# Supporting Information

# Ethynylflavones, Highly Potent and Selective Inhibitors of Cytochrome P450 1A1

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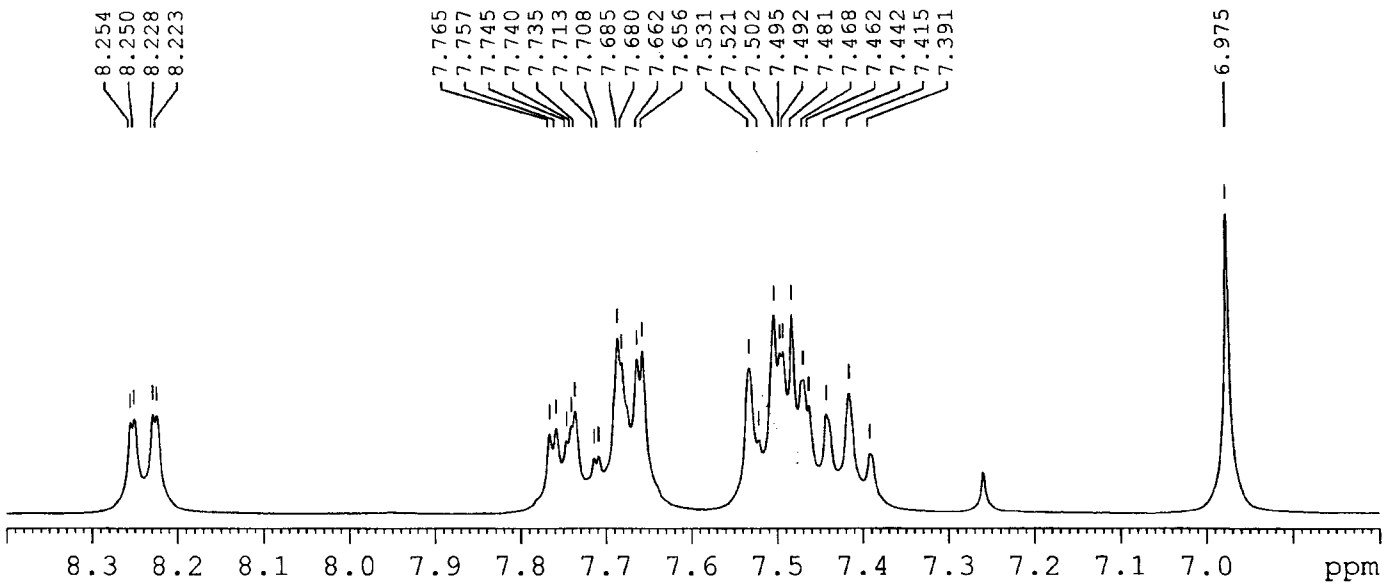
**Contents**

**Table S1.** The $K_i$ values of tested compounds for inhibition of P450s 1A1, 1A2, 1B1, 2A6, and 2B1

| | $IC_{50}$ (μM) | | | | |
|---|---|---|---|---|---|
| | P450 1A1 | P450 1A2 | P450 1B1 | P450 2A6 | P450 2B1 |
| αNF | 0.043±0.009 | 0.019±0.006 | 0.015±0.005 | >25 | 13.0±2.6 |
| 7E3PC | 0.74±0.08 | 2.97±0.33 | 1.72±0.23 | >25 | >25 |
| 2'EF | 1.64±0.30 | 0.23±0.01 | 0.61±0.06 | >25 | 15.7±8.23 |
| 3'EF | 0.041±0.004 | 0.80±0.12 | 0.16±0.03 | >25 | >25 |
| 4'EF | 0.039±0.003 | 3.26±0.63 | 0.13±0.01 | >25 | >25 |
| 5EF | 1.23±0.25 | 0.81±0.06 | 0.21±0.03 | >25 | >25 |
| 6EF | 0.035±0.011 | 6.20±0.61 | 0.54±0.05 | >25 | >25 |
| 7EF | 0.024±0.0002 | 0.52±0.06 | 0.42±0.06 | >25 | >25 |

The $K_i$ values are represented as the mean ± SE μM of three independent experiments. αNF, alpha-naphthoflavone. 7E3PC, 7-ethynyl-3-phenylcoumarin.

# 2'-Ethynyl flavone




Current Data Parameters

| | |
|---|---|
| NAME | 2'-Ethynylflavone |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

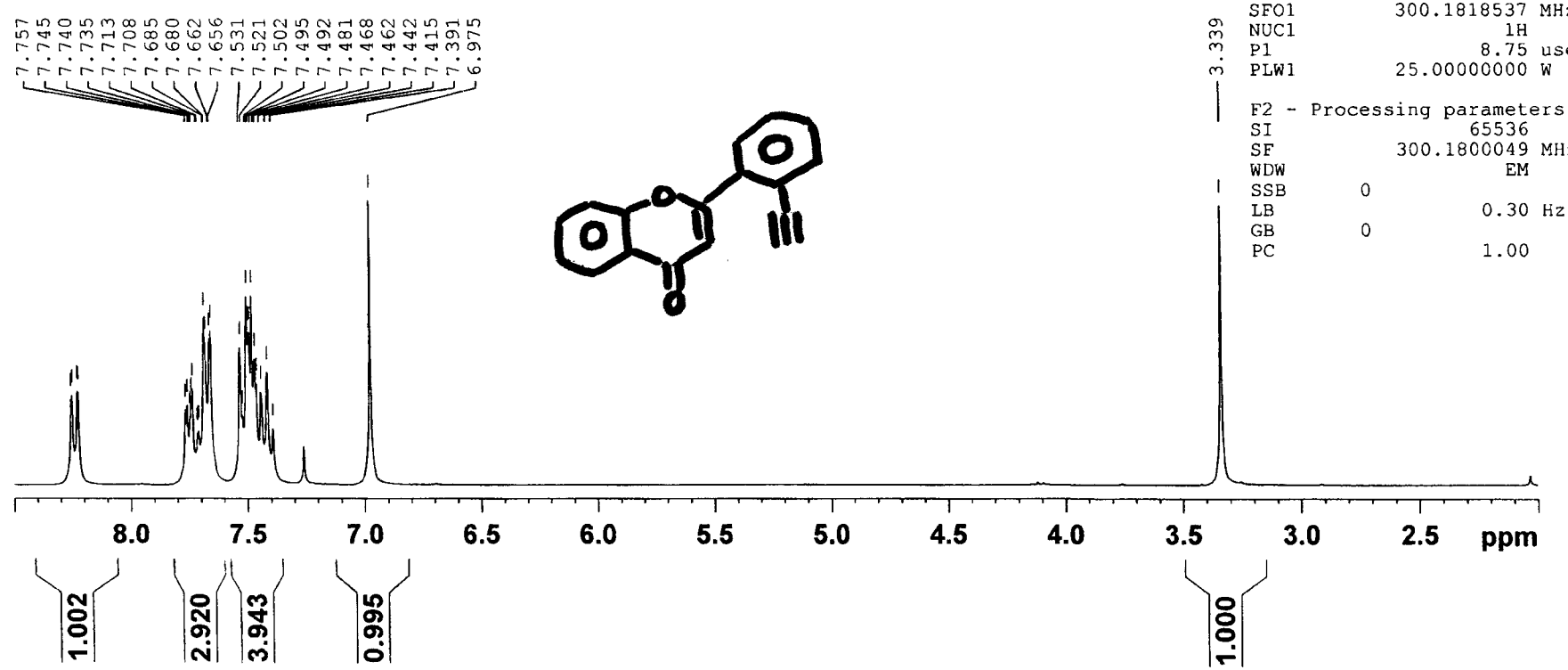
| | |
|---|---|
| Date_ | 20140502 |
| Time | 12.11 |
| INSTRUM | FOURIER300 |
| PROBHD | 5 mm DUL 13C-1 |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6103.516 Hz |
| FIDRES | 0.093132 Hz |
| AQ | 5.3687091 sec |
| RG | 26.3126 |
| DW | 81.920 usec |
| DE | 6.50 usec |
| TE | 295.6 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |

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

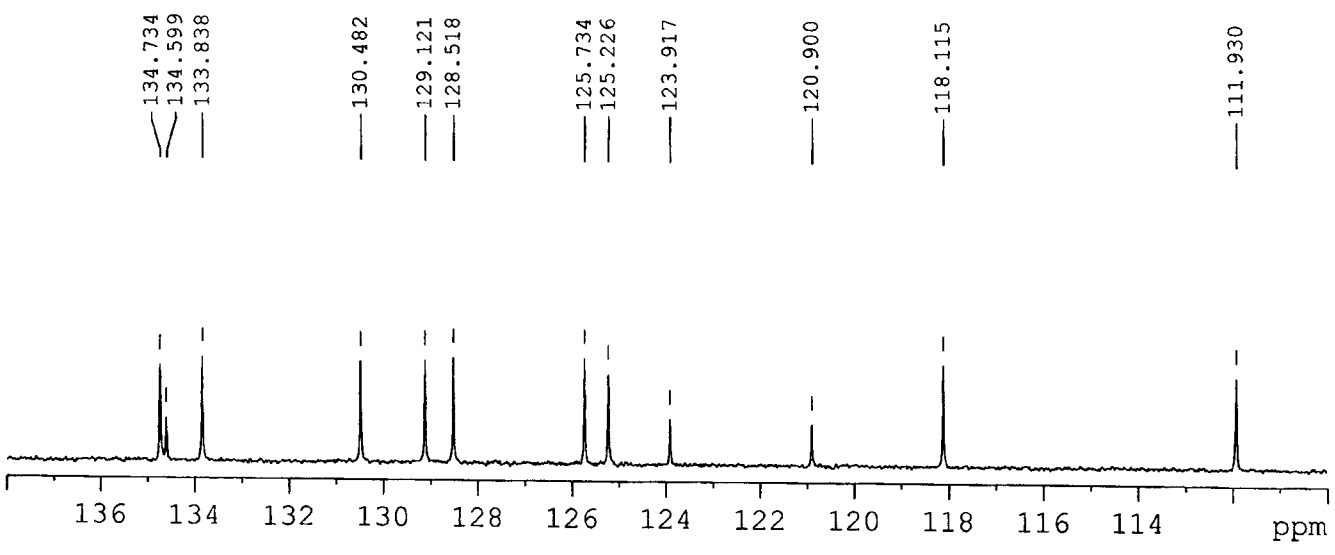
| | |
|---|---|
| SFO1 | 300.1818537 MHz |
| NUC1 | 1H |
| P1 | 8.75 usec |
| PLW1 | 25.00000000 W |

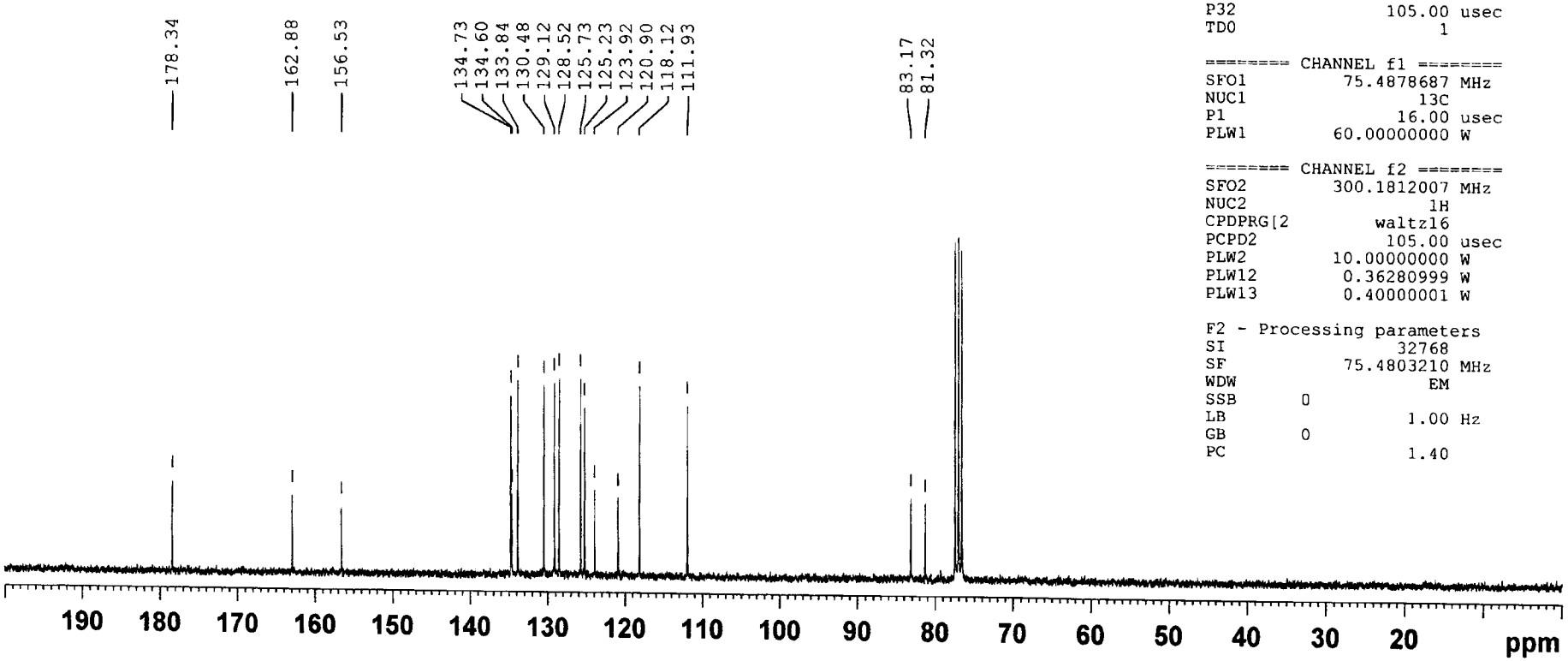
F2 - Processing parameters

| | |
|---|---|
| SI | 65536 |
| SF | 300.1800049 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |



# 2'-Ethynylflavone



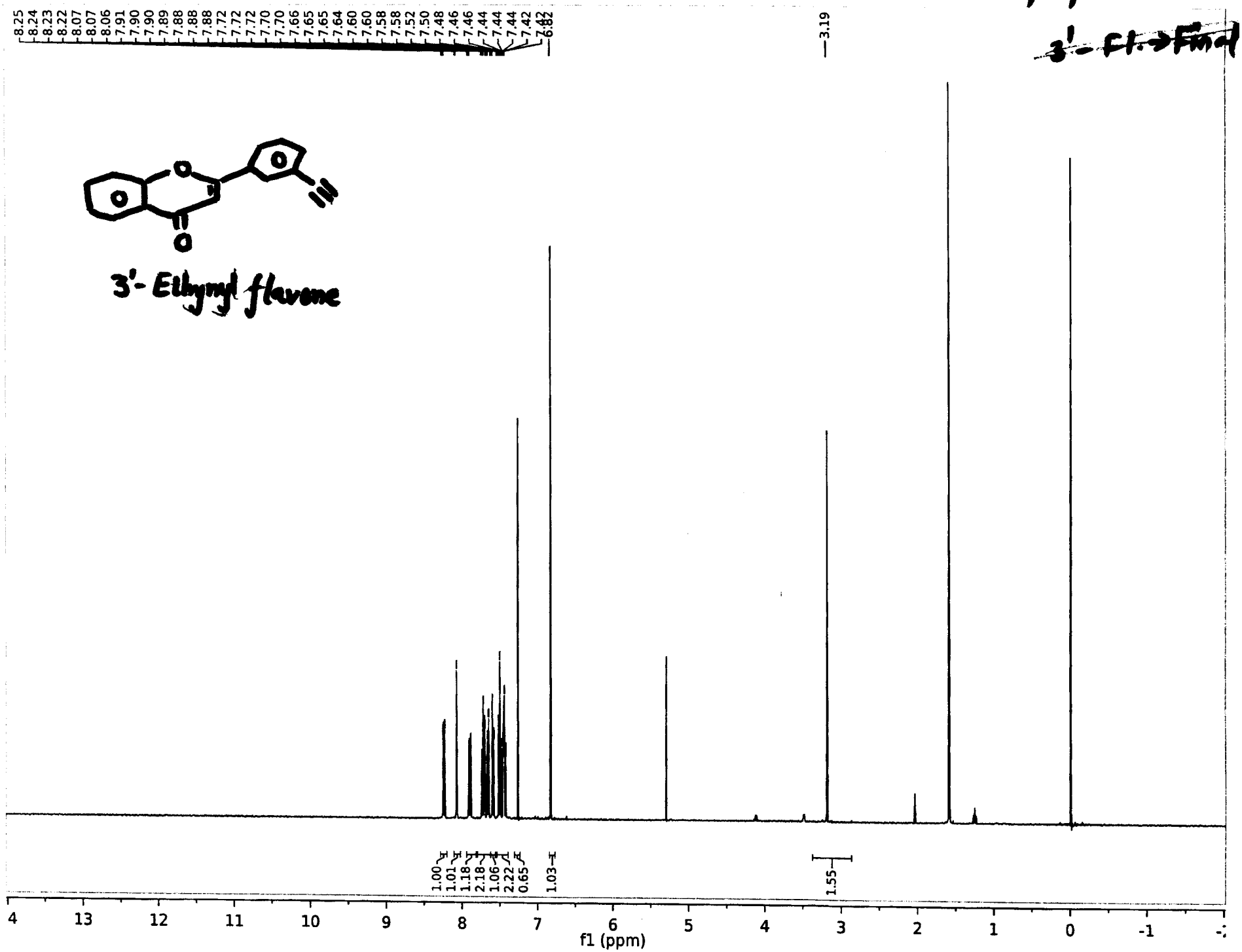

```
Current Data Parameters
NAME      2'-Ethynylflavone
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20140502
Time                 12.16
INSTRUM        FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   905
DS                     4
SWH           24414.063 Hz
FIDRES         0.372529 Hz
AQ             1.3421773 sec
RG               501.187
DW                20.480 usec
DE                 6.50 usec
TE                295.8 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001600 sec
D40            0.02432300 sec
L4                    34
L5                    49
P32               105.00 usec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4878687 MHz
NUC1                  13C
P1                 16.00 usec
PLW1          60.00000000 W

======== CHANNEL f2 ========
SFO2         300.1812007 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              105.00 usec
PLW2          10.00000000 W
PLW12          0.36280999 W
PLW13          0.40000001 W

F2 - Processing parameters
SI                    32768
SF           75.4803210 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

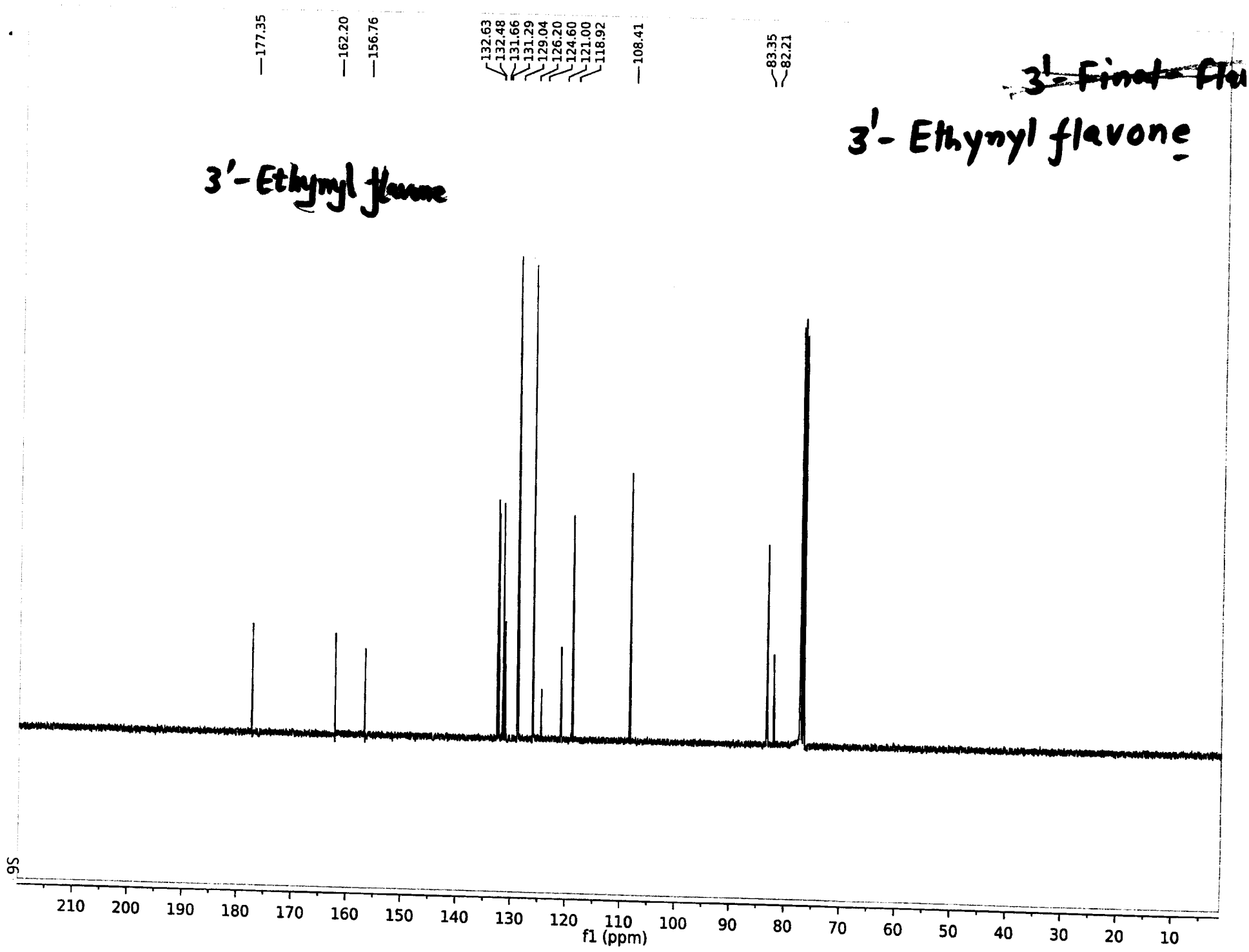
3'- Ethynyl Flavone

3'- Fl. → Final



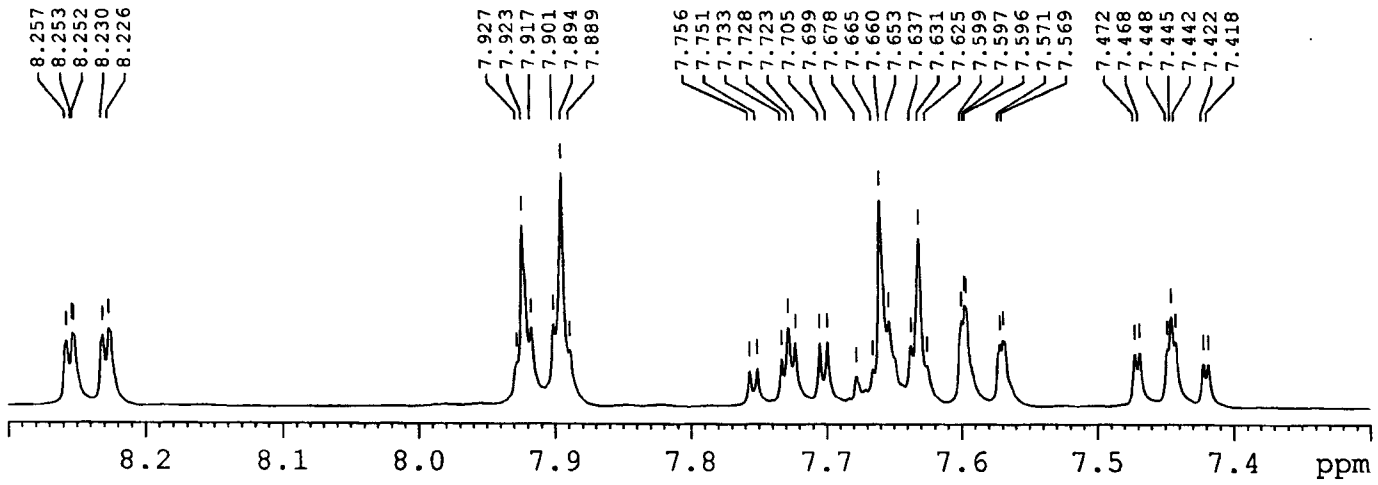
3'- Ethynyl flavone



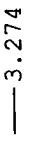

177.35
162.20
156.76
132.63
132.48
131.66
131.29
129.04
126.20
124.60
121.00
118.92
108.41
83.35
82.21
3'- Ethynyl flavone
3'- Ethynyl flavone
f1 (ppm)

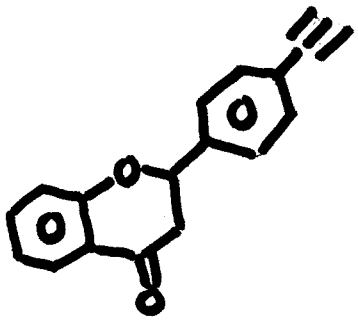
4'

4'EF

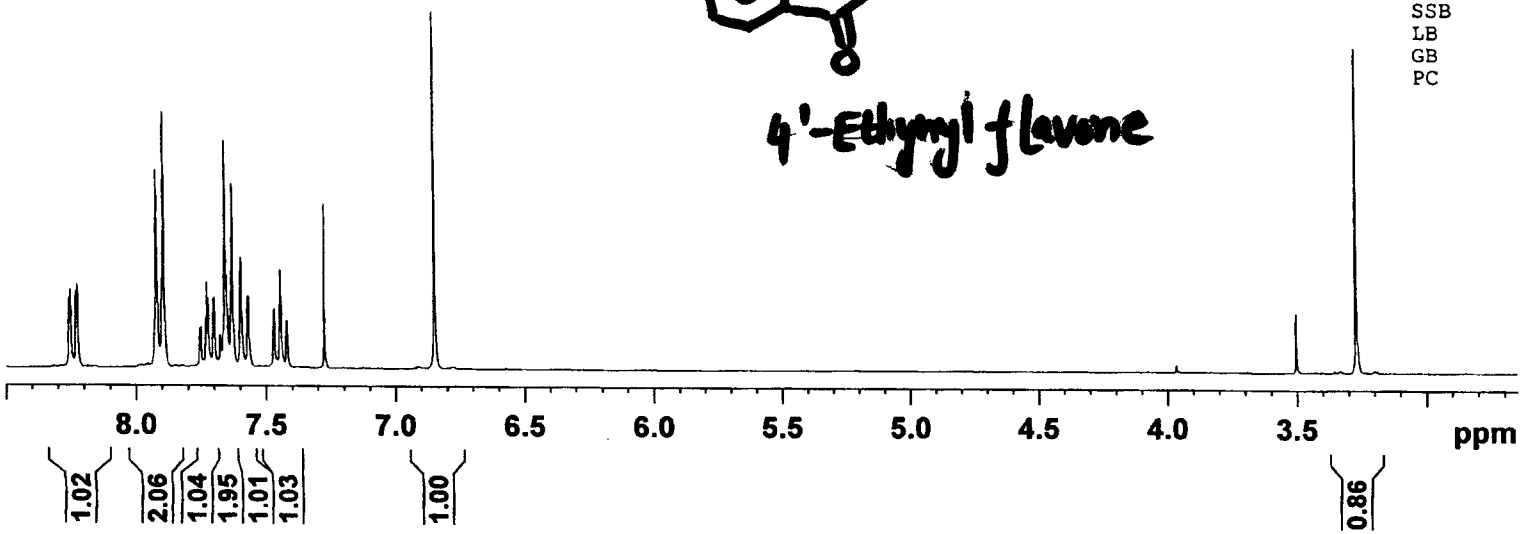






4'-Ethynyl flavone




Current Data Parameters

| | |
|---|---|
| NAME | 4'EF |
| EXPNO | 1 |
| PROCNO | 1 |

F2 - Acquisition Parameters

| | |
|---|---|
| Date_ | 20120730 |
| Time | 14.18 |
| INSTRUM | FOURIER300 |
| PROBHD | 5 mm DUL 13C-1 |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 6103.516 Hz |
| FIDRES | 0.093132 Hz |
| AQ | 5.3687091 sec |
| RG | 59.6078 |
| DW | 81.920 usec |
| DE | 6.50 usec |
| TE | 296.6 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |

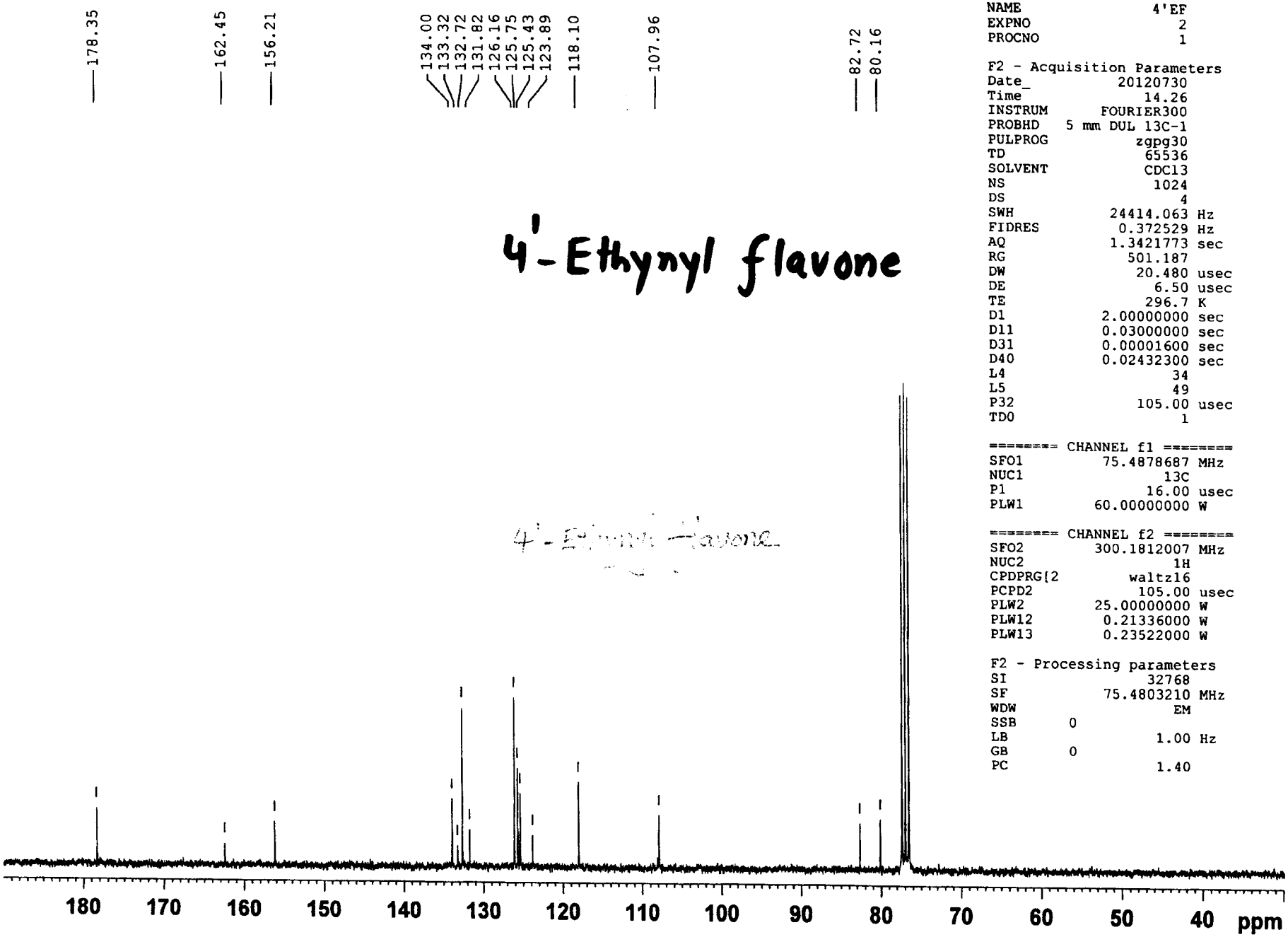
======== CHANNEL f1 ========

| | |
|---|---|
| SFO1 | 300.1818537 MHz |
| NUC1 | 1H |
| P1 | 8.75 usec |
| PLW1 | 25.00000000 W |

F2 - Processing parameters

| | |
|---|---|
| SI | 65536 |
| SF | 300.1800000 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.30 Hz |
| GB | 0 |
| PC | 1.00 |

4'EF




Current Data Parameters

| | |
|---|---|
| NAME | 4'EF |
| EXPNO | 2 |
| PROCNO | 1 |

F2 - Acquisition Parameters

| | |
|---|---|
| Date_ | 20120730 |
| Time | 14.26 |
| INSTRUM | FOURIER300 |
| PROBHD | 5 mm DUL 13C-1 |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 1024 |
| DS | 4 |
| SWH | 24414.063 Hz |
| FIDRES | 0.372529 Hz |
| AQ | 1.3421773 sec |
| RG | 501.187 |
| DW | 20.480 usec |
| DE | 6.50 usec |
| TE | 296.7 K |
| D1 | 2.00000000 sec |
| D11 | 0.03000000 sec |
| D31 | 0.00001600 sec |
| D40 | 0.02432300 sec |
| L4 | 34 |
| L5 | 49 |
| P32 | 105.00 usec |
| TD0 | 1 |

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

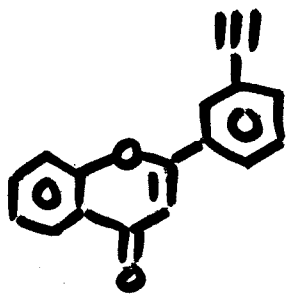
| | |
|---|---|
| SFO1 | 75.4878687 MHz |
| NUC1 | 13C |
| P1 | 16.00 usec |
| PLW1 | 60.00000000 W |

======== CHANNEL f2 ========

| | |
|---|---|
| SFO2 | 300.1812007 MHz |
| NUC2 | 1H |
| CPDPRG[2 | waltz16 |
| PCPD2 | 105.00 usec |
| PLW2 | 25.00000000 W |
| PLW12 | 0.21336000 W |
| PLW13 | 0.23522000 W |

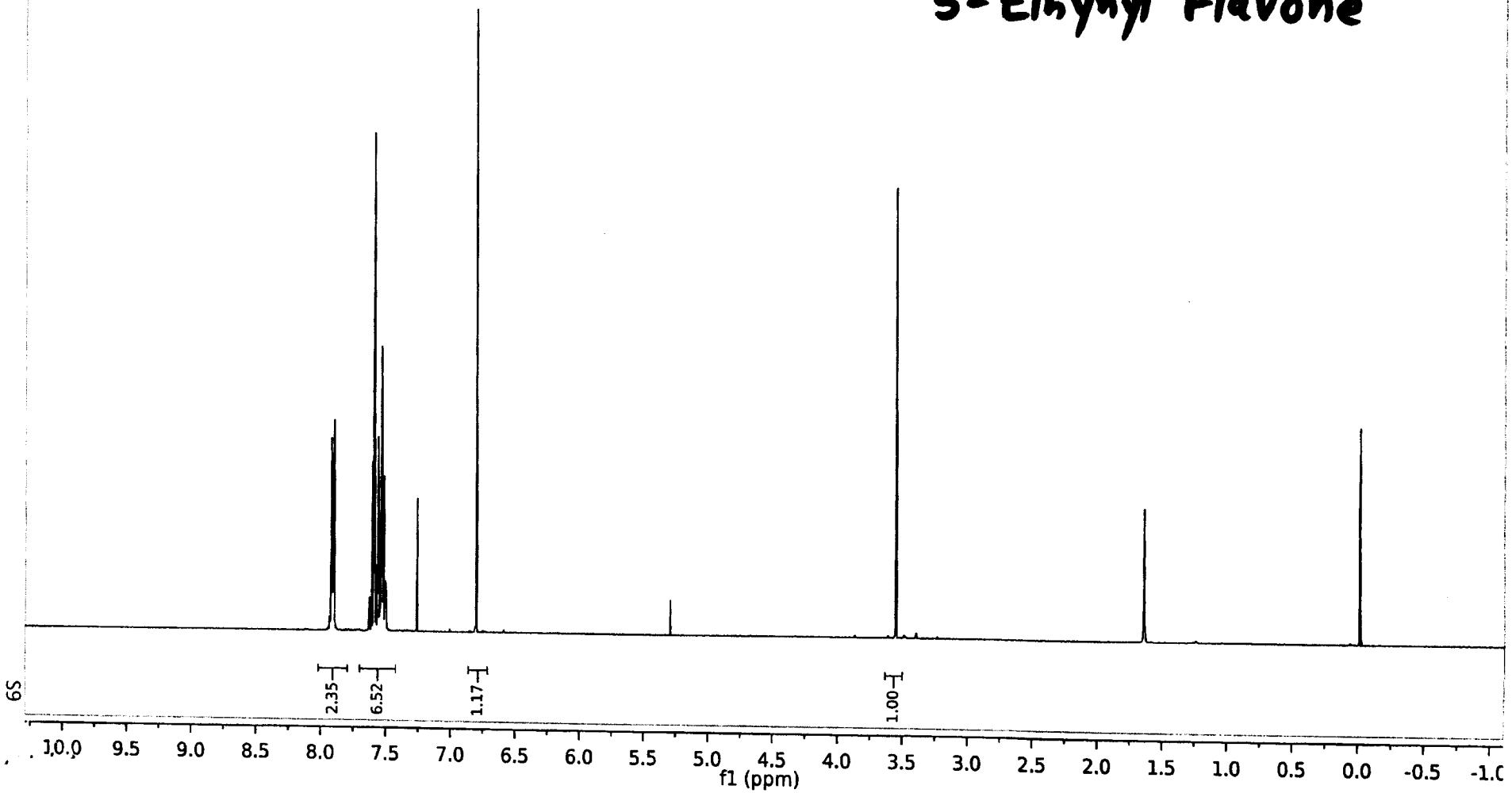
F2 - Processing parameters

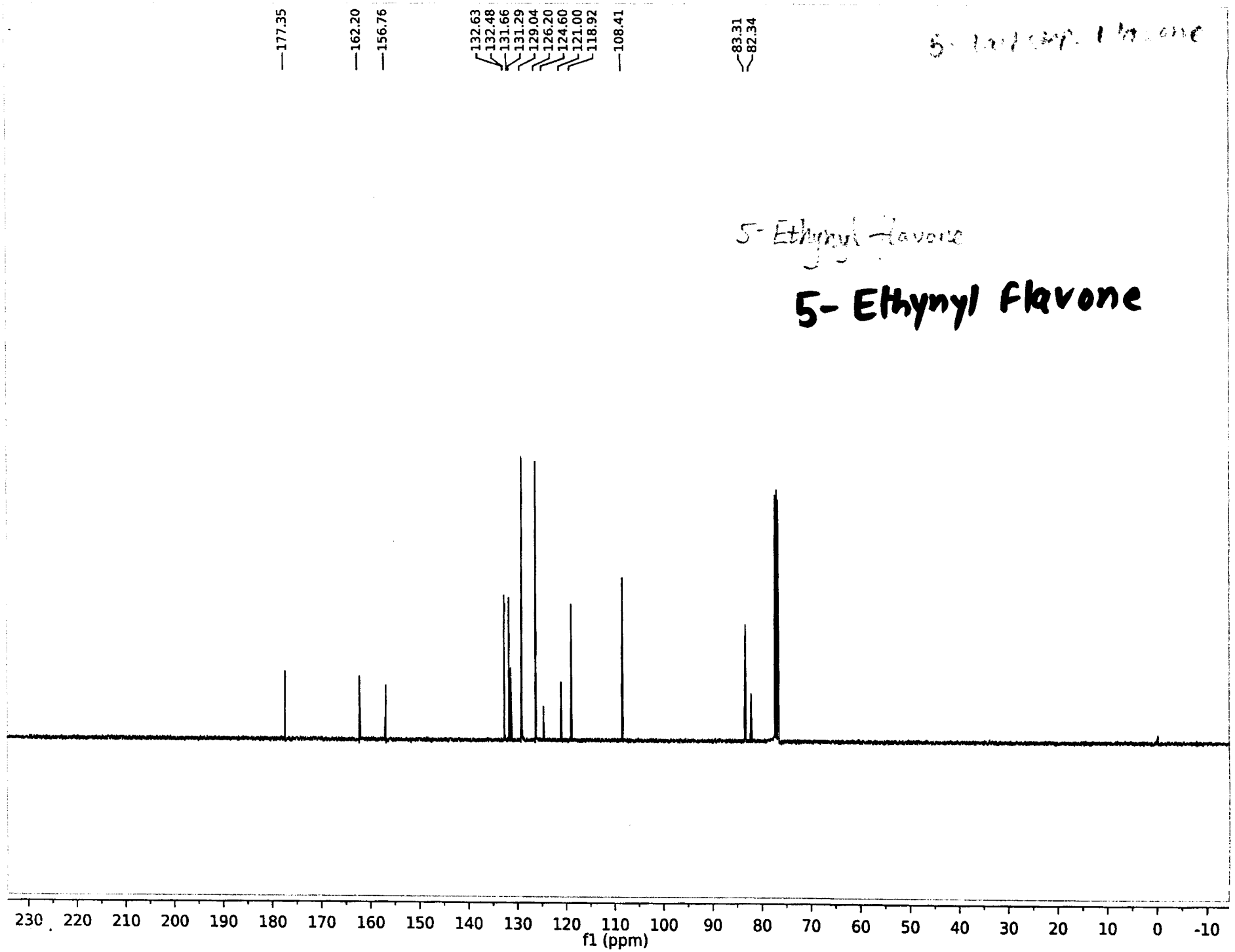
| | |
|---|---|
| SI | 32768 |
| SF | 75.4803210 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |



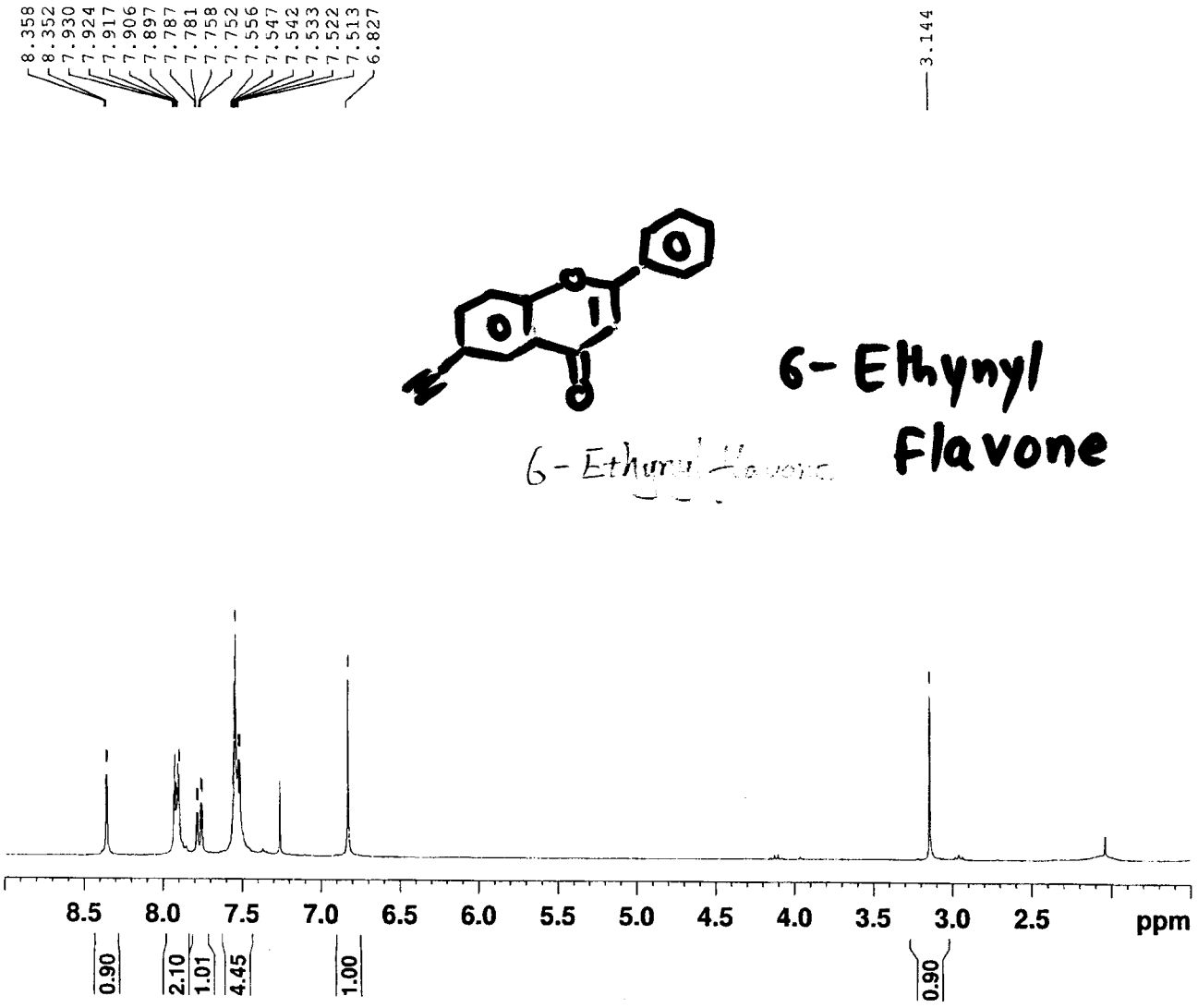
5-Ethynyl Flavone

# 5-Ethynyl Flavone



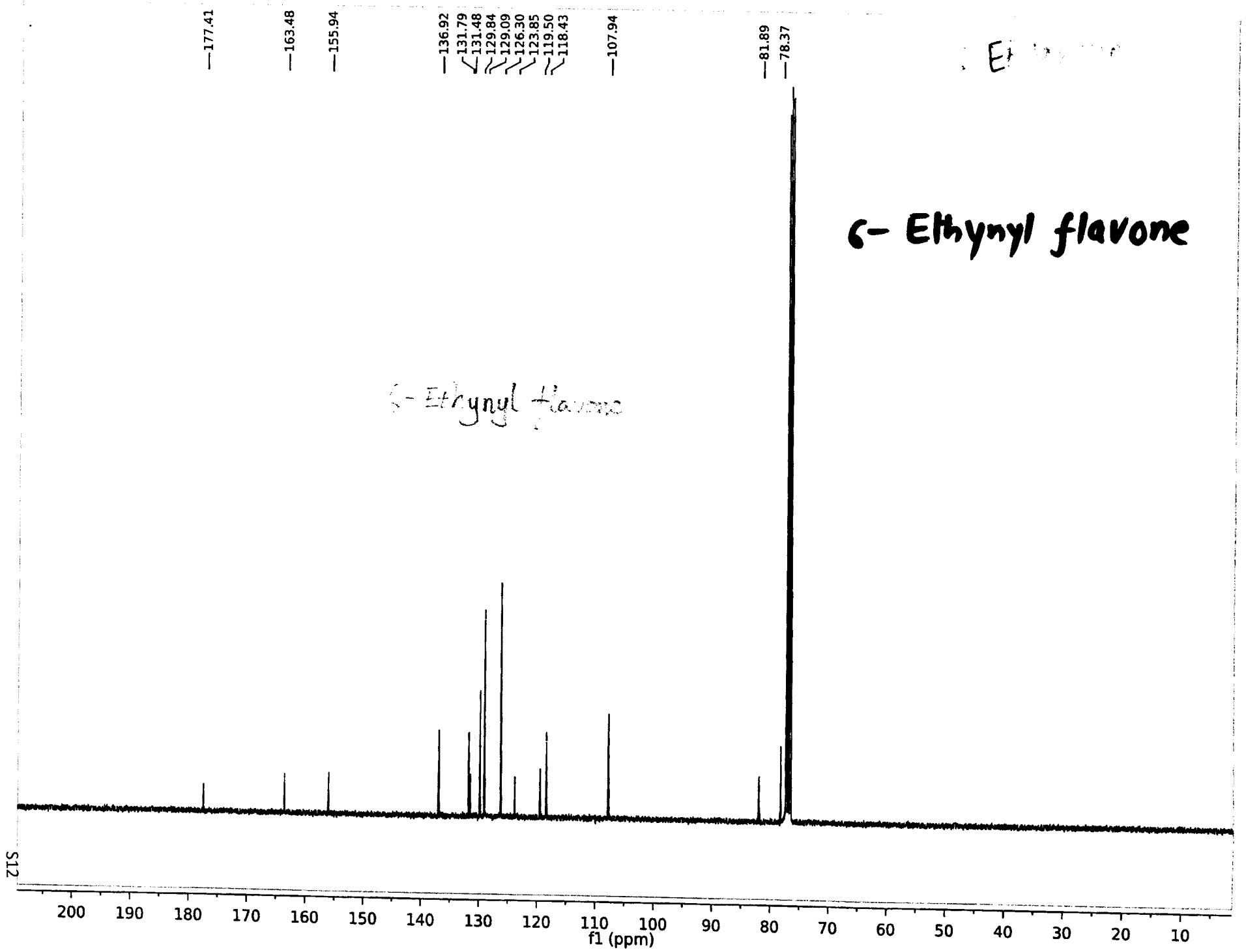

177.35
162.20
156.76
132.63
132.48
131.66
131.29
129.04
126.20
124.60
121.00
118.92
108.41
83.31
82.34
5- Ethynyl flavone
5- Ethynyl Flavone
S10
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

6EF

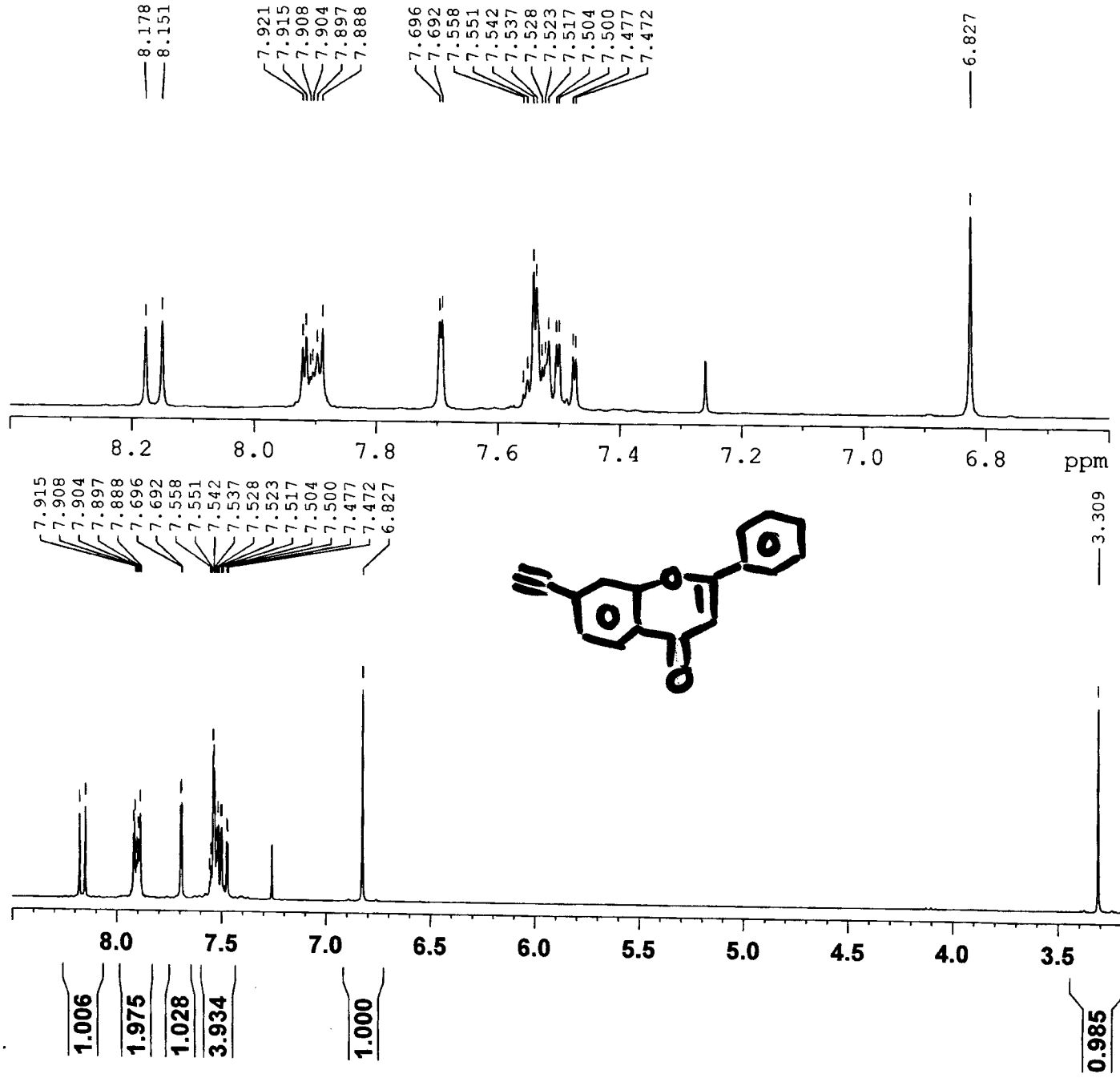



6EF

```
Current Data Parameters
NAME      6-ethynylflavone
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130114
Time                 14.34
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES               0.093132 Hz
AQ                5.3687091 sec
RG                   51.6302
DW                   81.920 usec
DE                    6.50 usec
TE                   296.5 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            300.1818537 MHz
NUC1                    1H
P1                    8.75 usec
PLW1           25.00000000 W

F2 - Processing parameters
SI                   65536
SF              300.1800049 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

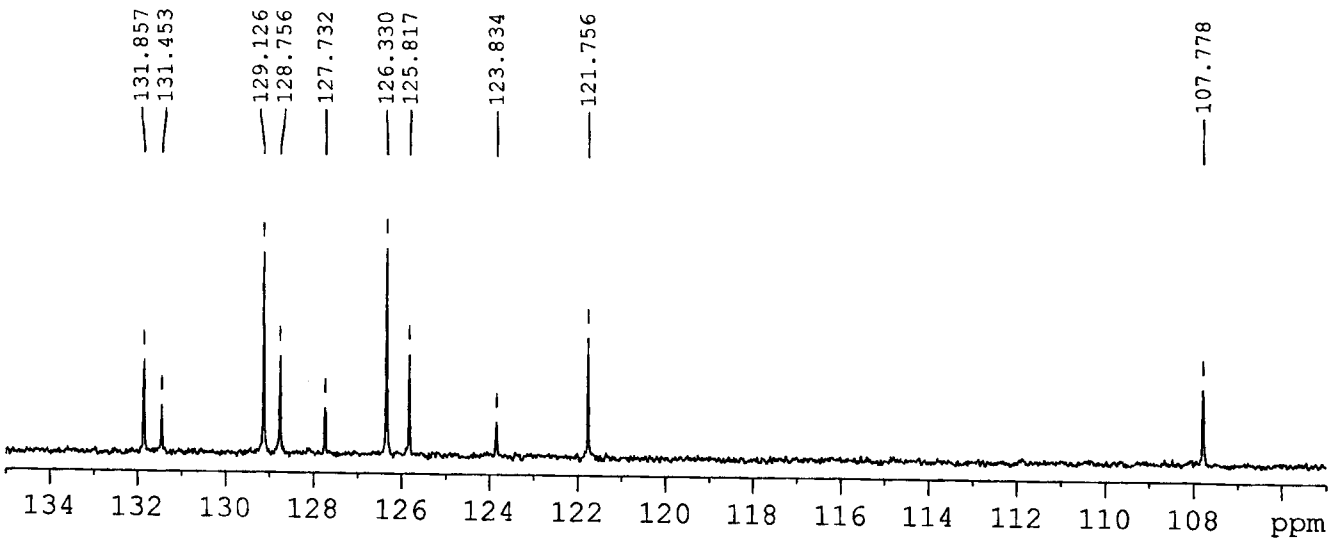

177.41
163.48
155.94
136.92
131.79
131.48
129.84
129.09
126.30
123.85
119.50
118.43
107.94
81.89
78.37
6- Ethynyl flavone
6- Ethynyl flavone
S12
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

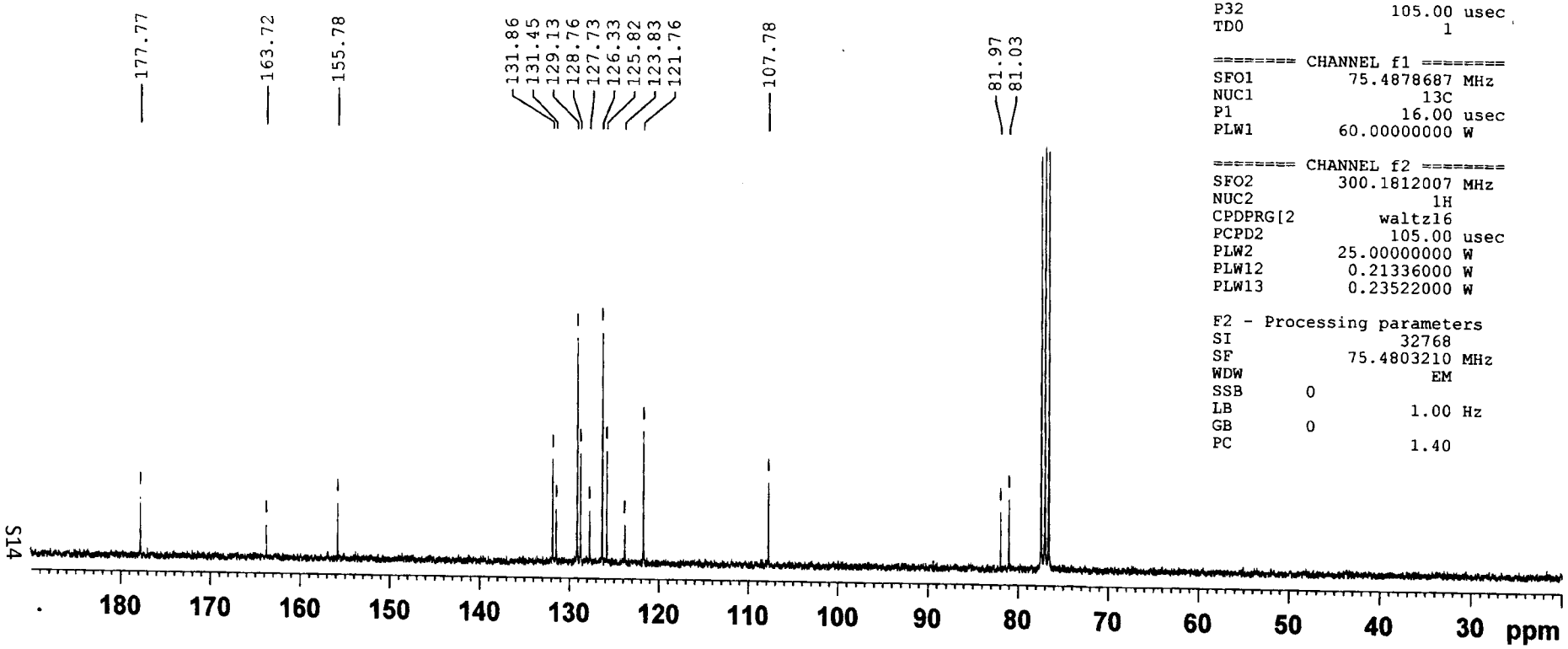
7-Ethynylflavone




```
Current Data Parameters
NAME      7-ethynylflavone
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20121003
Time                 15.35
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6103.516 Hz
FIDRES           0.093132 Hz
AQ               5.3687091 sec
RG                  45.8507
DW                  81.920 usec
DE                   6.50 usec
TE                  297.5 K
D1               1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          300.1818537 MHz
NUC1                    1H
P1                   8.75 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI                   65536
SF            300.1800050 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

7-Ethynylflavone




S14

```
Current Data Parameters
NAME      7-ethynylflavone
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20121003
Time                 15.45
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     909
DS                       4
SWH              24414.063 Hz
FIDRES               0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   297.6 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001600 sec
D40            0.02432300 sec
L4                      34
L5                      49
P32                 105.00 usec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4878687 MHz
NUC1                   13C
P1                   16.00 usec
PLW1          60.00000000 W

======== CHANNEL f2 ========
SFO2          300.1812007 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               105.00 usec
PLW2          25.00000000 W
PLW12          0.21336000 W
PLW13          0.23522000 W

F2 - Processing parameters
SI                    32768
SF             75.4803210 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

# Atlantic Microlab, Inc.

Sample No. 2'EF

**6180 Atlantic Blvd. Suite M**
**Norcross, GA 30071**
***www.atlanticmicrolab.com***

Company/School Xavier University of Louisiana
Dept. Chemistry
Address 1 Drexel Dr
City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 10/22/2013
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0046569

| Element | Theory | Found | |
|---|---|---|---|
| C | 82.91 | 81.67 | 81.68 |
| H | 4.09 | 4.21 | 4.35 |
| | | | |
| | | | |
| | | | |
| | | | |

Single ☐ Duplicate ☒

Elements Present: C, H, O

Analyze for: C, H

Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____

To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____

Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

mforooze@xula.edu

Date Received OCT 29 2013 Date Completed OCT 30 2013

Remarks:

# Atlantic Microlab, Inc.

Sample No. 3'EF

**6180 Atlantic Blvd. Suite M**
**Norcross, GA 30071**
***www.atlanticmicrolab.com***

Company/School Xavier University of Louisiana
Dept. Chemistry
Address 1 Drexel Dr
City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 10/22/2013
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# PO046569

| Element | Theory | Found | |
|---|---|---|---|
| C | 82.91 | 81.33 | 81.44 |
| H | 4.09 | 4.09 | 4.20 |
| | | | |
| | | | |
| | | | |
| | | | |

Single ☐ Duplicate ☒

Elements Present: C, H, O

Analyze for: C, H

Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____

To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____

Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

mforooze@xula.edu

Date Received OCT 29 2013 Date Completed OCT 30 2013

Remarks:

# Atlantic Microlab, Inc.

Sample No. 4'EF

**6180 Atlantic Blvd. Suite M**
**Norcross, GA 30071**
***www.atlanticmicrolab.com***

Company/School Xavier University of Louisiana
Dept. Chemistry
Address 1 Drexel Dr
City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 10/23/2013
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0046569

| Element | Theory | Found | |
|---|---|---|---|
| C | 82.91 | 82.50 | 82.36 |
| H | 4.09 | 4.26 | 4.39 |
| | | | |
| | | | |
| | | | |
| | | | |

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
Include Email Address or FAX # Below
mforooze@xula.edu

Date Received OCT 29 2013 Date Completed OCT 30 2013
Remarks:

# Atlantic Microlab, Inc.

Sample No. SEF

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School Xavier University of Louisiana
Dept. Chemistry
Address 1 Drexel Dr
City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 10/22/2013
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0046569

| Element | Theory | Found | |
|---|---|---|---|
| C | 82.91 | 82.04 | 82.07 |
| H | 4.09 | 4.20 | 4.29 | |
| | | | |
| | | | |
| | | | |
| | | | |

Single ☐ Duplicate ☒

Elements Present: C, H, O

Analyze for: C, H

Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____

To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____

Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

mforooze@xula.edu

Date Received OCT 29 2013 Date Completed OCT 30 2013

Remarks:

# Atlantic Microlab, Inc.

Sample No. 6 EF

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School Xavier University of Louisiana
Dept. Chemistry
Address 1 Drexel Dr
City, State, Zip New Orleans, LA 70125
Name Jiawang Liu Date 07/26/2013
Phone (504) 638-4036

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P0042436

| Element | Theory | Found | |
|---|---|---|---|
| C | 82.91 | 80.86 | 80.62 |
| H | 4.09 | 4.53 | 4.41 |
| | | | |
| | | | |
| | | | |
| | | | |

Single ☐ Duplicate ☒
Elements Present: C, H, O
Analyze for: C, H
Hygroscopic ☐ Explosive ☐
M.P. _____ B.P. _____
To be dried: Yes ☐ No ☒
Temp. _____ Vac. _____ Time _____
Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.
Include Email Address or FAX # Below
mforooze@xula.edu

Date Received AUG 0 5 2013 Date Completed AUG 0 6 2013
Remarks:

# Atlantic Microlab, Inc.

Sample No. 7EF

6180 Atlantic Blvd. Suite M
Norcross, GA 30071
www.atlanticmicrolab.com

Company/School Xavier University of Louisiana
Dept. Chemistry
Address 1 Drexel Dr
City, State, Zip New Orleans, LA 70125

Professor/Supervisor: Dr Maryam Foroozesh
PO# / CC# P00372 18

Name Jiawang Liu Date
Phone (504) 638-4036

| Element | Theory | Found | |
|---|---|---|---|
| C | 82.91 | 81.91 | 81.83 |
| H | 4.09 | 4.22 | 4.10 |
| | | | |
| | | | |
| | | | |
| | | | |

Single ☐ Duplicate ☒

Elements Present: C, H, O

Analyze for: C, H

Hygroscopic ☐ Explosive ☐
M.P. 144°C B.P.

To be dried: Yes ☐ No ☒
Temp. Vac. Time

Rush Service ☐ Rush service guarantees analyses will be completed and results available by 5 PM EST on the day the sample is received by 11 AM.

Include Email Address or FAX # Below

mforooze@xula.edu

Date Received OCT 18 2012 Date Completed OCT 19 2012

Remarks: