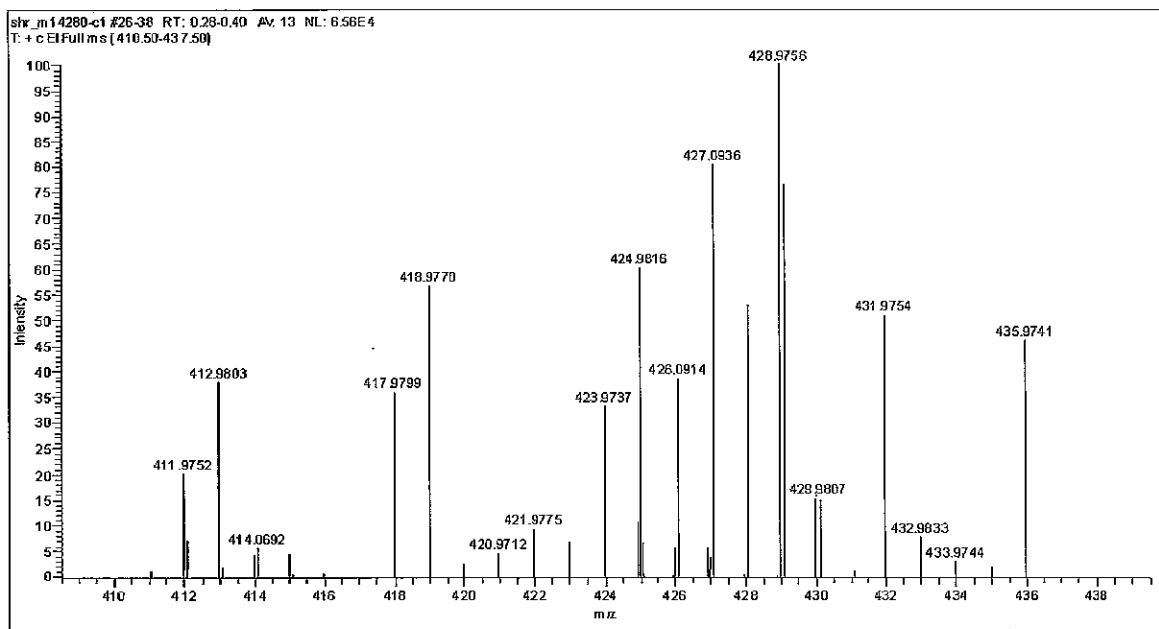
===== CHANNEL f2 =====  
CPDPRG2 bi\_waltz85\_256  
NUC2 1H  
PCPD2 90.00 usec  
PLW2 20.00000000 W  
PLW12 0.71358001 W  
PLW13 0.57800001 W  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127731 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





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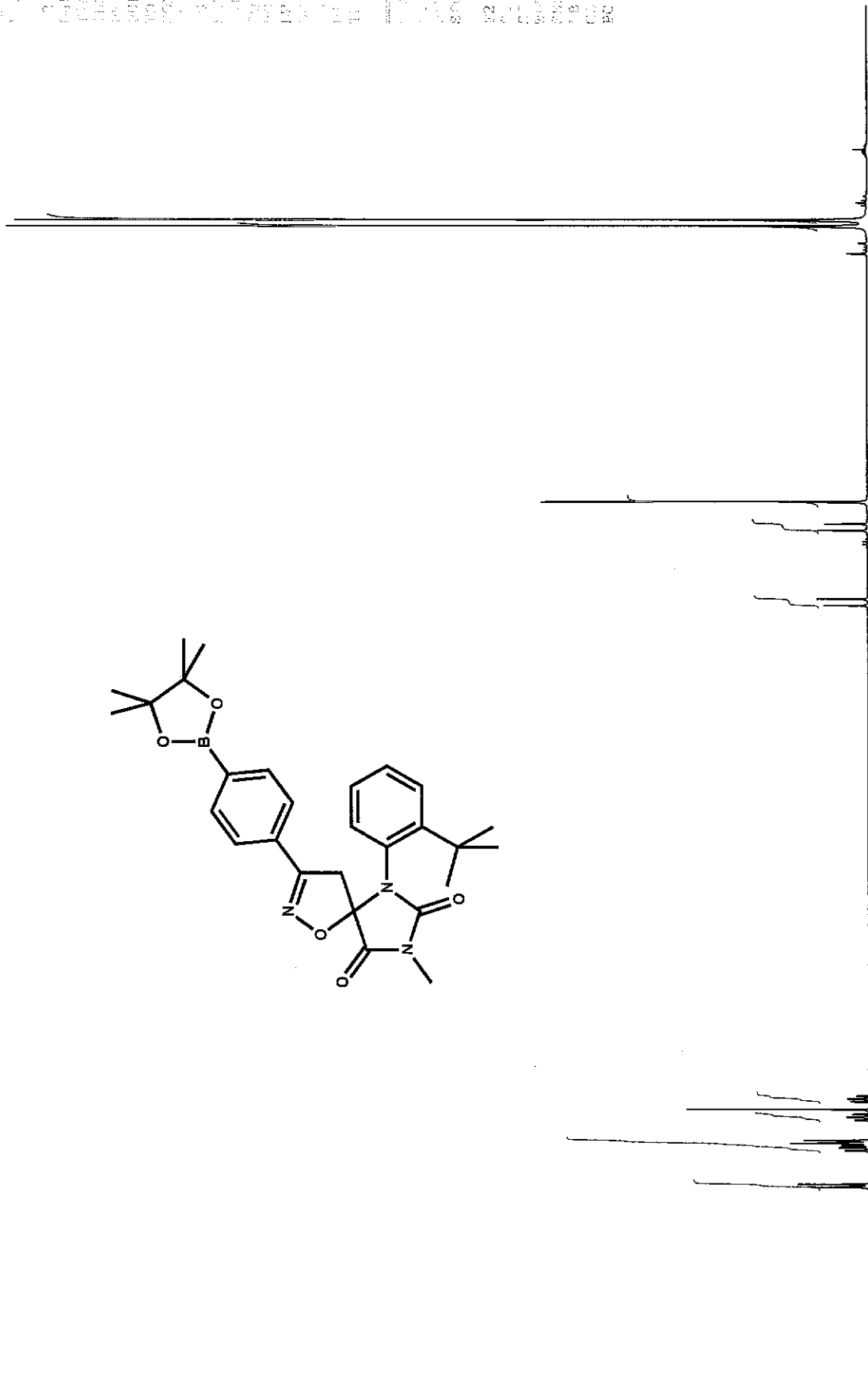
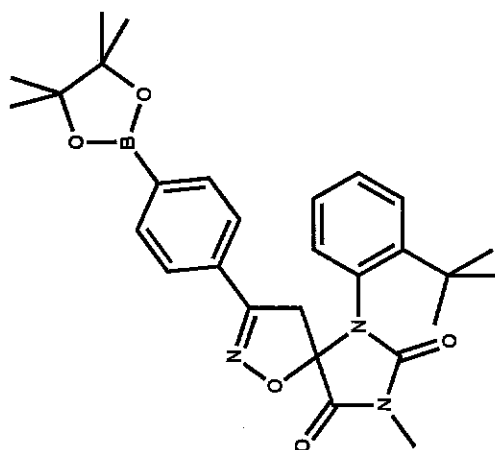
Low Resolution EI SpectrumHigh Resolution EI Spectrum

Name Sarah Harding  
 WBS R-00366-09-003  
 SLH074s  
 CSIRO Av400X\_1H CDCl3 C:\har97c 8

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1 - 1H NMR spectrum  
 NAME: SLH074s  
 DATE: 10/10/01  
 TIME: 10:00

2 - Acquisition parameters  
 Date: 10/11/01  
 Time: 10:19  
 Name: SLH074s  
 File: 101010101  
 Exp: 1  
 F1: 400.136095 MHz  
 F2: 101.625000 MHz  
 F3: 101.625000 MHz  
 F4: 101.625000 MHz  
 F5: 101.625000 MHz  
 F6: 101.625000 MHz  
 F7: 101.625000 MHz  
 F8: 101.625000 MHz  
 F9: 101.625000 MHz  
 F10: 101.625000 MHz  
 F11: 101.625000 MHz  
 F12: 101.625000 MHz  
 F13: 101.625000 MHz  
 F14: 101.625000 MHz  
 F15: 101.625000 MHz  
 F16: 101.625000 MHz  
 F17: 101.625000 MHz  
 F18: 101.625000 MHz  
 F19: 101.625000 MHz  
 F20: 101.625000 MHz  
 F21: 101.625000 MHz  
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 F24: 101.625000 MHz  
 F25: 101.625000 MHz  
 F26: 101.625000 MHz  
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 F29: 101.625000 MHz  
 F30: 101.625000 MHz  
 F31: 101.625000 MHz  
 F32: 101.625000 MHz  
 F33: 101.625000 MHz  
 F34: 101.625000 MHz  
 F35: 101.625000 MHz  
 F36: 101.625000 MHz  
 F37: 101.625000 MHz  
 F38: 101.625000 MHz  
 F39: 101.625000 MHz  
 F40: 101.625000 MHz  
 F41: 101.625000 MHz  
 F42: 101.625000 MHz  
 F43: 101.625000 MHz  
 F44: 101.625000 MHz  
 F45: 101.625000 MHz  
 F46: 101.625000 MHz  
 F47: 101.625000 MHz  
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 F49: 101.625000 MHz  
 F50: 101.625000 MHz  
 F51: 101.625000 MHz  
 F52: 101.625000 MHz  
 F53: 101.625000 MHz  
 F54: 101.625000 MHz  
 F55: 101.625000 MHz  
 F56: 101.625000 MHz  
 F57: 101.625000 MHz  
 F58: 101.625000 MHz  
 F59: 101.625000 MHz  
 F60: 101.625000 MHz  
 F61: 101.625000 MHz  
 F62: 101.625000 MHz  
 F63: 101.625000 MHz  
 F64: 101.625000 MHz  
 F65: 101.625000 MHz  
 F66: 101.625000 MHz  
 F67: 101.625000 MHz  
 F68: 101.625000 MHz  
 F69: 101.625000 MHz  
 F70: 101.625000 MHz  
 F71: 101.625000 MHz  
 F72: 101.625000 MHz  
 F73: 101.625000 MHz  
 F74: 101.625000 MHz  
 F75: 101.625000 MHz  
 F76: 101.625000 MHz  
 F77: 101.625000 MHz  
 F78: 101.625000 MHz  
 F79: 101.625000 MHz  
 F80: 101.625000 MHz  
 F81: 101.625000 MHz  
 F82: 101.625000 MHz  
 F83: 101.625000 MHz  
 F84: 101.625000 MHz  
 F85: 101.625000 MHz  
 F86: 101.625000 MHz  
 F87: 101.625000 MHz  
 F88: 101.625000 MHz  
 F89: 101.625000 MHz  
 F90: 101.625000 MHz  
 F91: 101.625000 MHz  
 F92: 101.625000 MHz  
 F93: 101.625000 MHz  
 F94: 101.625000 MHz  
 F95: 101.625000 MHz  
 F96: 101.625000 MHz  
 F97: 101.625000 MHz  
 F98: 101.625000 MHz  
 F99: 101.625000 MHz  
 F100: 101.625000 MHz



Name Sarah Harding  
 WBS R-00366-09-003  
 SLH074S  
 CSIRO Av400X\_13C CDC13 C:\har97c 31

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36.69  
 36.52  
 32.47  
 25.32  
 24.81  
 24.78

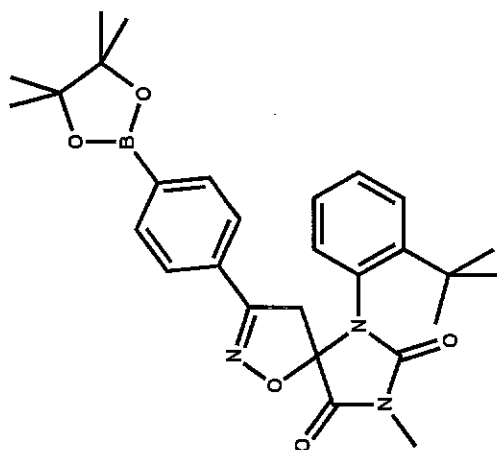
84.08

97.13

135.07  
 132.24  
 130.31  
 130.20  
 129.79  
 128.15  
 127.51  
 125.72

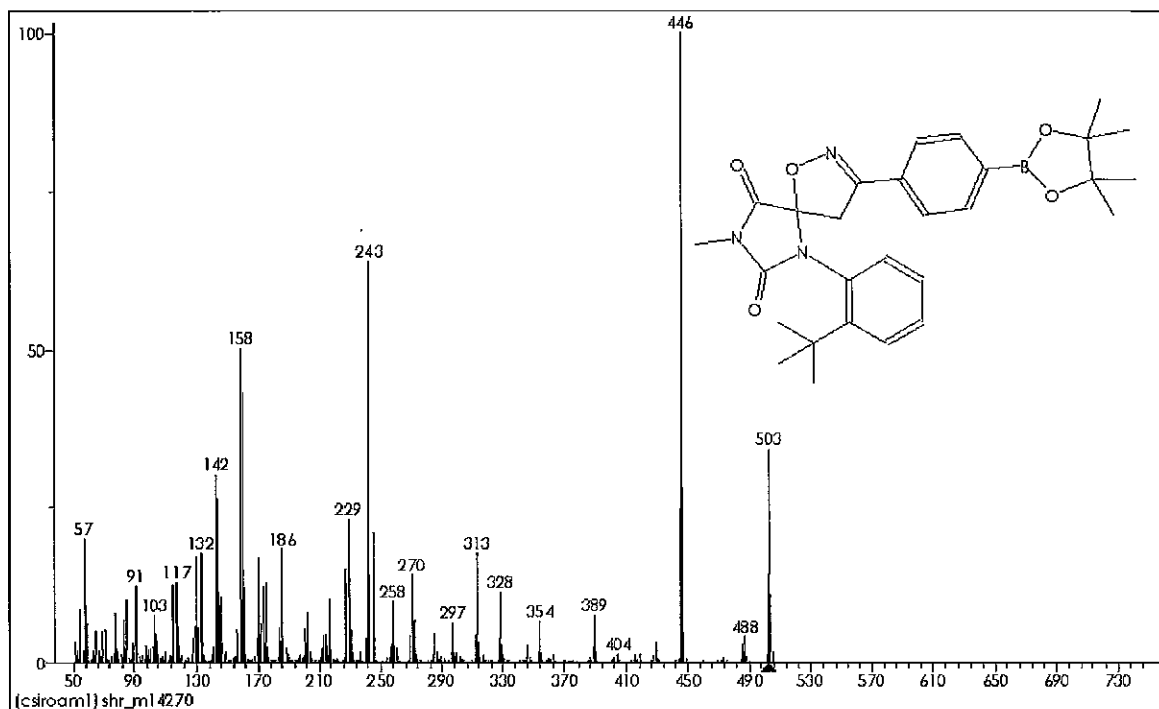
156.07  
 155.41  
 148.31

169.11





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Low Resolution EI SpectrumHigh Resolution EI Spectrum