

## Supplementary Material

### Synthesis of some novel 1-aryl-1*H*-1,2,3-triazole-4-carboxamides and ethyl 1-aryl-5-(1,2,3-triazol-1-yl)-1*H*-pyrazole-4-carboxylates

Marialuce Avigliano,<sup>#,a</sup> Debora De Francesco,<sup>#,b</sup> Antonella Brizzi, Marco Paolino, Federico Corelli,\*  
and Claudia Mugnaini

*Department of Biotechnology, Chemistry and Pharmacy, University of Siena, 53100 Siena, Italy*

<sup>a</sup>*Present address: School of Pharmacy and Pharmaceutical Sciences, Redwood Building, King Edward VII Ave., Cardiff CF10 3NB, UK*

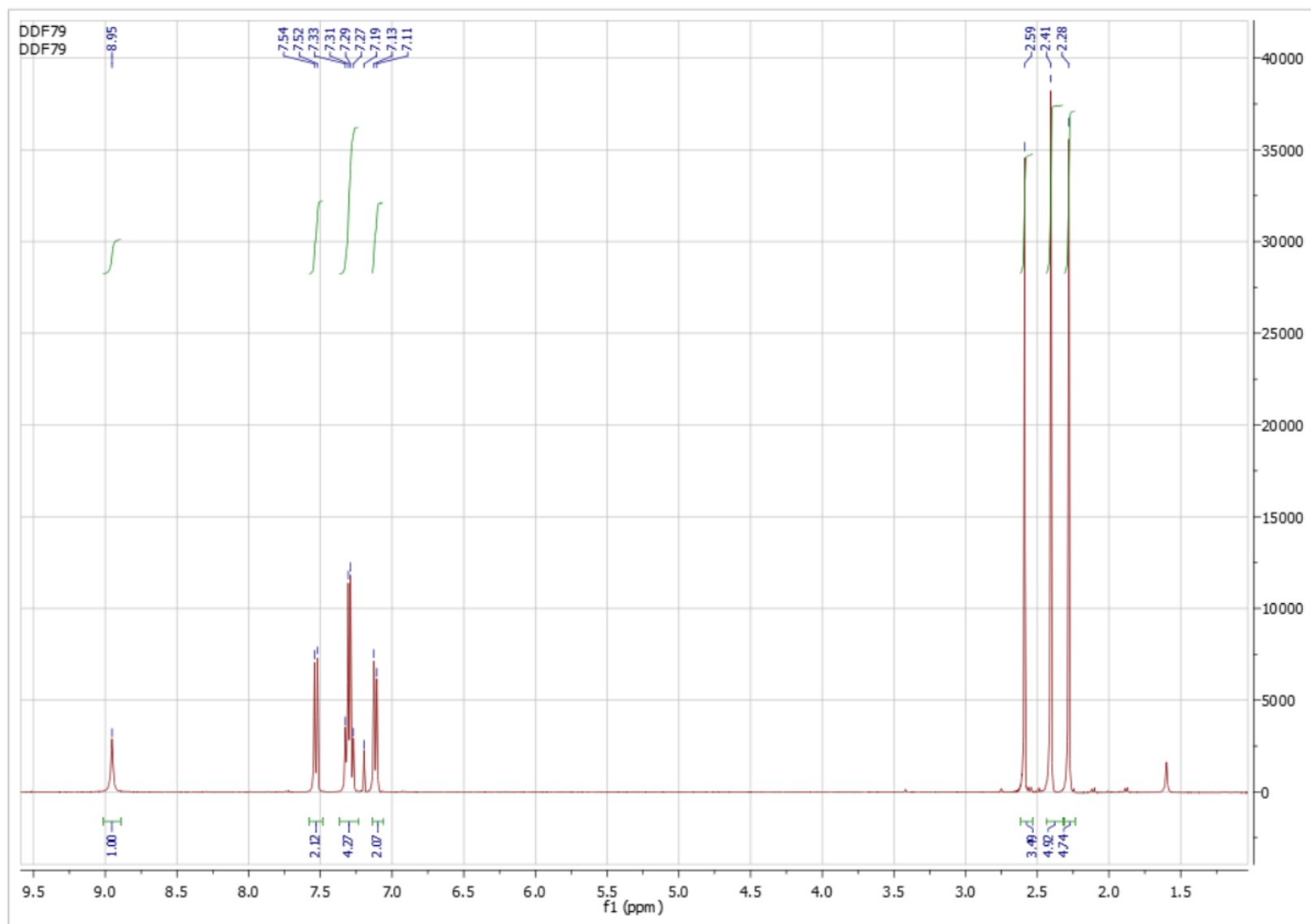
<sup>b</sup>*Present address: GreenBone Ortho SpA, Via A. Einstein 8, 48018 Faenza (RA), Italy*

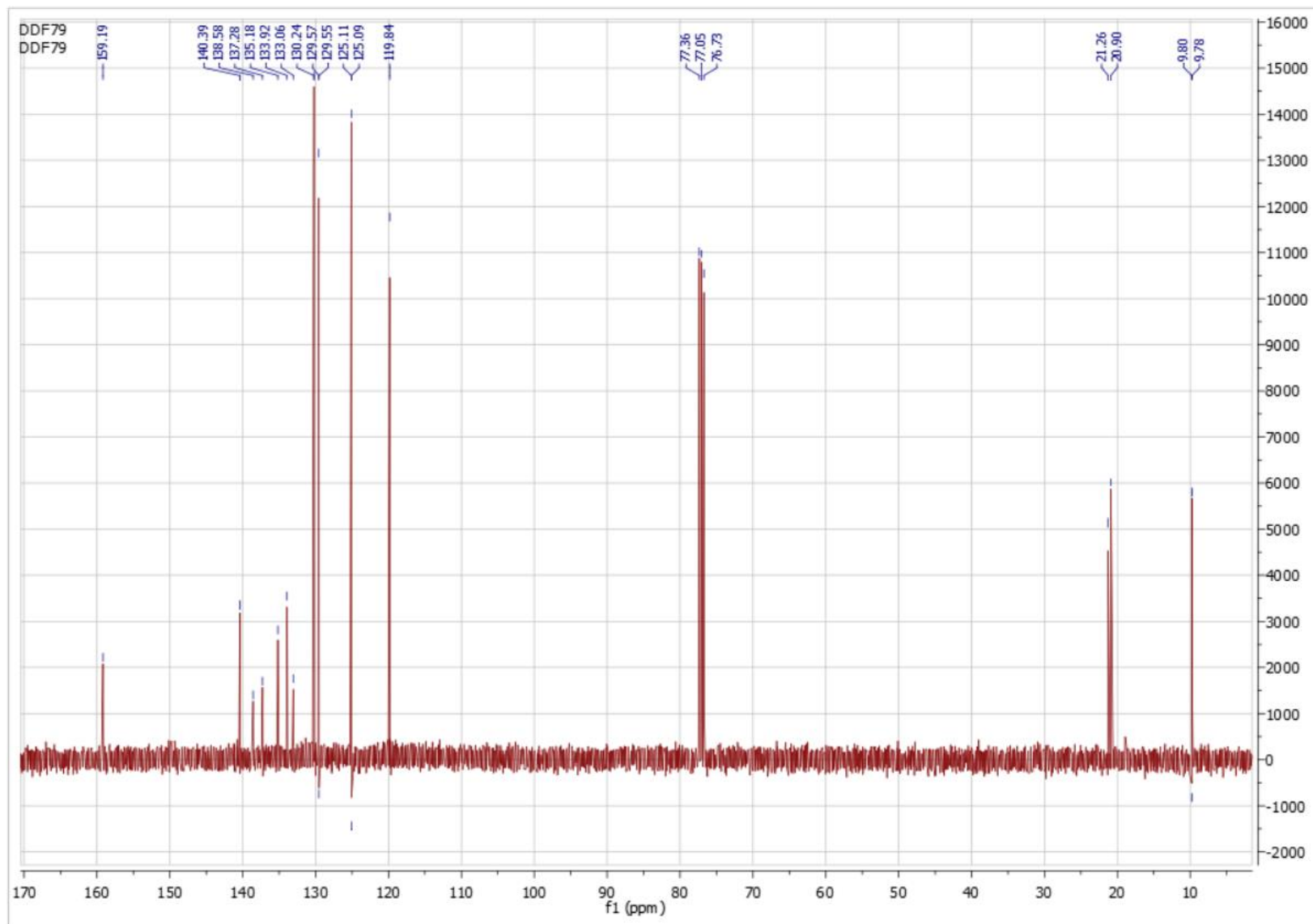
<sup>#</sup>*These authors contributed equally to this work*

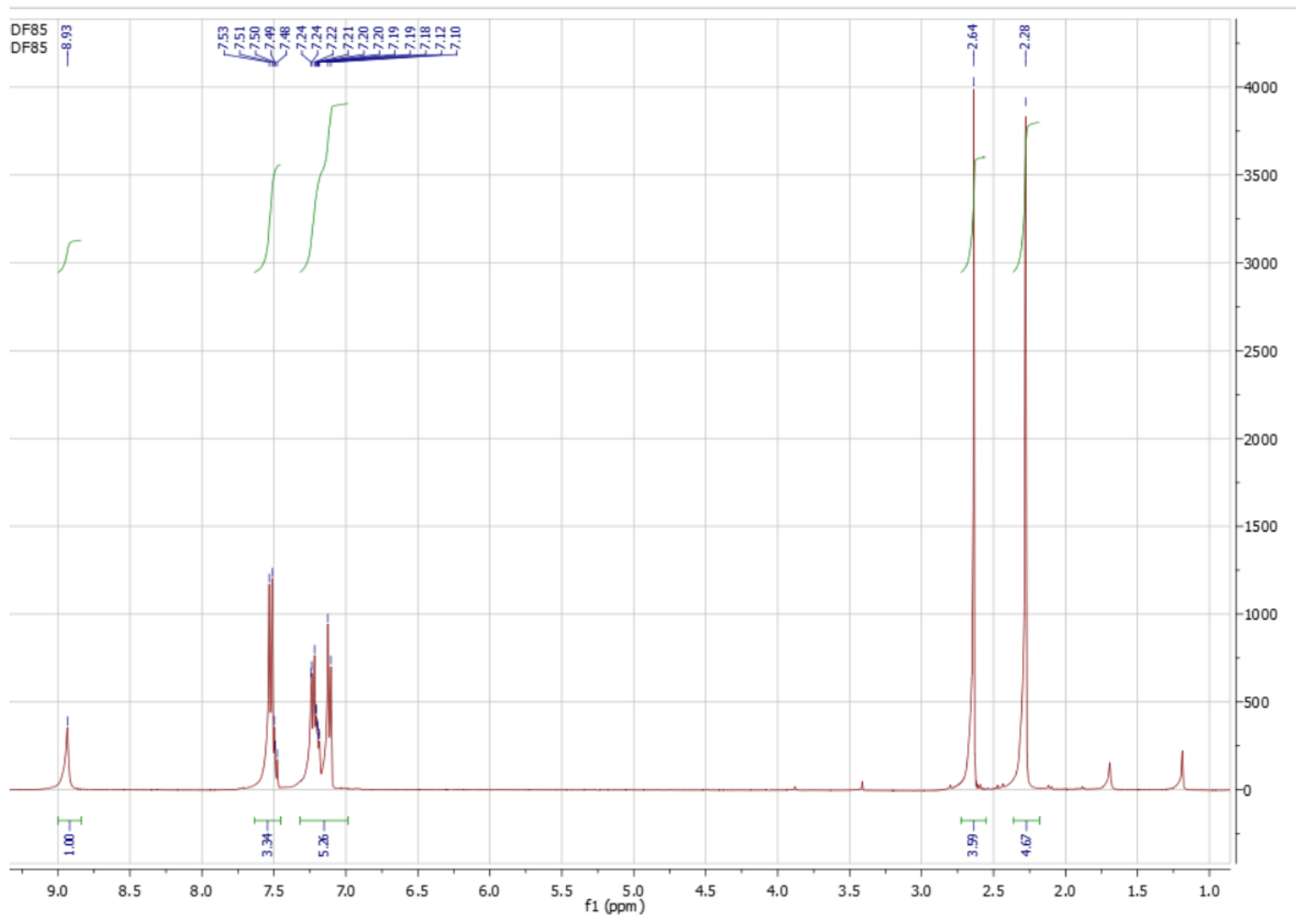
Email: [federico.corelli@unisi.it](mailto:federico.corelli@unisi.it)

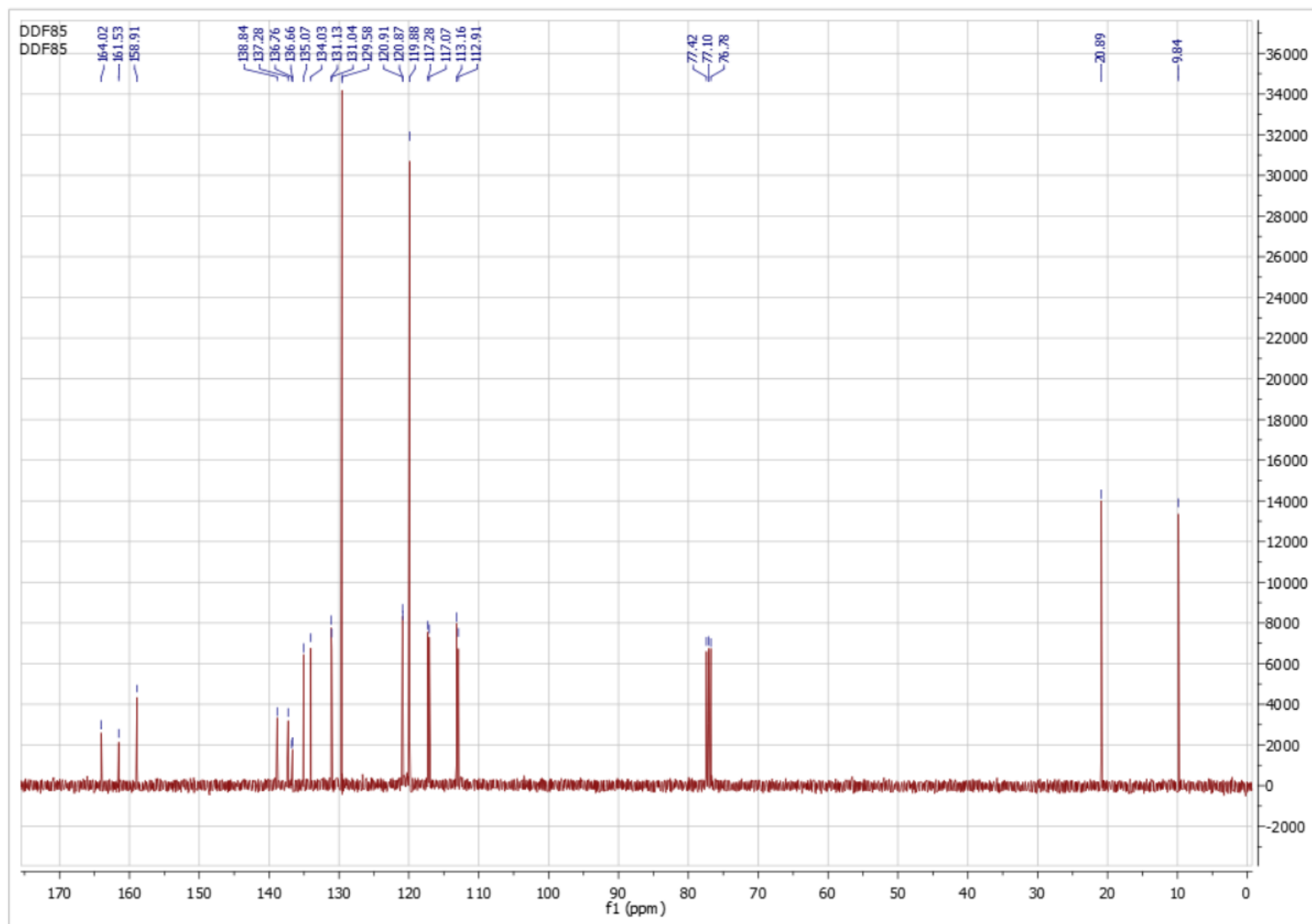
### Table of Contents

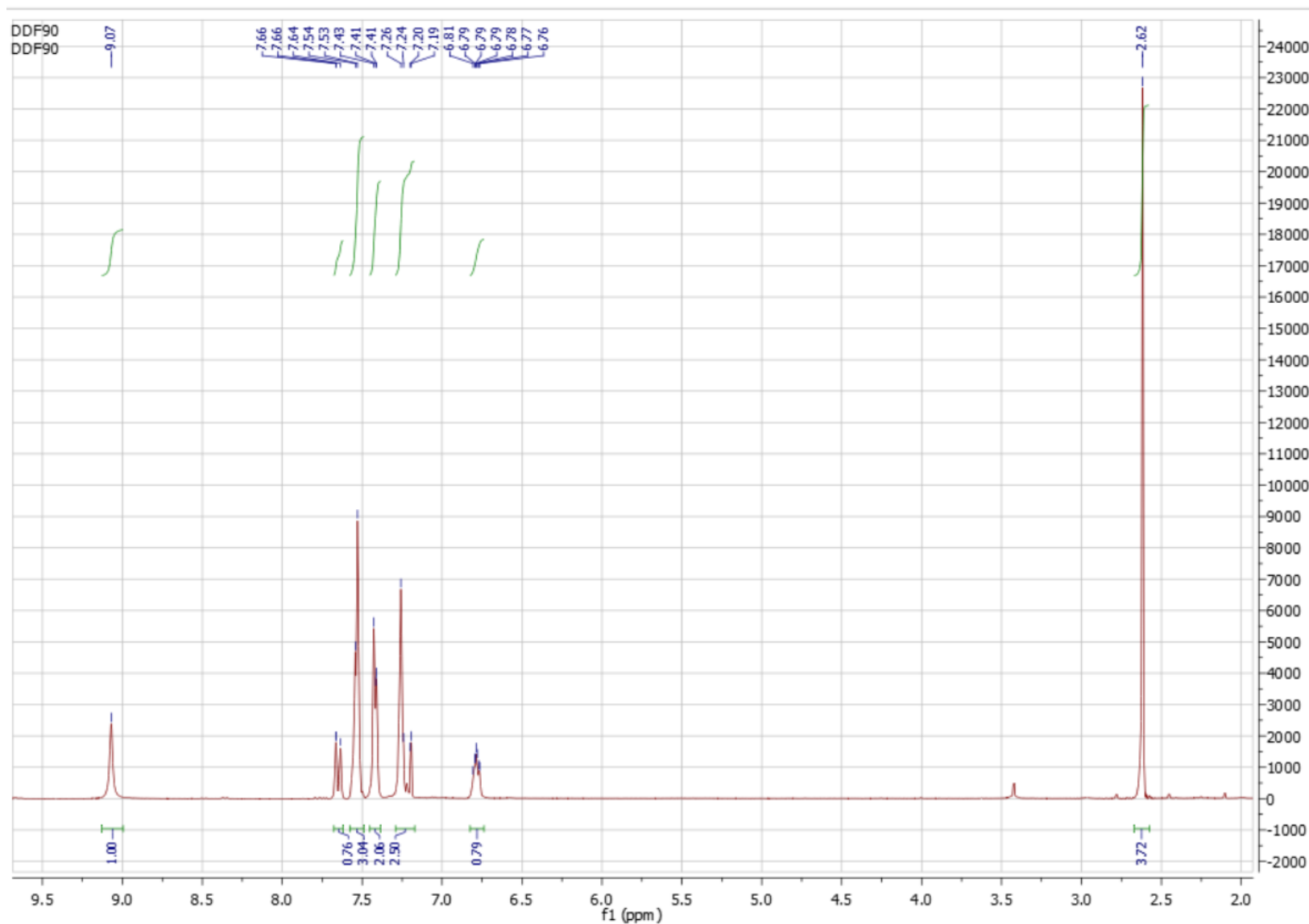
Copies of the <sup>1</sup>H-NMR spectra, <sup>13</sup>C-NMR spectra and HPLC traces of compounds **2a-i** and **3a-d**.....S2

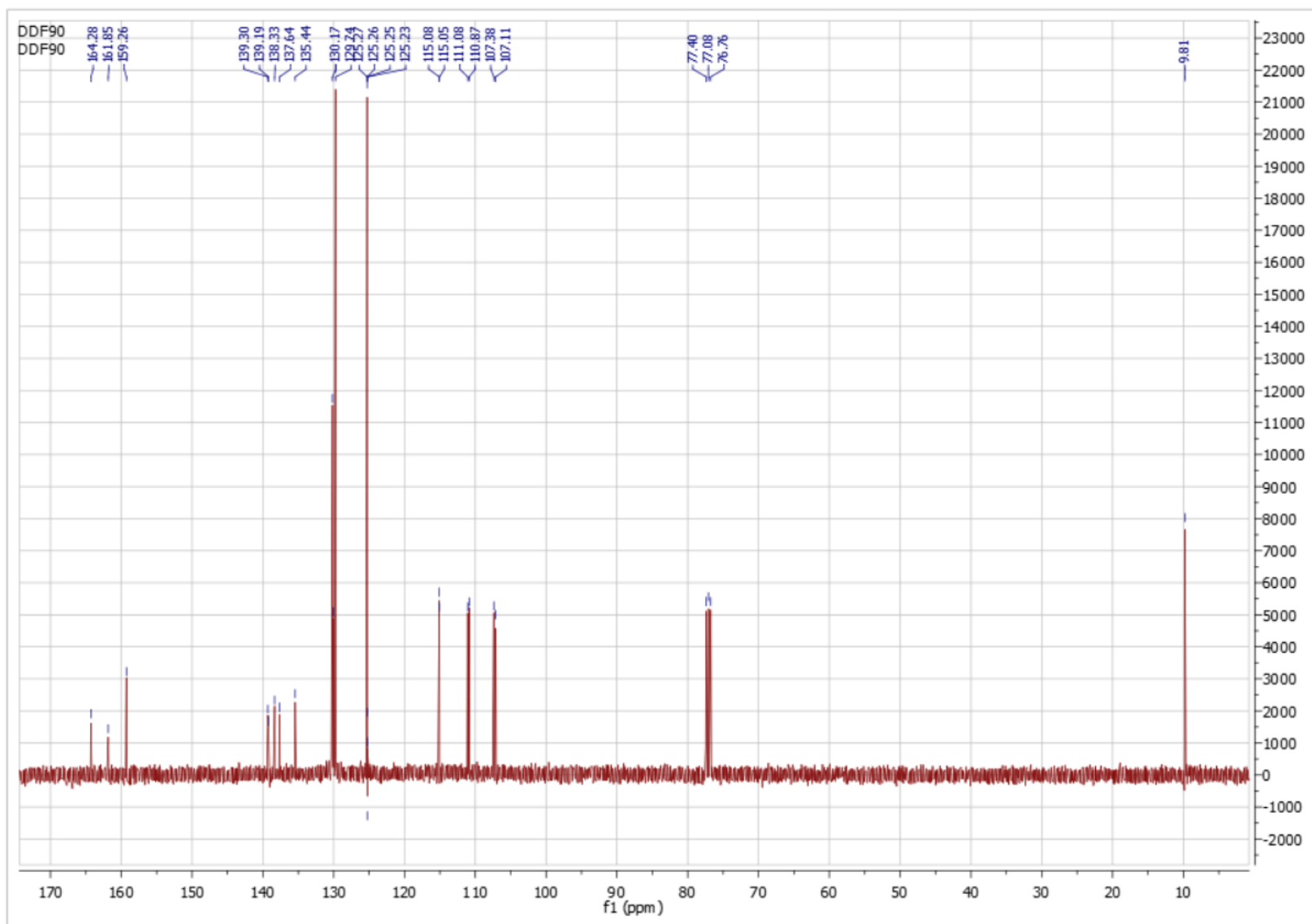
 $^1\text{H}$ -NMR spectrum of compound **2a**

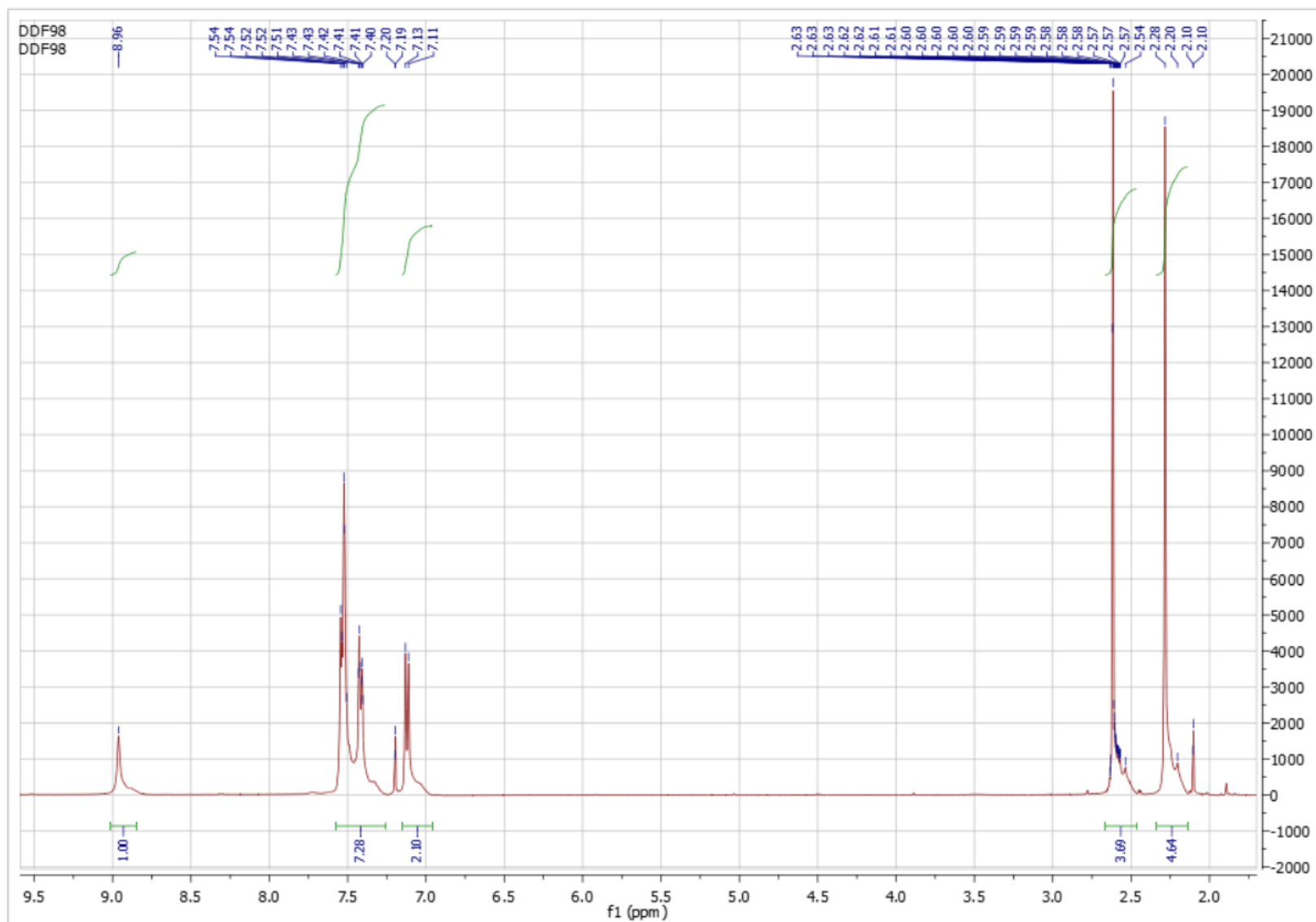
 $^{13}\text{C}$ -NMR spectrum of compound **2a**

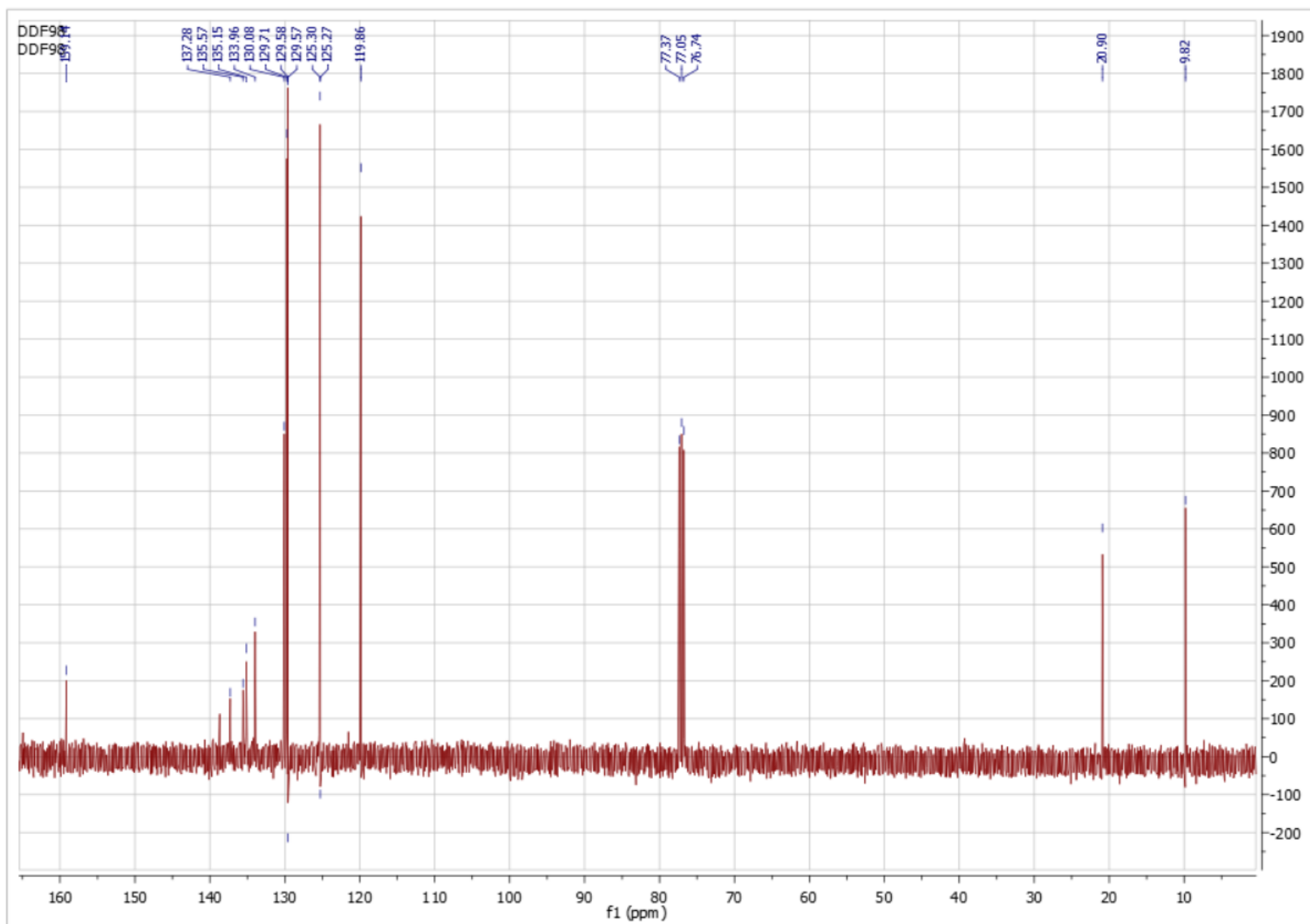
<sup>1</sup>H-NMR spectrum of compound **2b**

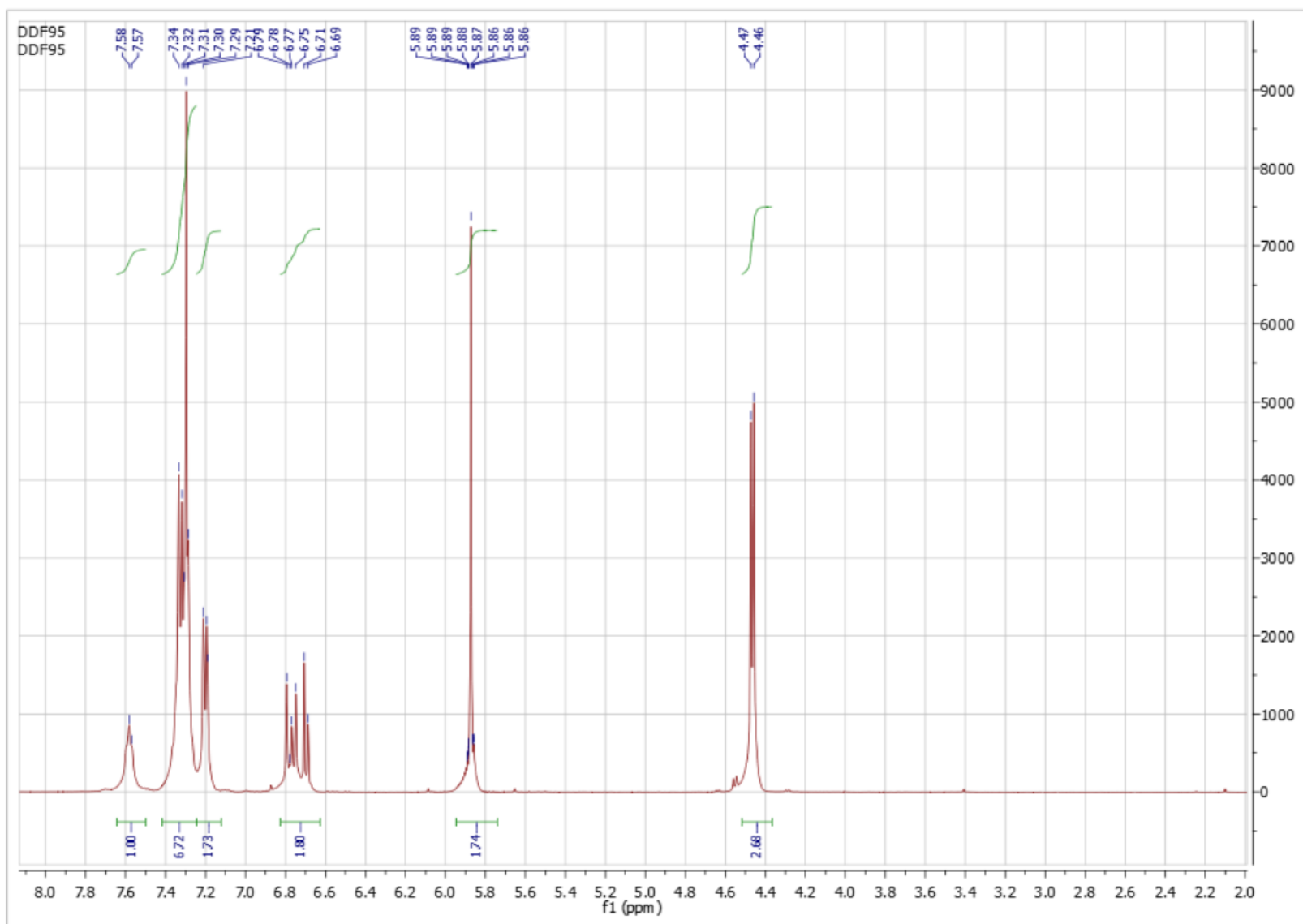
<sup>13</sup>C-NMR spectrum of compound **2b**

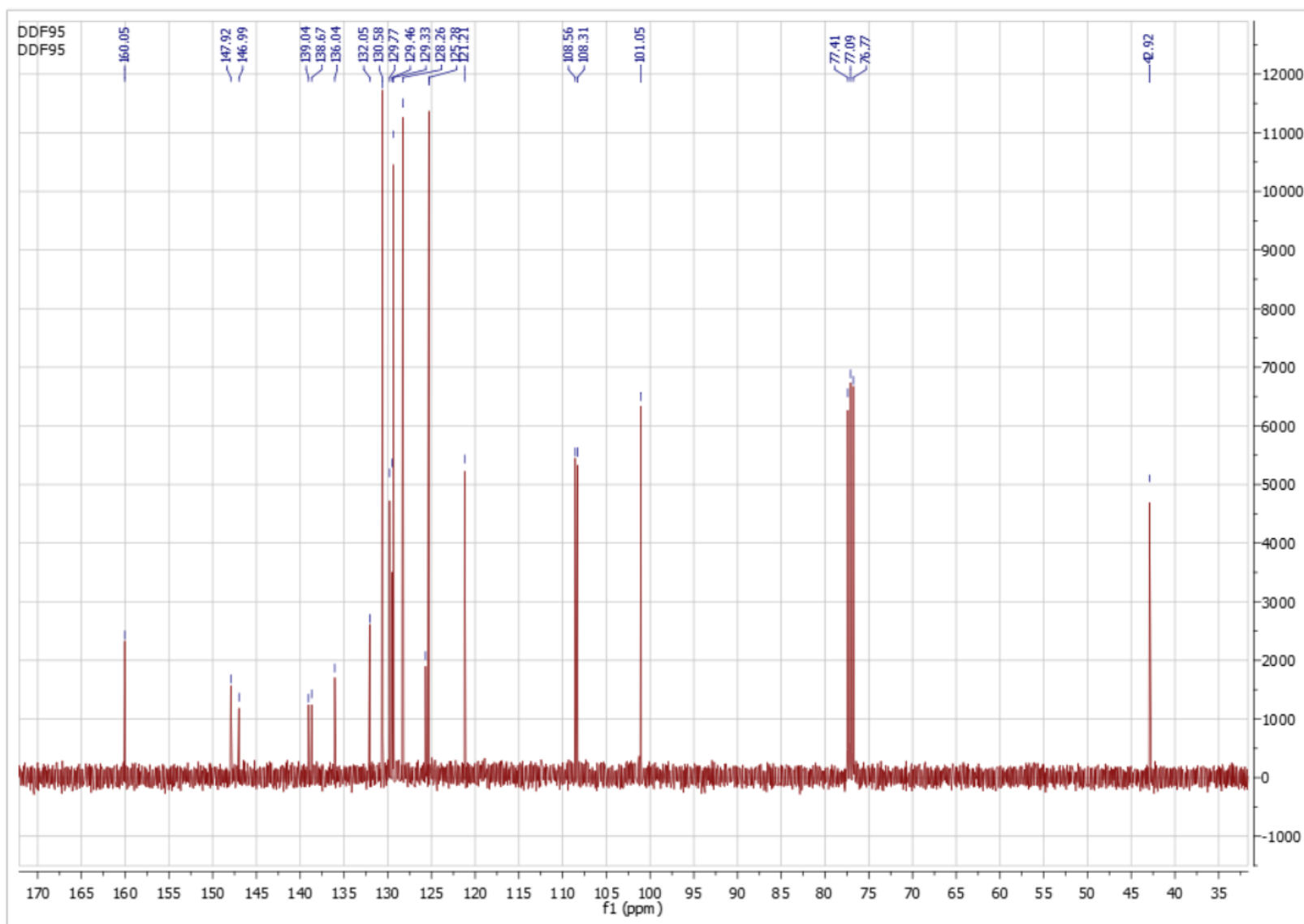
<sup>1</sup>H-NMR spectrum of compound 2c

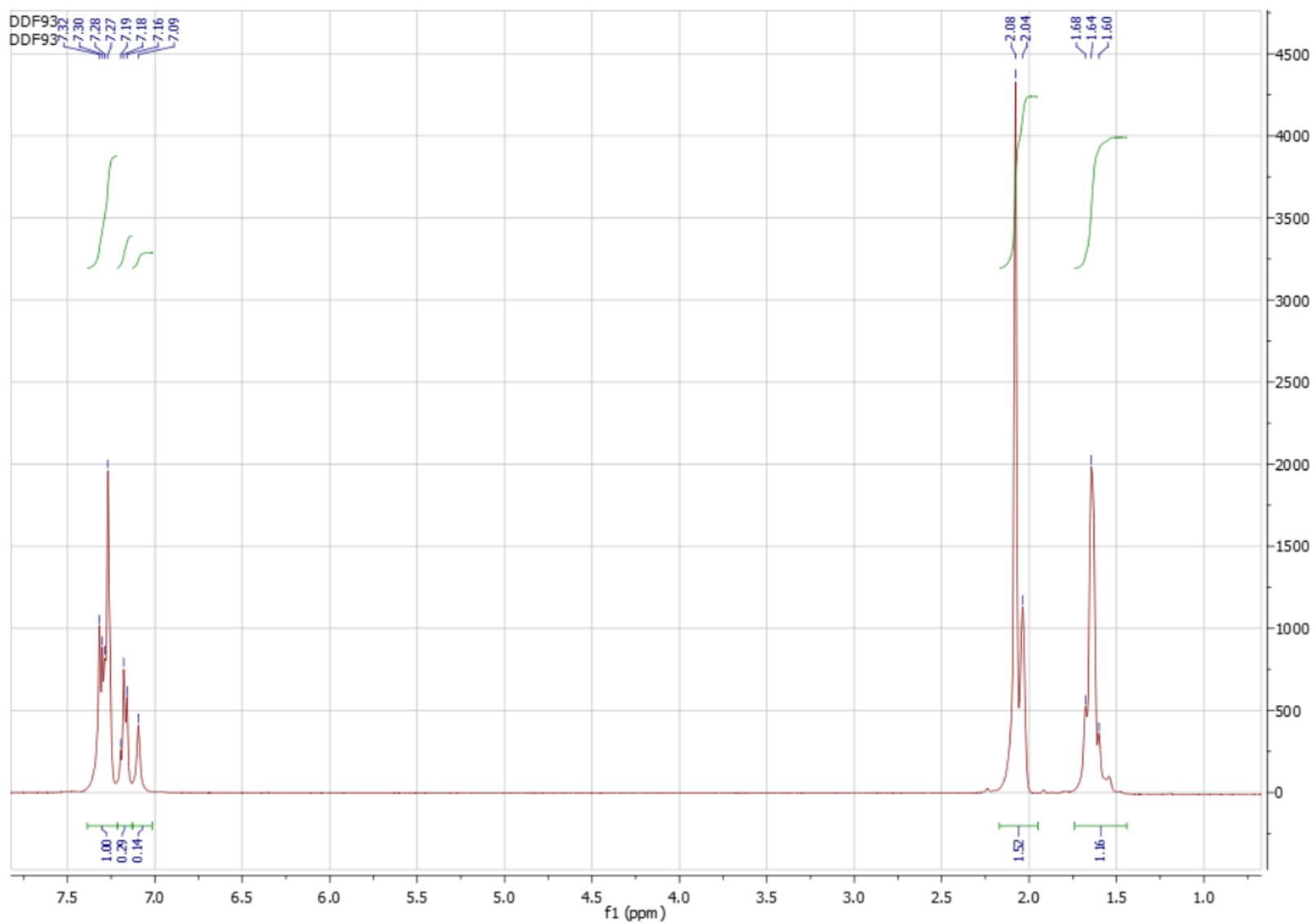
<sup>13</sup>C-NMR spectrum of compound **2c**

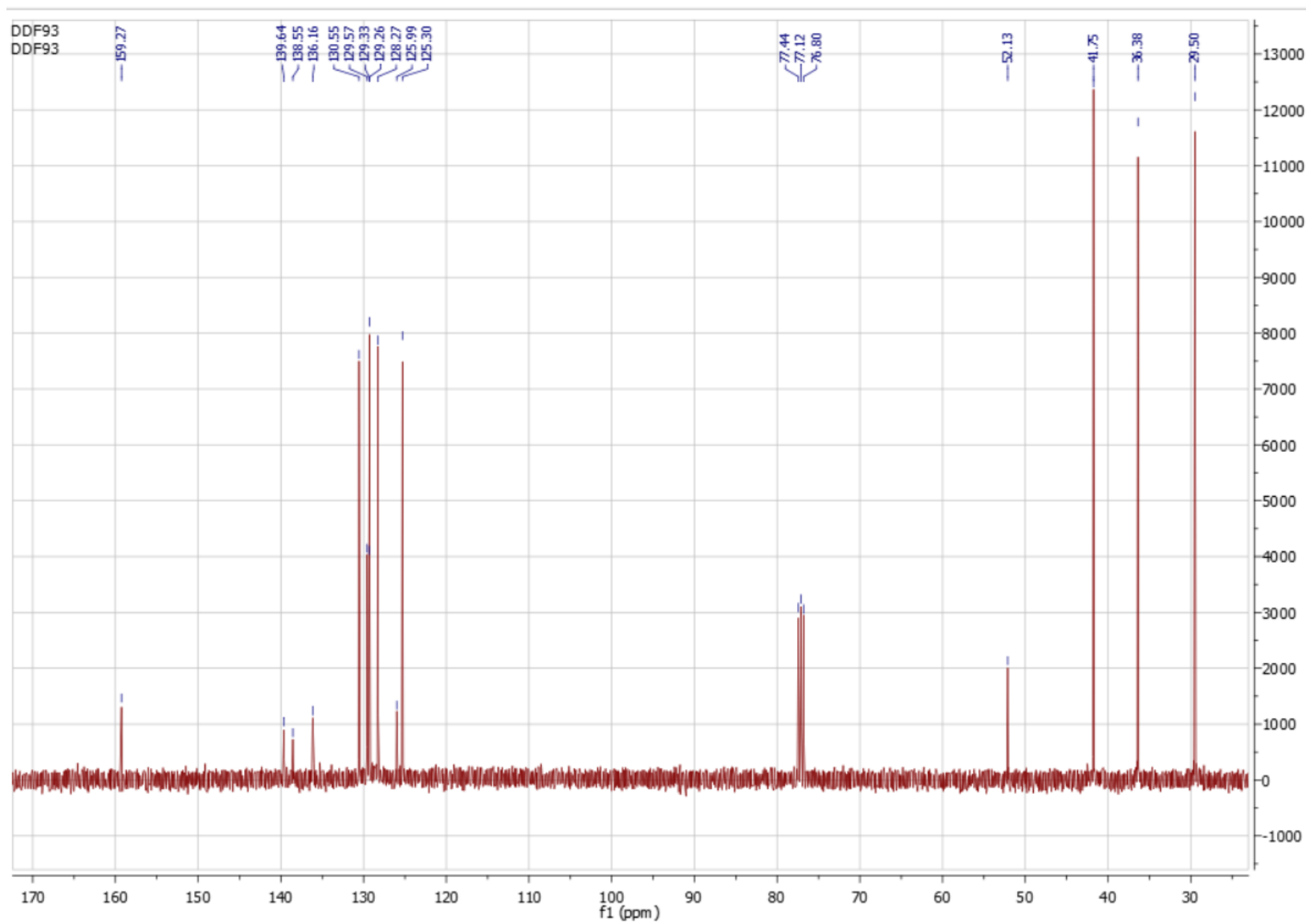
<sup>1</sup>H-NMR spectrum of compound **2d**

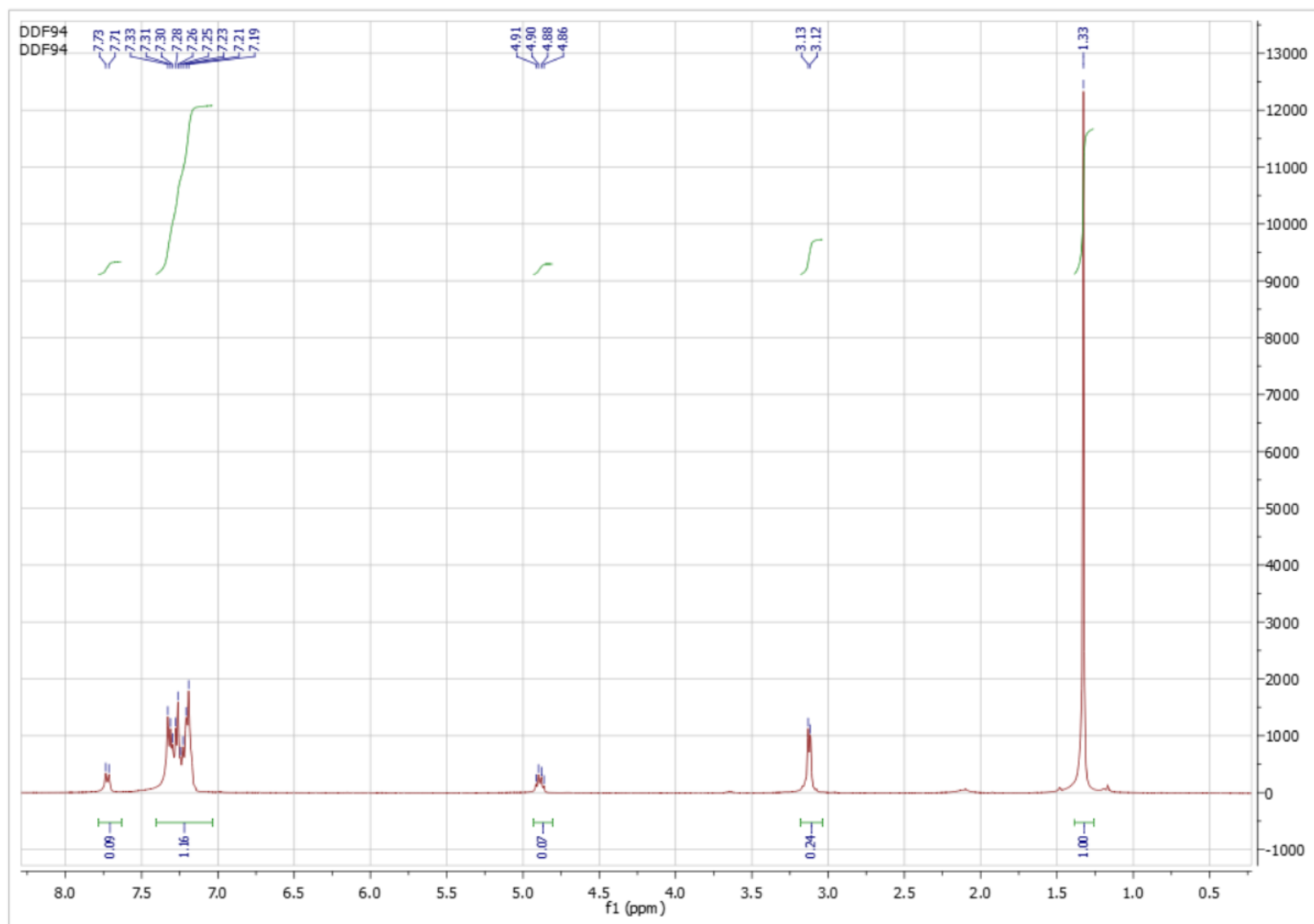
<sup>13</sup>C-NMR spectrum of compound 2d

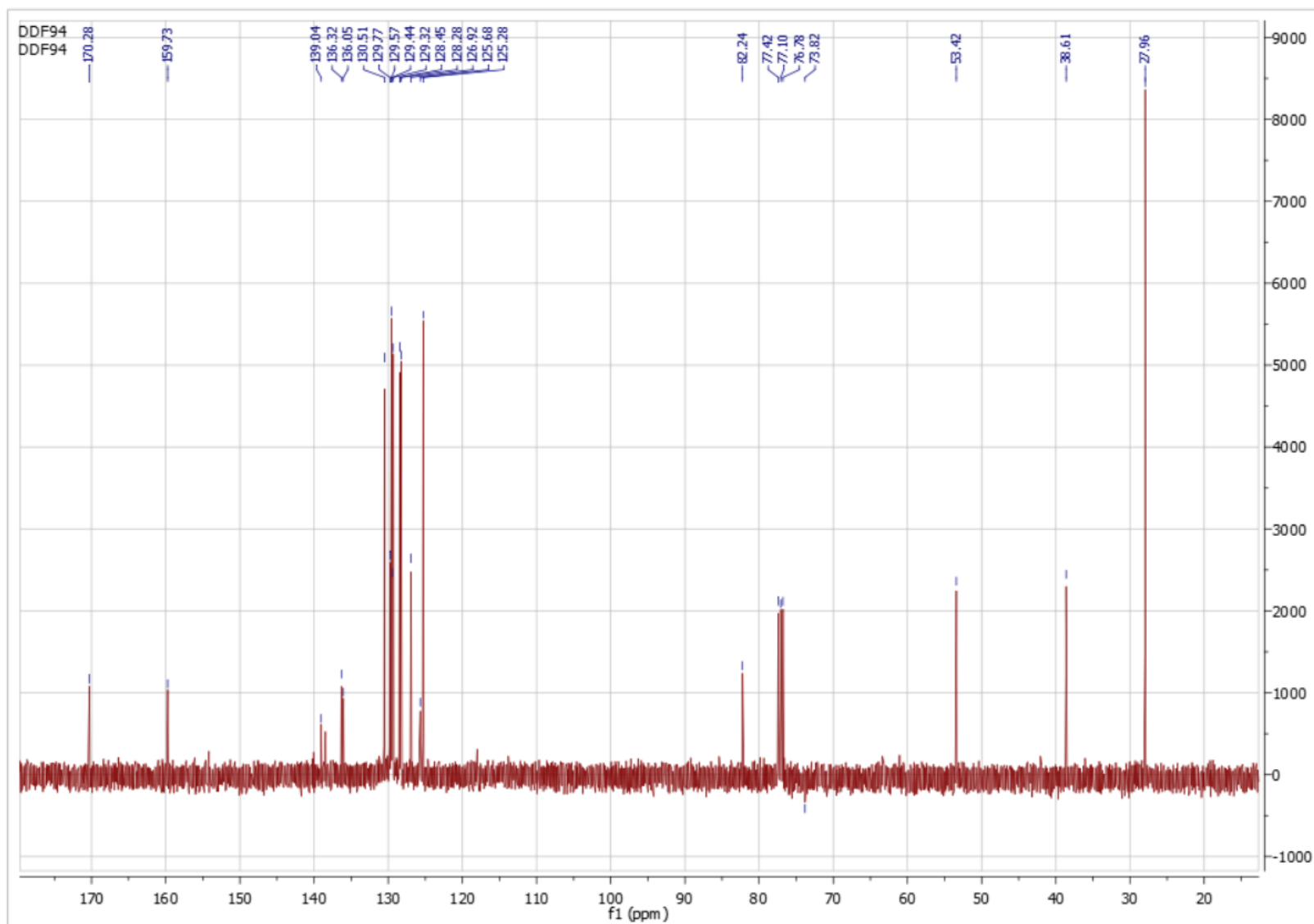
<sup>1</sup>H-NMR spectrum of compound **2e**

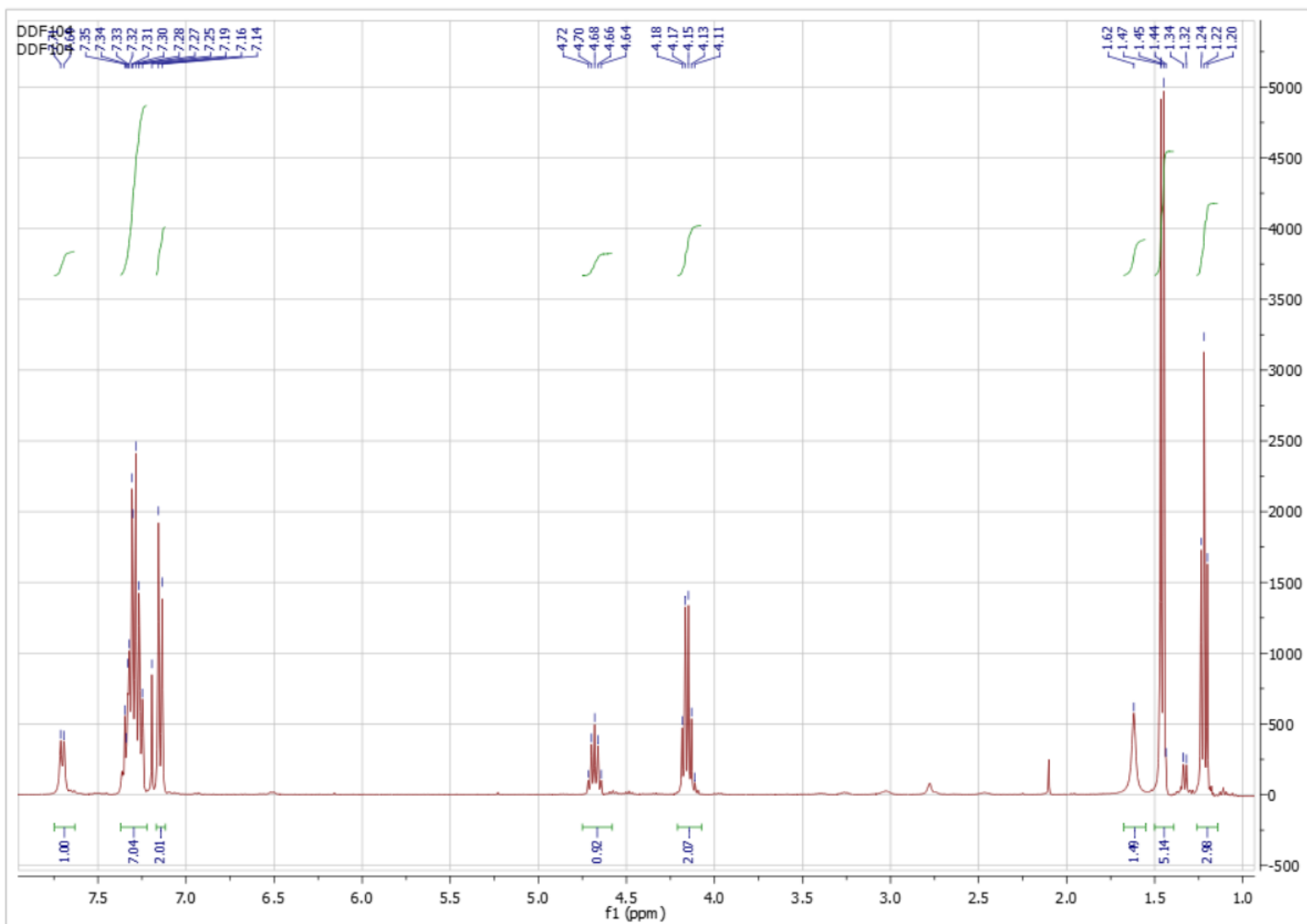
 $^{13}\text{C}$ -NMR spectrum of compound **2e**

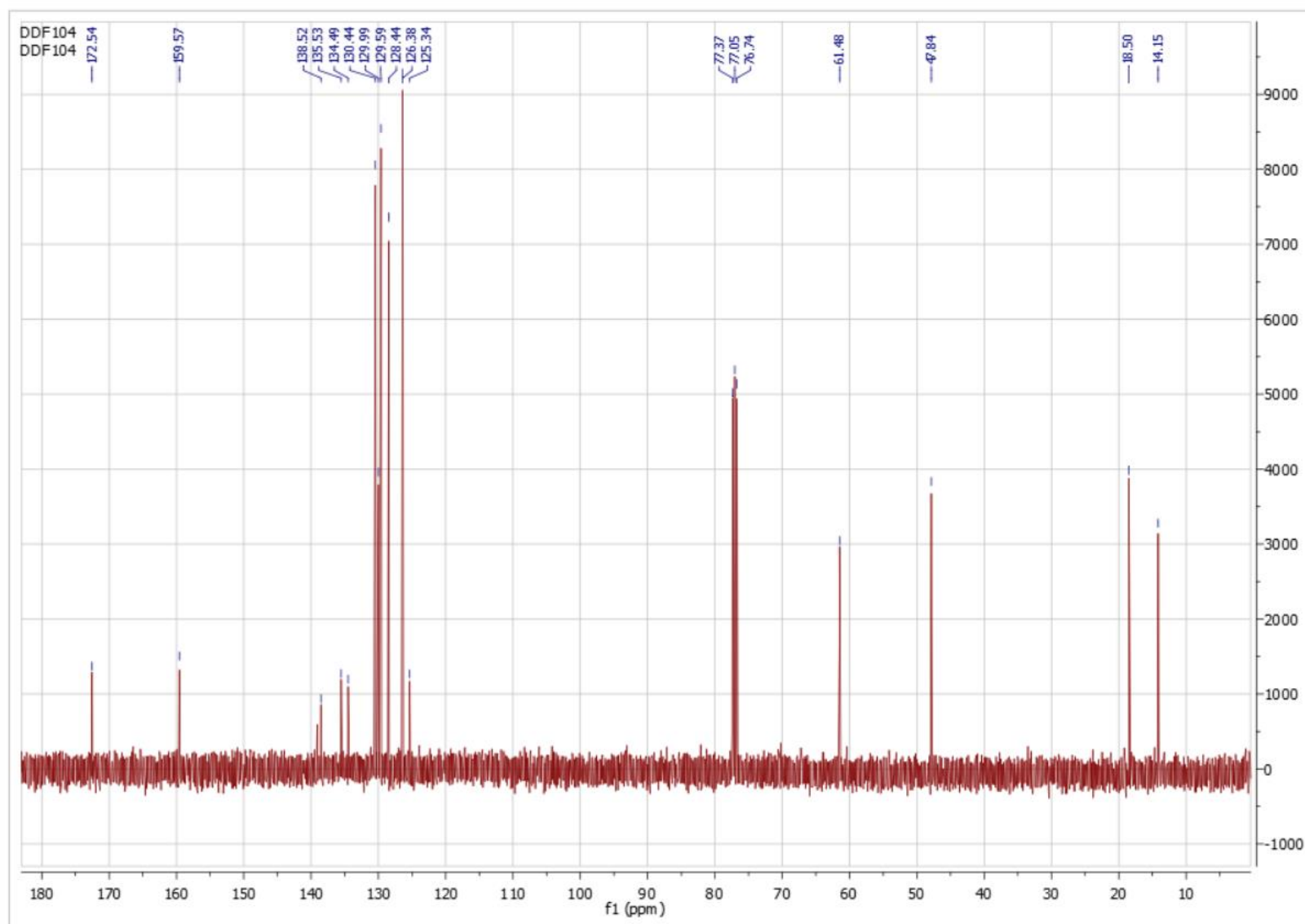
<sup>1</sup>H-NMR spectrum of compound **2f**

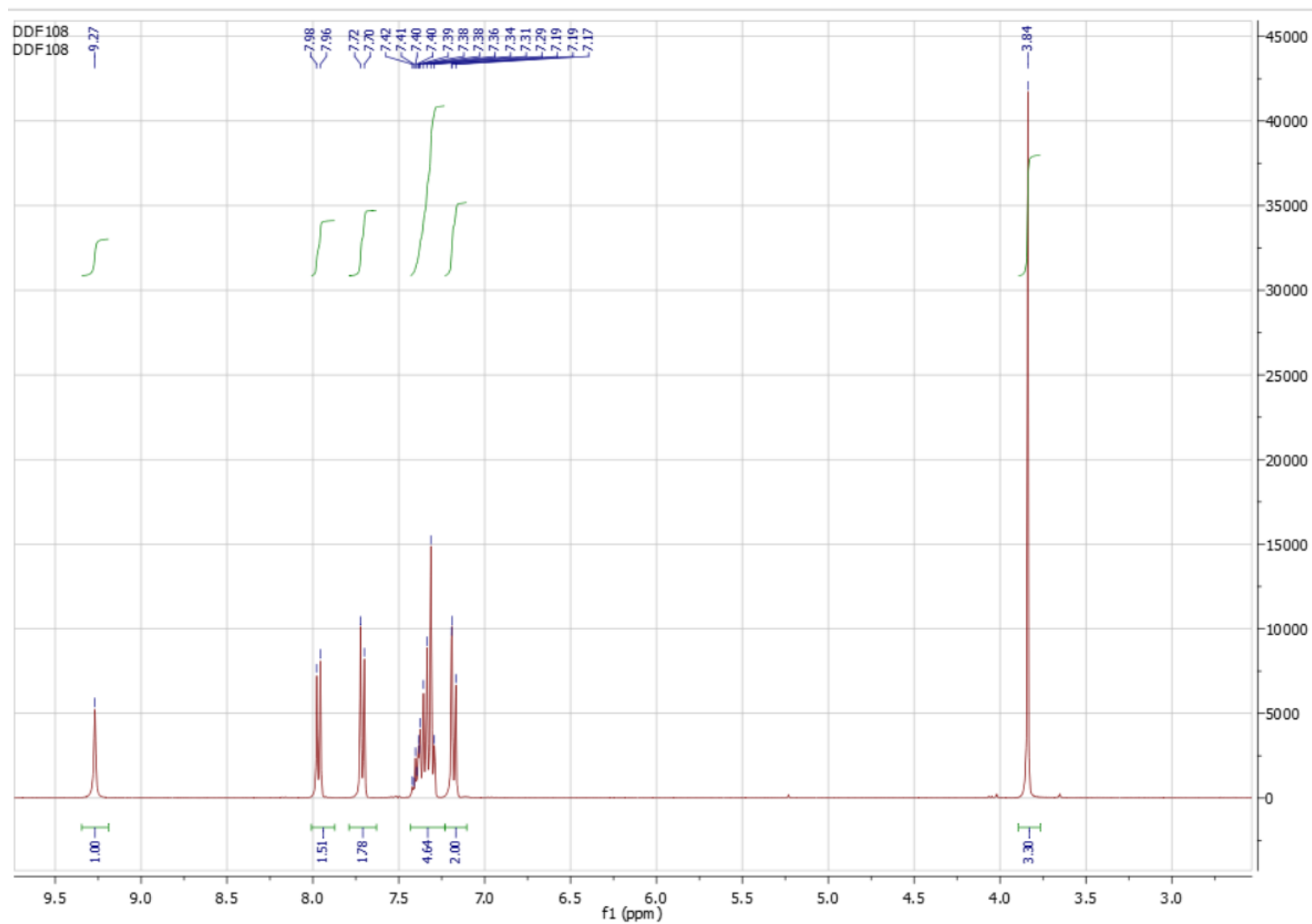
 $^{13}\text{C}$ -NMR spectrum of compound **2f**

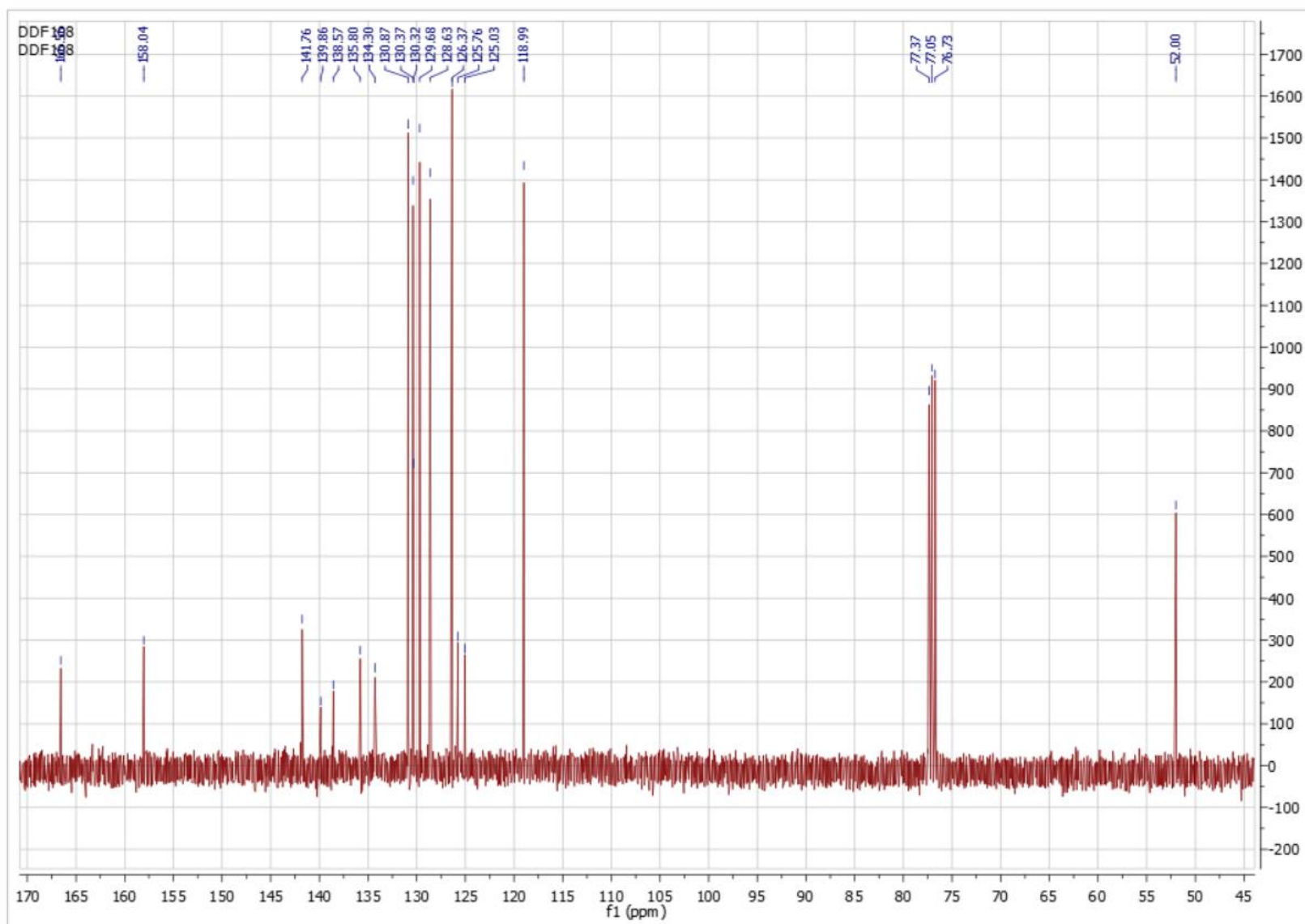
<sup>1</sup>H-NMR spectrum of compound **2g**

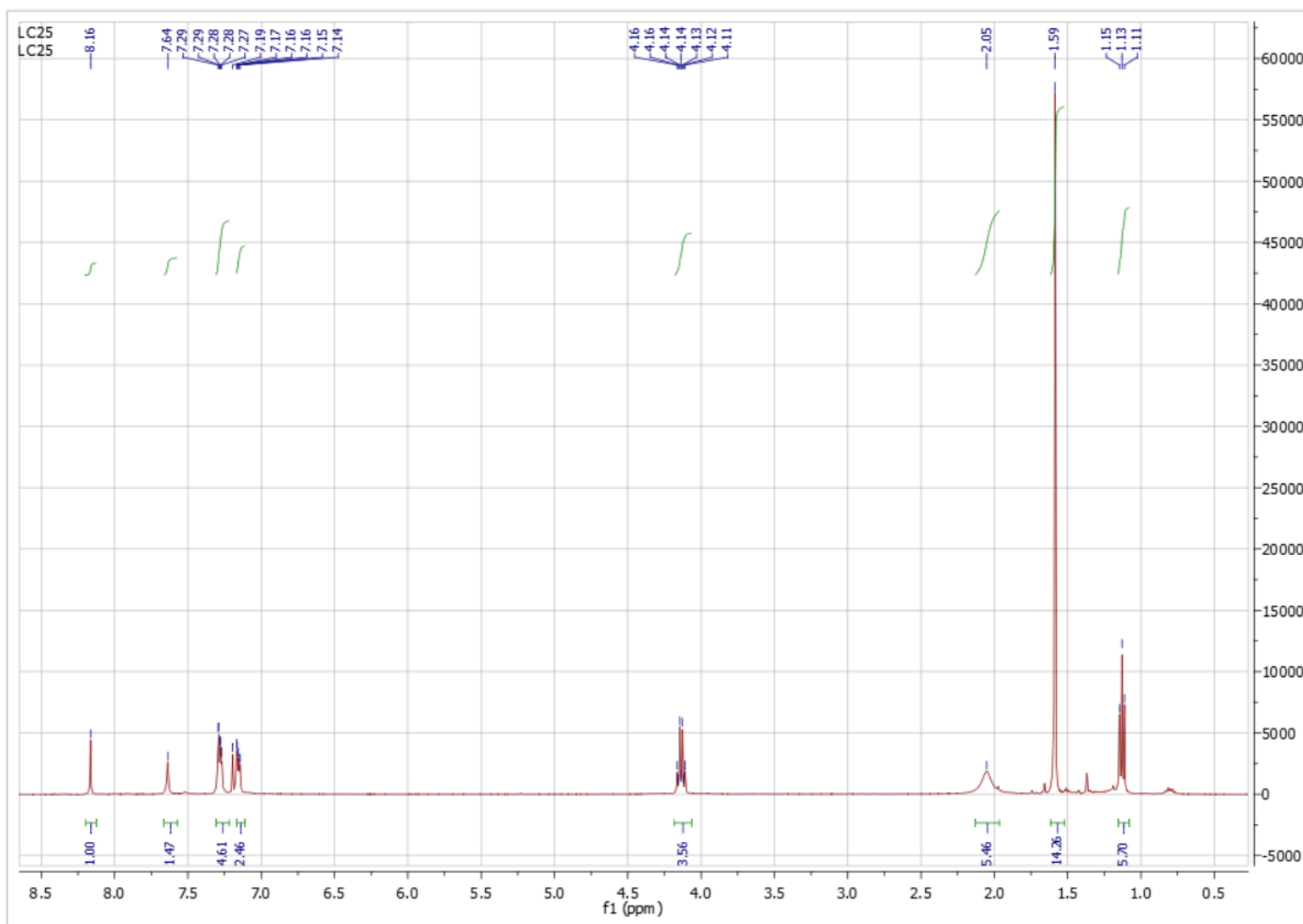
<sup>13</sup>C-NMR spectrum of compound **2g**

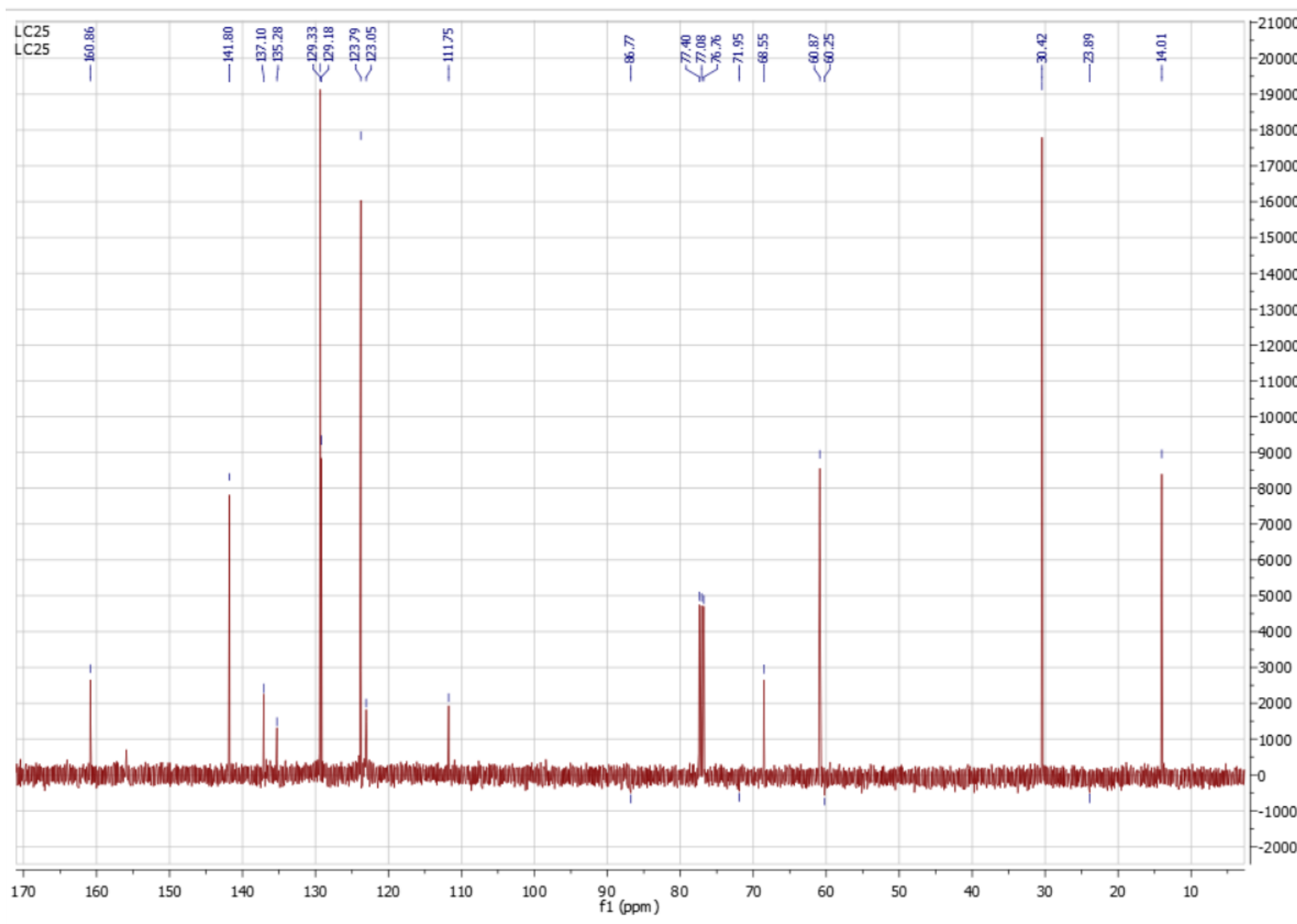
<sup>1</sup>H-NMR spectrum of compound **2h**

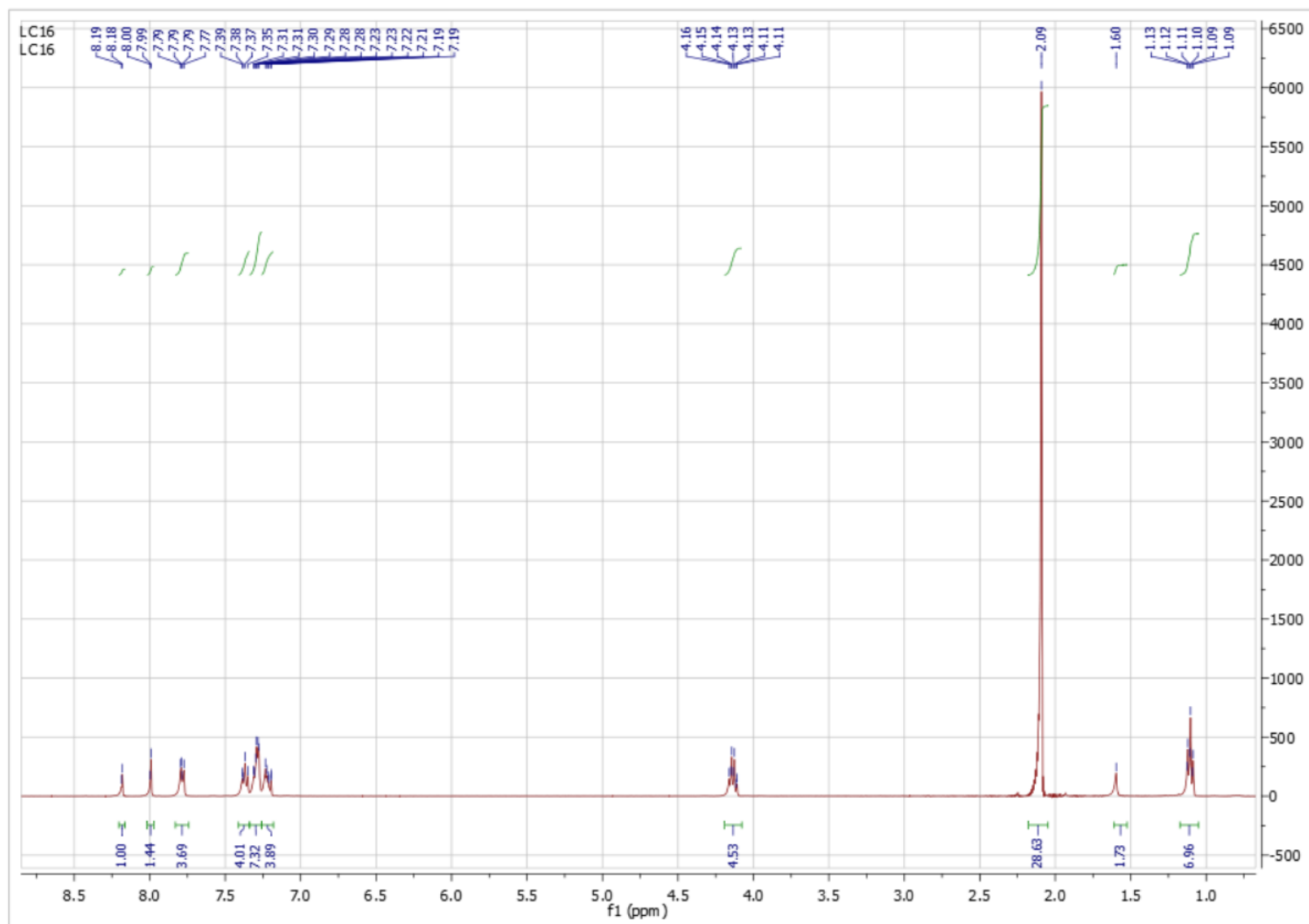
<sup>13</sup>C-NMR spectrum of compound **2h**

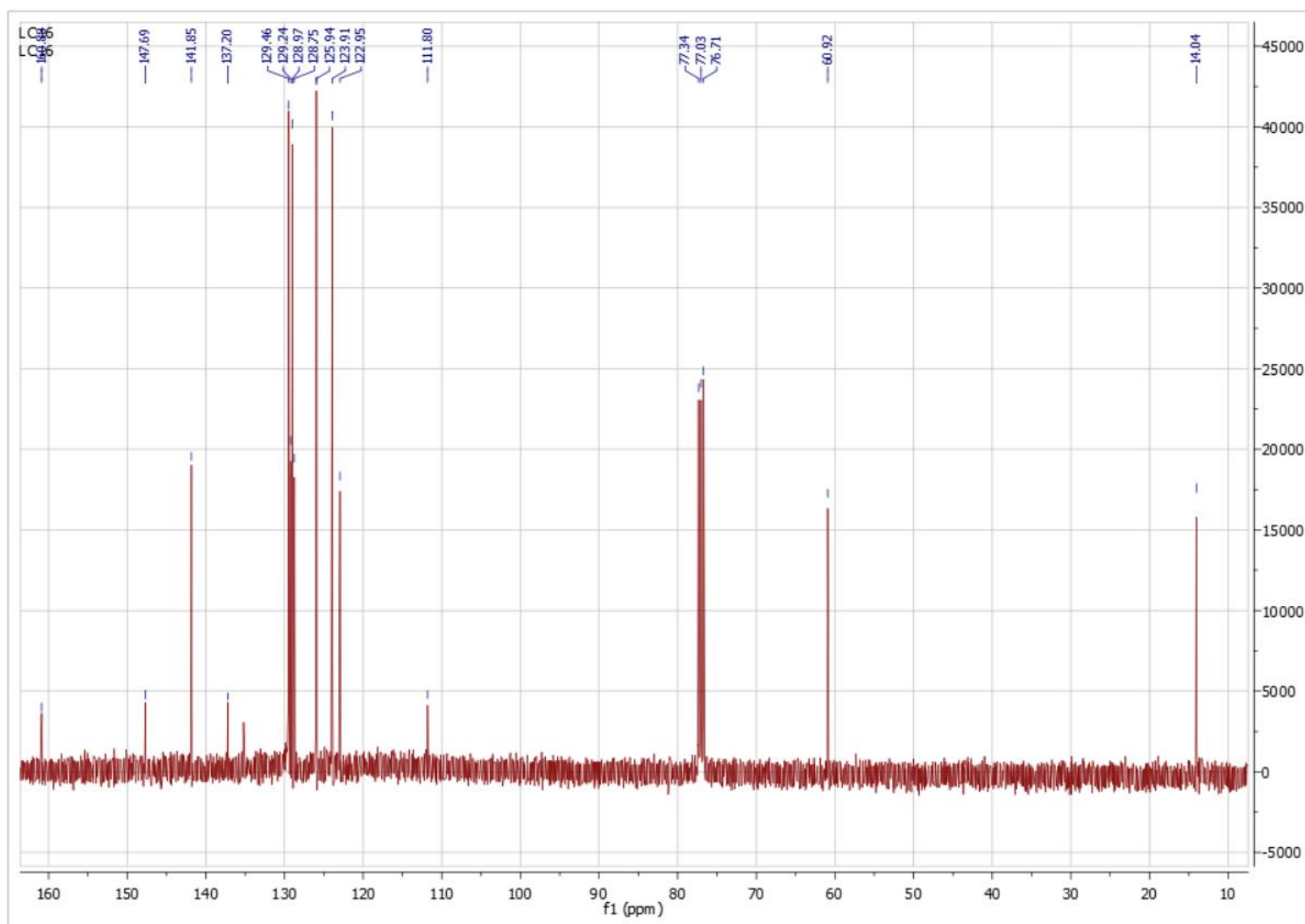
<sup>1</sup>H-NMR spectrum of compound **2i**

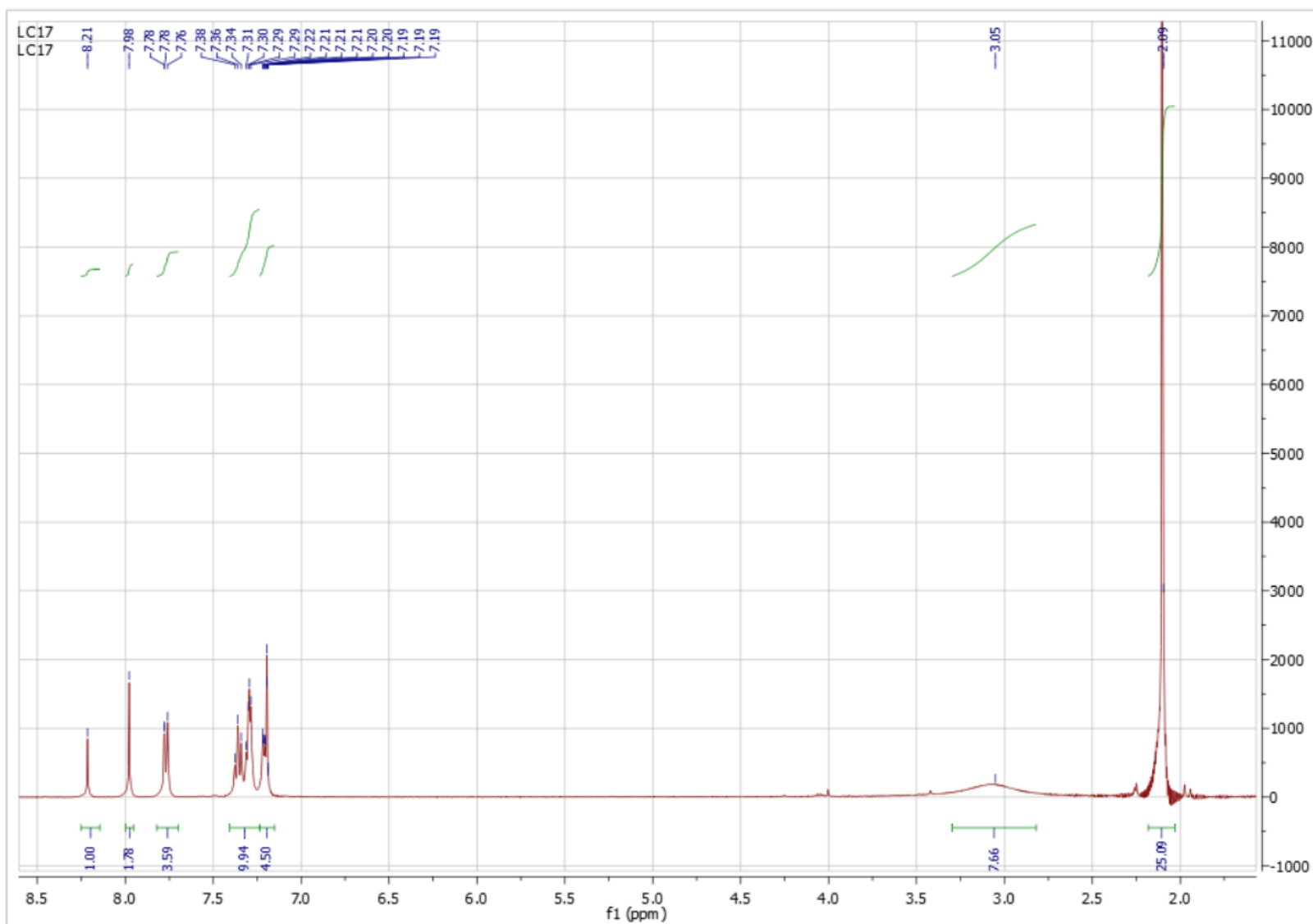
 $^{13}\text{C}$ -NMR spectrum of compound **2i**

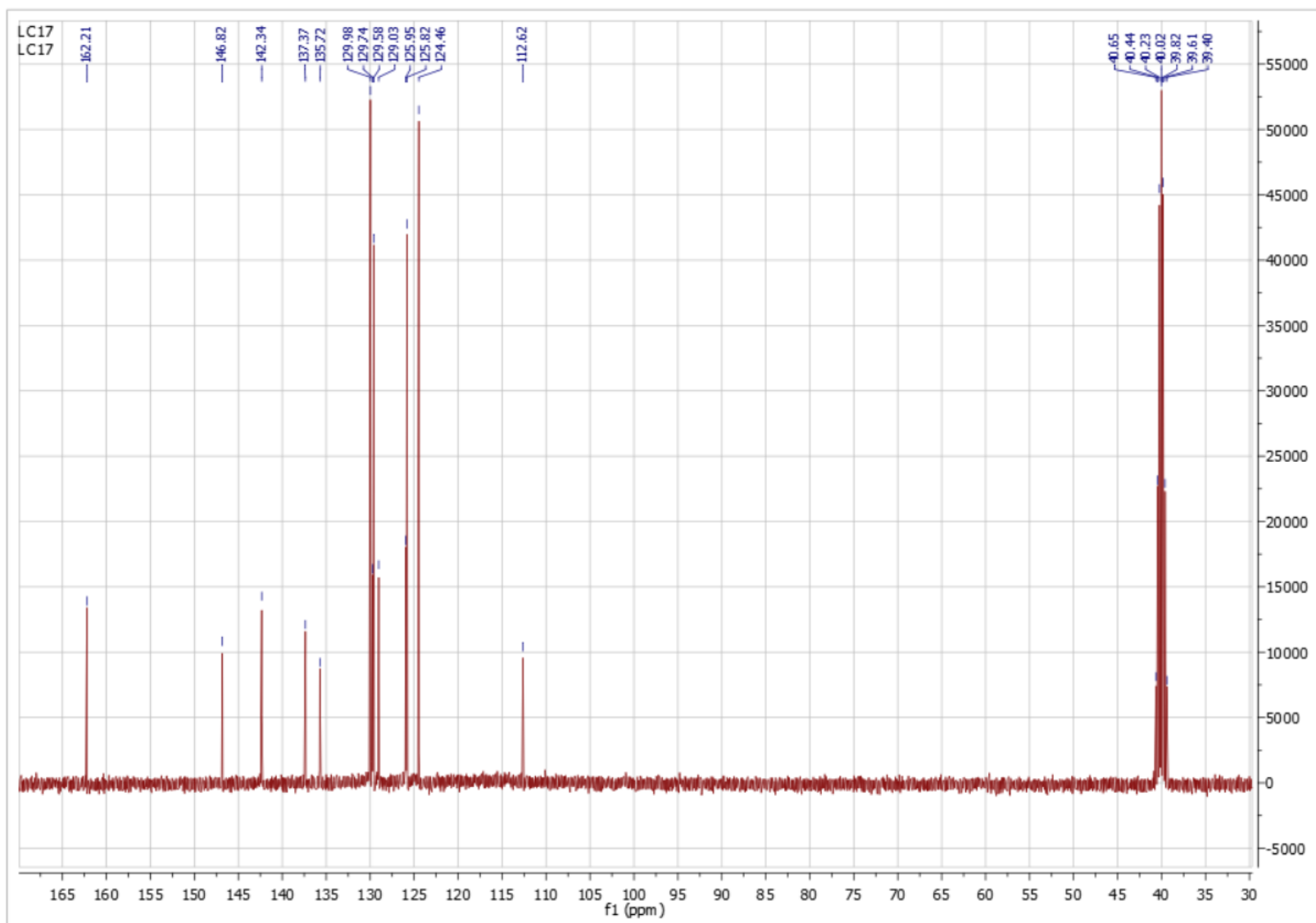
<sup>1</sup>H-NMR spectrum of compound **3a**

 $^{13}\text{C}$ -NMR spectrum of compound **3a**

<sup>1</sup>H-NMR spectrum of compound **3c**

<sup>13</sup>C-NMR spectrum of compound **3c**

<sup>1</sup>H-NMR spectrum of compound **3d**

 $^{13}\text{C}$ -NMR spectrum of compound **3d**

## Openlynx Report -

Sample: 32

Date:18-Jan-2018

Vial:1:D,3

Time:18:29:59

File:I-0227944-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

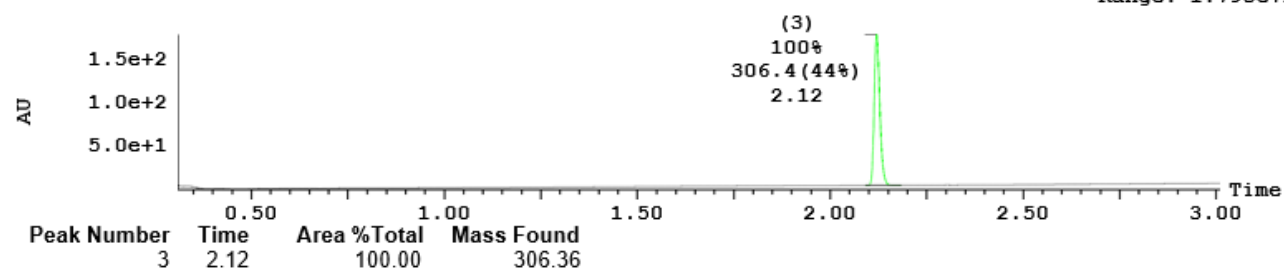
## Compound 2a

Sample 32 Vial 1:D,3 ID File I-0227944-001 Date 18-Jan-2018 Time 18:29:59 Description Met Gen

3: UV Detector: TIC

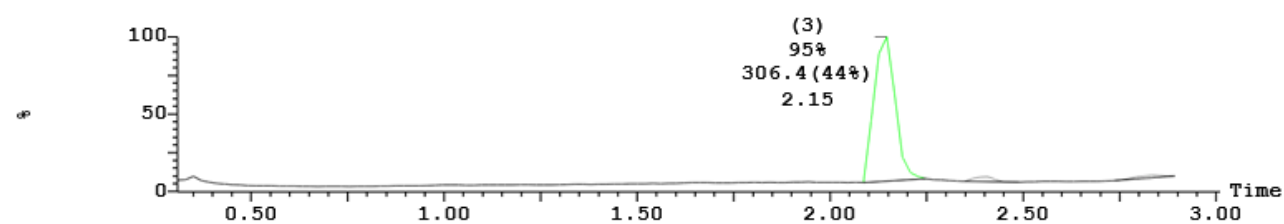
1.797e+2

Range: 1.793e+2



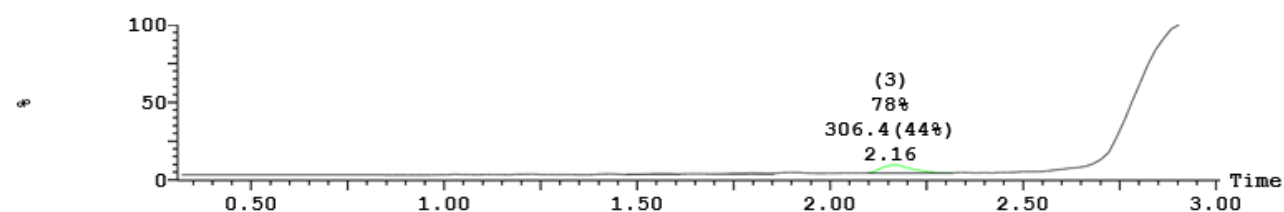
1: MS ES+ :TIC

2.9e+009



2: MS ES- :TIC

4.2e+007



| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 2.15 | 307.36     |

3: (Time: 2.12)

1:MS ES+

3.6e+007



## Openlynx Report -

Sample: 32

Date: 18-Jan-2018

Vial: 1:D,3

Time: 18:29:59

File: I-0227944-001

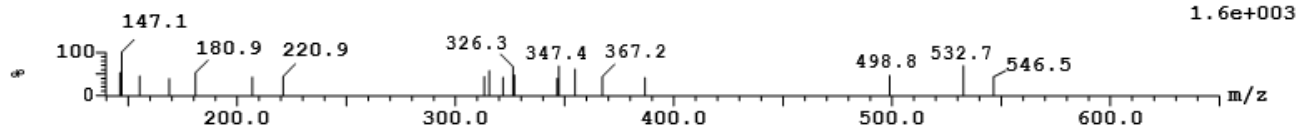
Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
|---------|------|------------|

|   |      |  |
|---|------|--|
| 3 | 2.15 |  |
|---|------|--|

3: (Time: 2.12)

2: MS ES-  
1.6e+003

## Openlynx Report -

Sample: 33

Date: 18-Jan-2018

Vial: 1:D,4

Time: 18:34:03

File: I-0227945-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

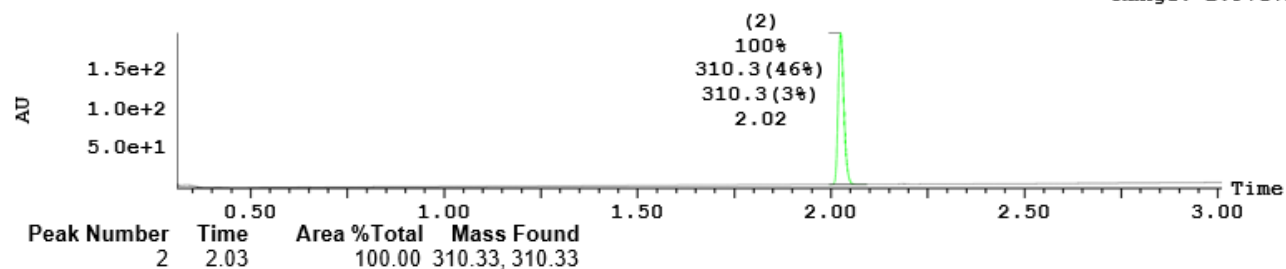
## Compound 2b

Sample 33 Vial 1:D,4 ID File I-0227945-001 Date 18-Jan-2018 Time 18:34:03 Description Met Gen

3: UV Detector: TIC

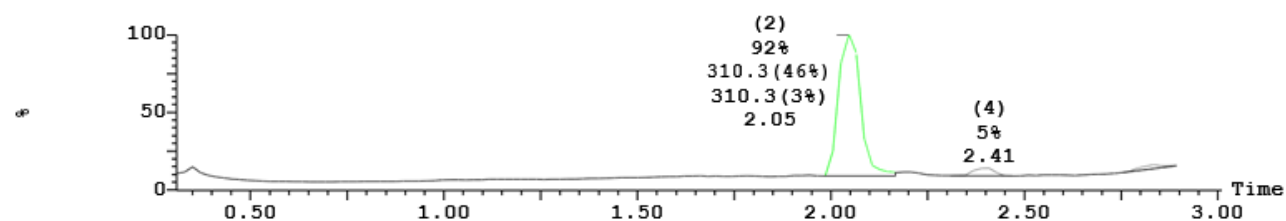
1.973e+2

Range: 1.97e+2



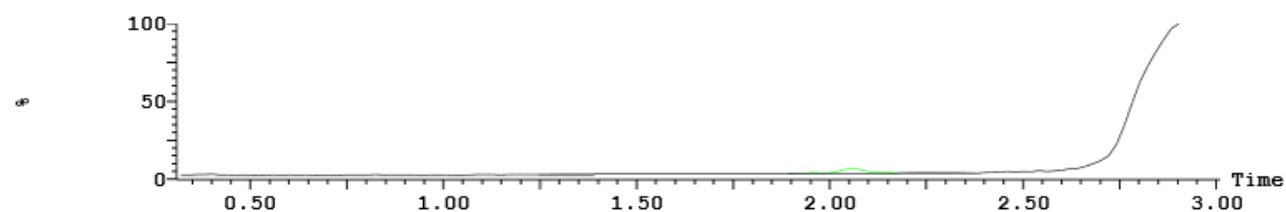
1: MS ES+ :TIC

1.8e+009



2: MS ES- :TIC

4.4e+007

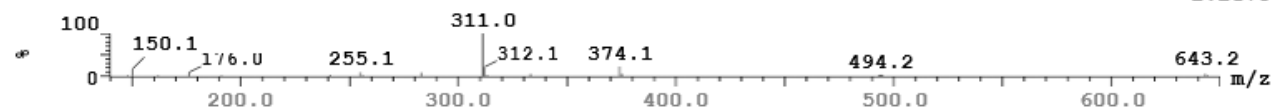


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 2       | 2.05 | 311.33     |

2: (Time: 2.03)

1:MS ES+

2.2e+007



## Openlynx Report -

Sample: 33

Date: 18-Jan-2018

Vial: 1:D,4

Time: 18:34:03

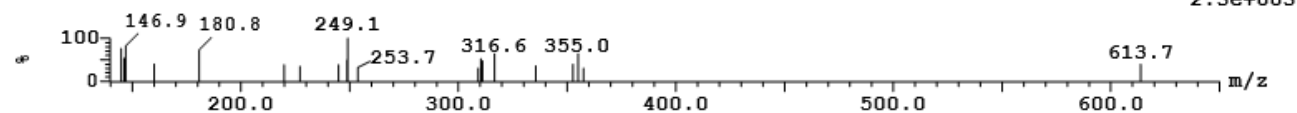
File: I-0227945-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 2       | 2.05 | 309.33     |

2: (Time: 2.03)

2:MS ES-  
2.3e+003

## Openlynx Report -

Sample: 34

Date: 18-Jan-2018

Vial: 1:D,5

Time: 18:38:09

File: I-0227946-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

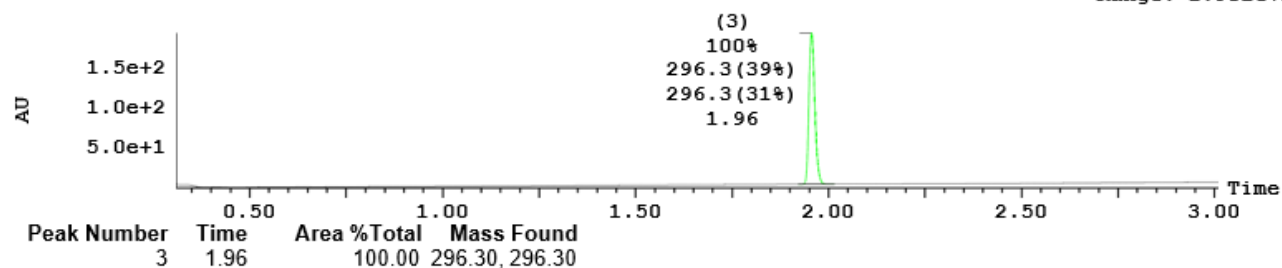
## Compound 2c

Sample 34 Vial 1:D,5 ID File I-0227946-001 Date 18-Jan-2018 Time 18:38:09 Description Met Gen

3: UV Detector: TIC

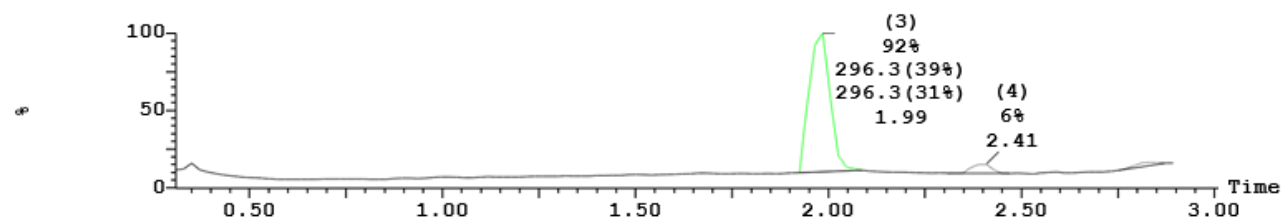
1.936e+2

Range: 1.932e+2



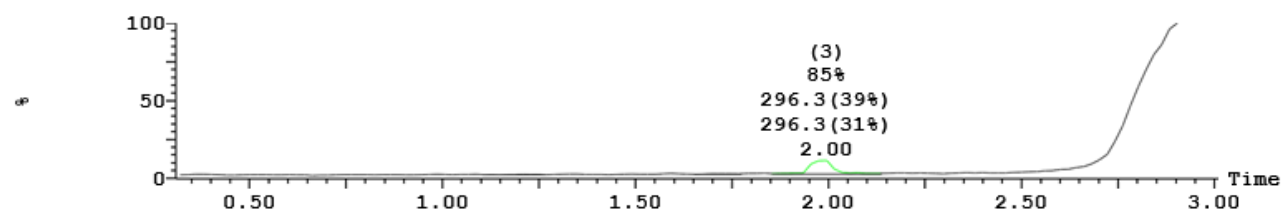
1: MS ES+ :TIC

1.8e+009



2: MS ES- :TIC

4.3e+007

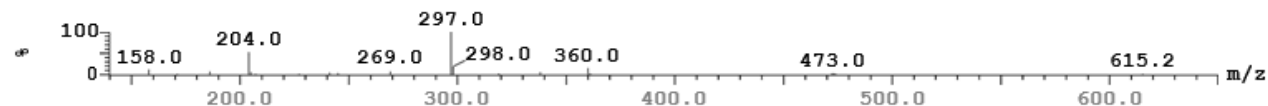


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 1.99 | 297.30     |

3: (Time: 1.96)

1:MS ES+

1.8e+007



## Openlynx Report -

Sample: 34

Vial:1:D,5

File:I-0227946-001

Date:18-Jan-2018

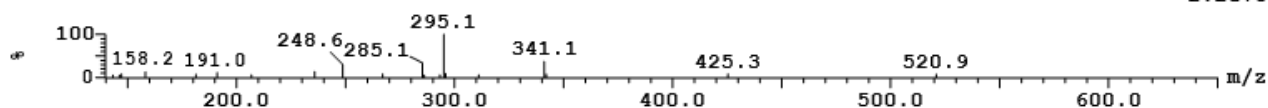
Time:18:38:09

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 1.99 | 295.30     |

3: (Time: 1.96)

2:MS ES-  
2.2e+004

## Openlynx Report -

Sample: 35

Date: 18-Jan-2018

Vial: 1:D,6

Time: 18:42:15

File: I-0227947-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

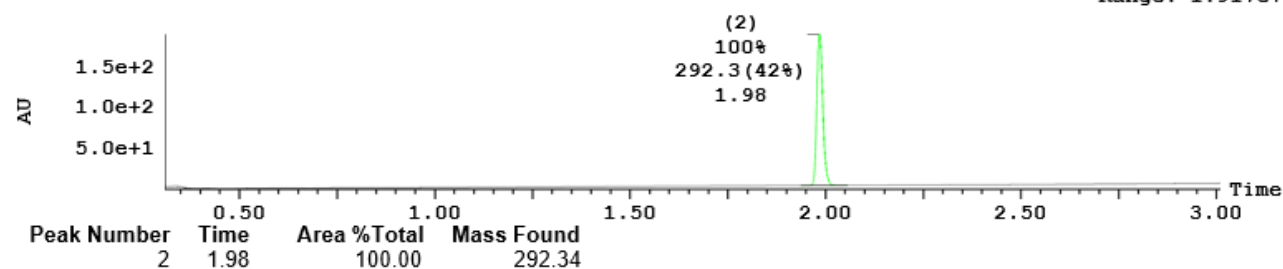
## Compound 2d

Sample 35 Vial 1:D,6 ID File I-0227947-001 Date 18-Jan-2018 Time 18:42:15 Description Met Gen

3: UV Detector: TIC

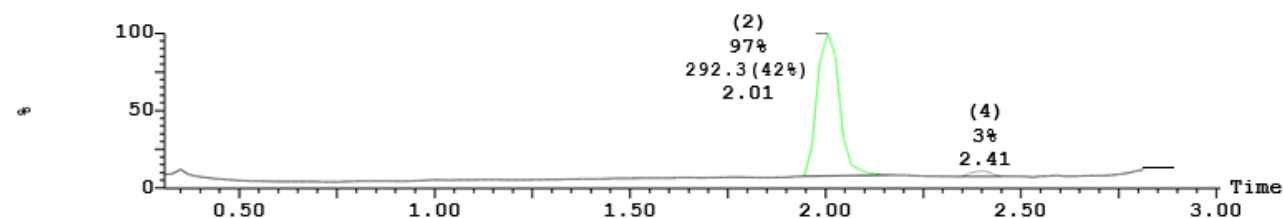
1.92e+2

Range: 1.917e+2



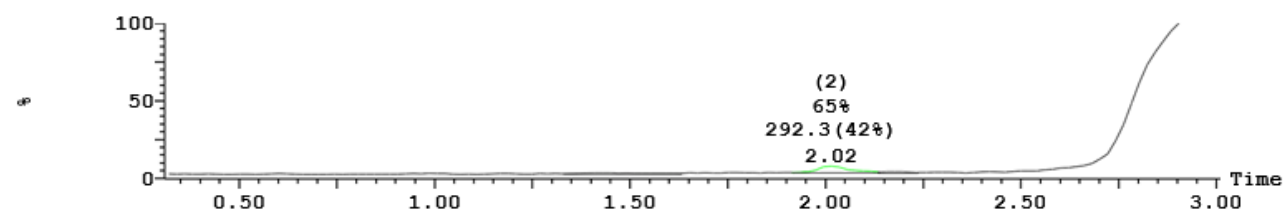
1: MS ES+ :TIC

2.4e+009



2: MS ES- :TIC

4.3e+007

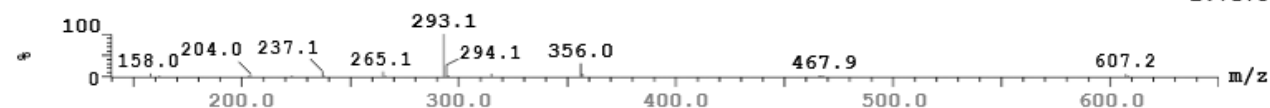


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 2       | 2.01 | 293.34     |

2: (Time: 1.98)

1:MS ES+

2.7e+007



## Openlynx Report -

Sample: 35

Date: 18-Jan-2018

Vial: 1:D,6

Time: 18:42:15

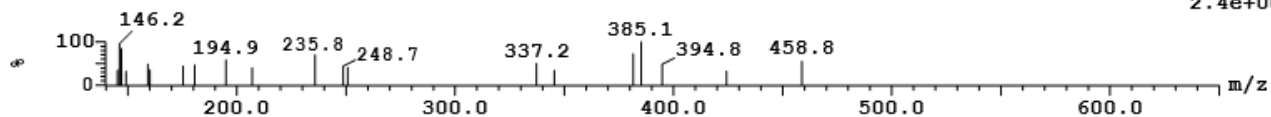
File: I-0227947-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 2       | 2.01 |            |

2: (Time: 1.98)

2:MS ES-  
2.4e+003

## Openlynx Report -

Sample: 37

Vial:1:D,8

File:I-0227949-001

Date:18-Jan-2018

Time:18:50:27

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

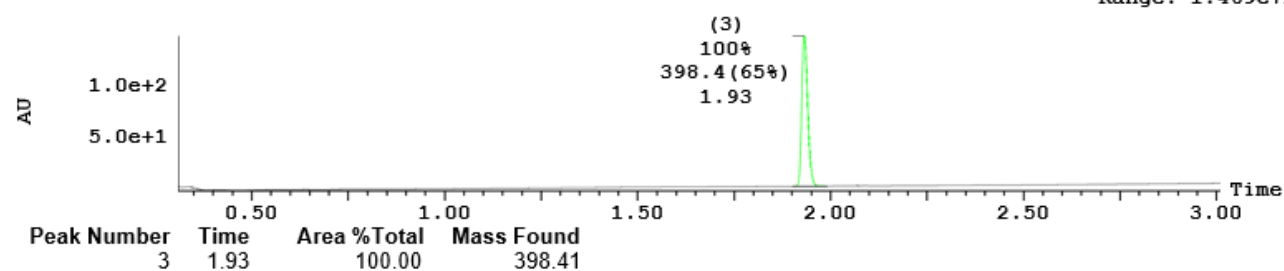
## Compound 2e

Sample 37 Vial 1:D,8 ID File I-0227949-001 Date 18-Jan-2018 Time 18:50:27 Description Met Gen

3: UV Detector: TIC

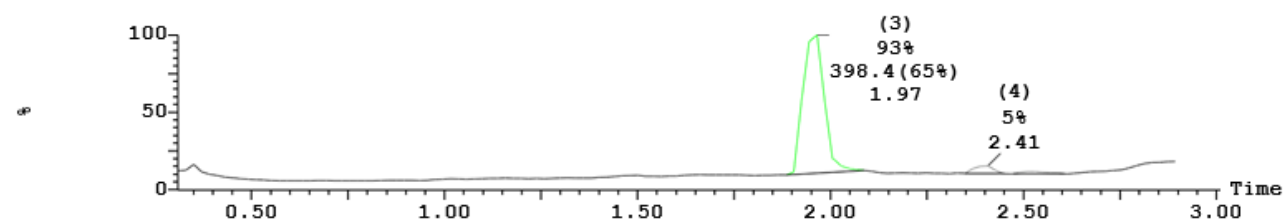
1.473e+2

Range: 1.469e+2



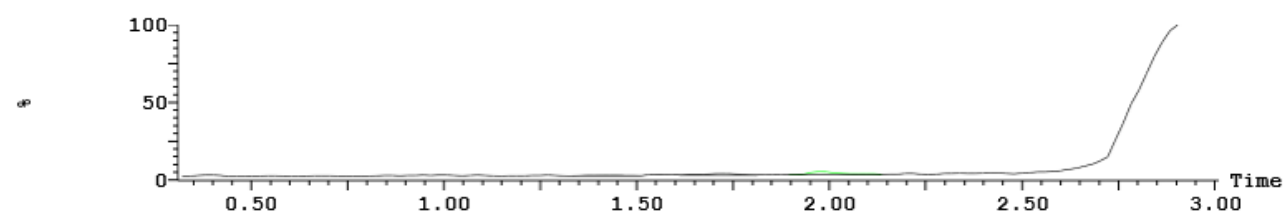
1: MS ES+ :TIC

1.7e+009



2: MS ES- :TIC

4.4e+007

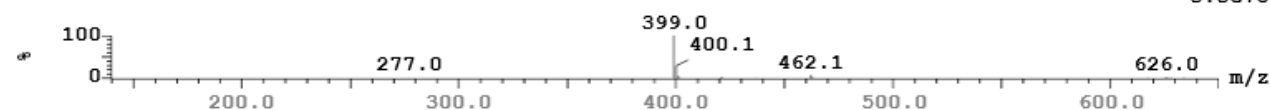


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 1.97 | 399.41     |

3: (Time: 1.93)

1:MS ES+

3.3e+007



## Openlynx Report -

Sample: 37

Date: 18-Jan-2018

Vial: 1:D,8

Time: 18:50:27

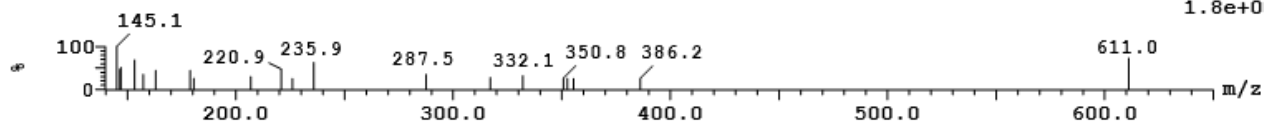
File: I-0227949-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 1.97 |            |

3: (Time: 1.93)

2:MS ES-  
1.8e+003

## Openlynx Report -

Sample: 36

Date: 18-Jan-2018

Vial: 1:D,7

Time: 18:46:21

File: I-0227948-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

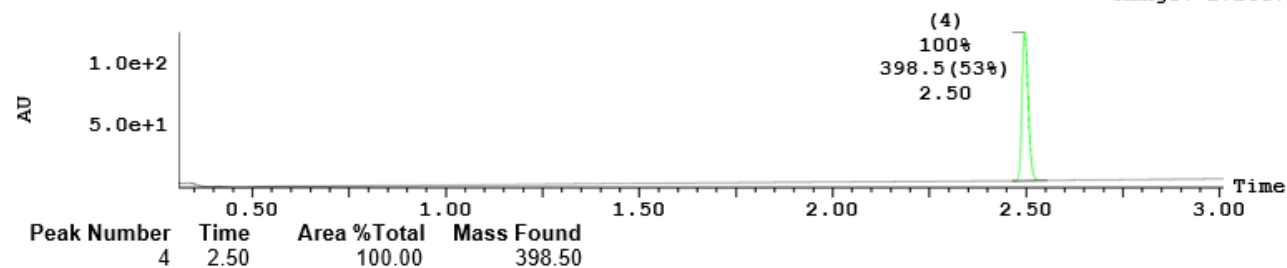
## Compound 2f

Sample 36 Vial 1:D,7 ID File I-0227948-001 Date 18-Jan-2018 Time 18:46:21 Description Met Gen

## 3: UV Detector: TIC

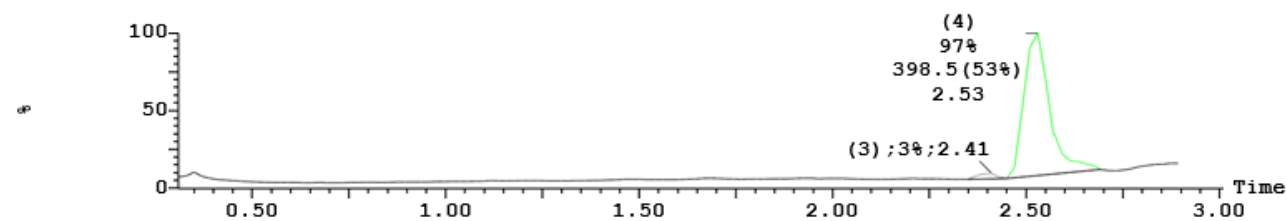
1.264e+2

Range: 1.26e+2



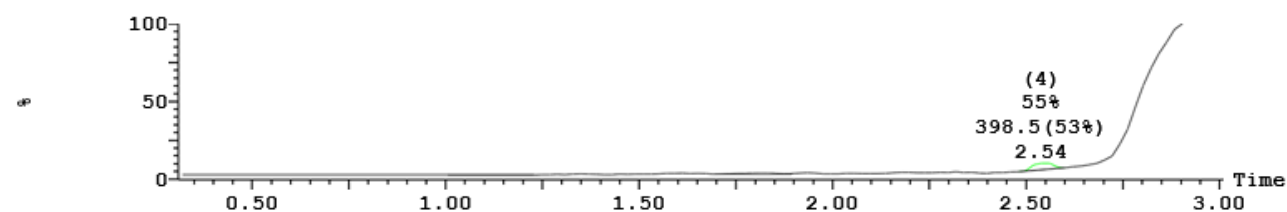
## 1: MS ES+ :TIC

2.8e+009



## 2: MS ES- :TIC

4.2e+007

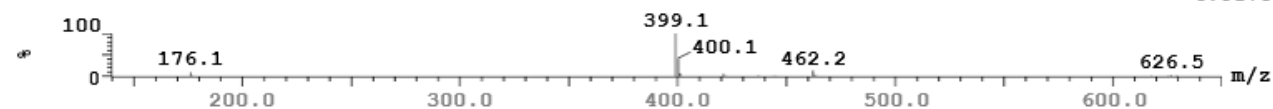


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 4       | 2.53 | 399.50     |

## 4: (Time: 2.50)

1:MS ES+

4.8e+007



## Openlynx Report -

Sample: 36

Date: 18-Jan-2018

Vial: 1:D,7

Time: 18:46:21

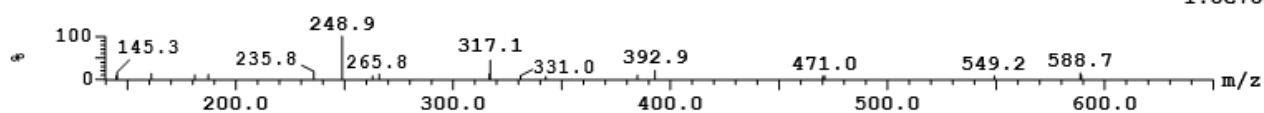
File: I-0227948-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 4       | 2.53 |            |

4: (Time: 2.50)

2:MS ES-  
1.0e+004

## Openlynx Report -

Sample: 38

Vial:1:D,9

File:I-0227950-001

Date:18-Jan-2018

Time:18:54:35

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

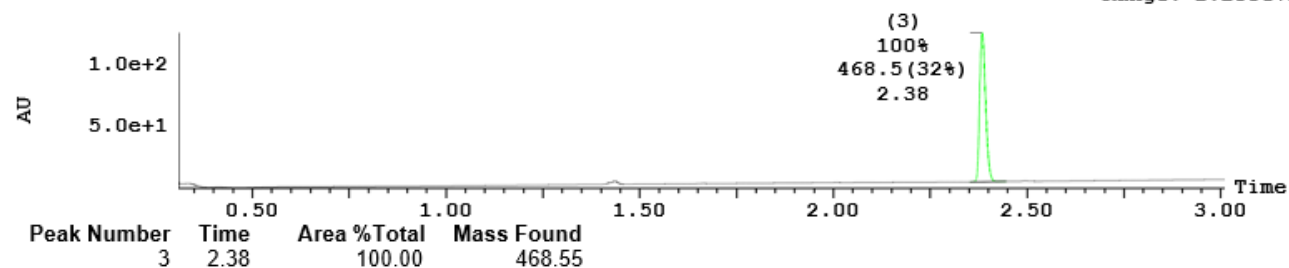
## Compound 2g

Sample 38 Vial 1:D,9 ID File I-0227950-001 Date 18-Jan-2018 Time 18:54:35 Description Met Gen

3: UV Detector: TIC

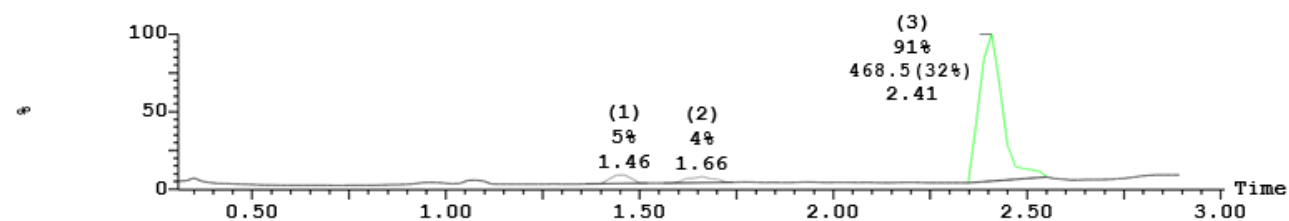
1.259e+2

Range: 1.255e+2



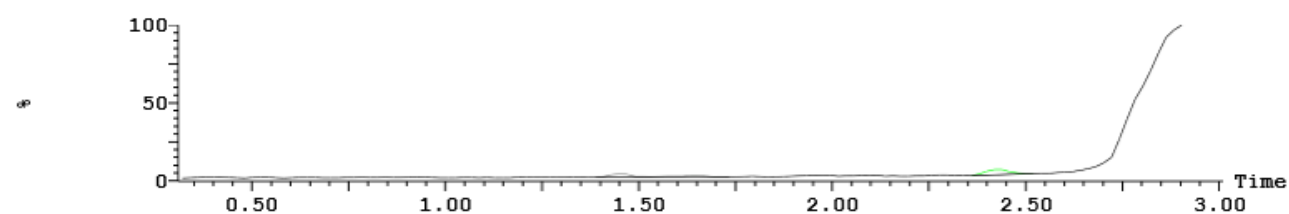
1: MS ES+ :TIC

3.8e+009



2: MS ES- :TIC

4.0e+007

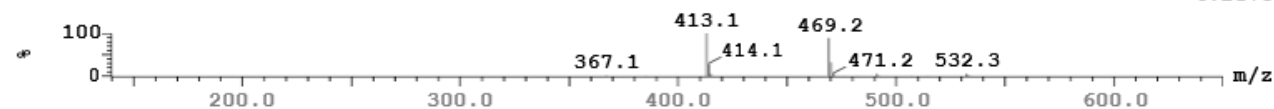


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 2.41 | 469.55     |

3: (Time: 2.38)

1:MS ES+

4.2e+007



## Openlynx Report -

Sample: 38

Date: 18-Jan-2018

Vial: 1:D,9

Time: 18:54:35

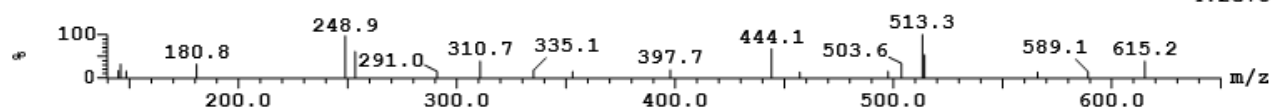
File: I-0227950-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 2.41 |            |

3: (Time: 2.38)

2:MS ES-  
4.2e+003

## Openlynx Report -

Sample: 39

Vial:1:D,10

File:I-0227951-001

Date:18-Jan-2018

Time:18:58:42

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

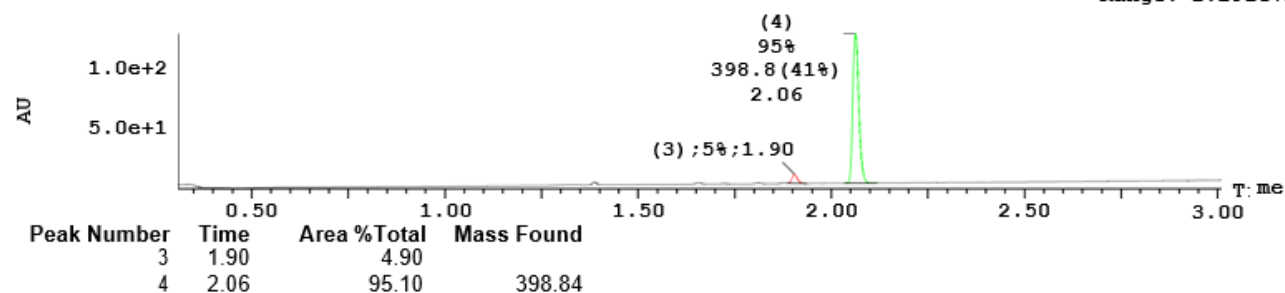
## Compound 2h

Sample 39 Vial 1:D,10 ID File I-0227951-001 Date 18-Jan-2018 Time 18:58:42 Description Met Gen

3: UV Detector: TIC

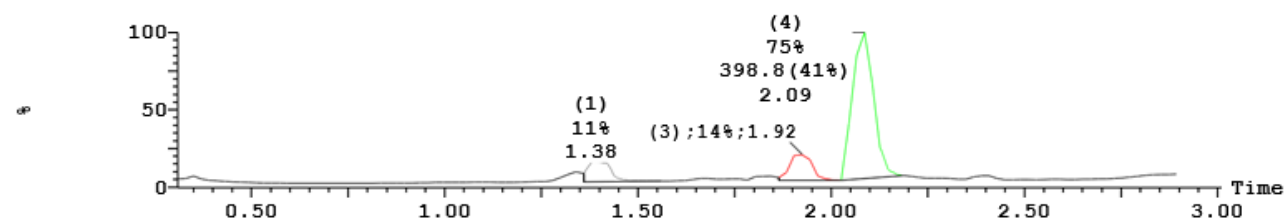
1.294e+2

Range: 1.291e+2



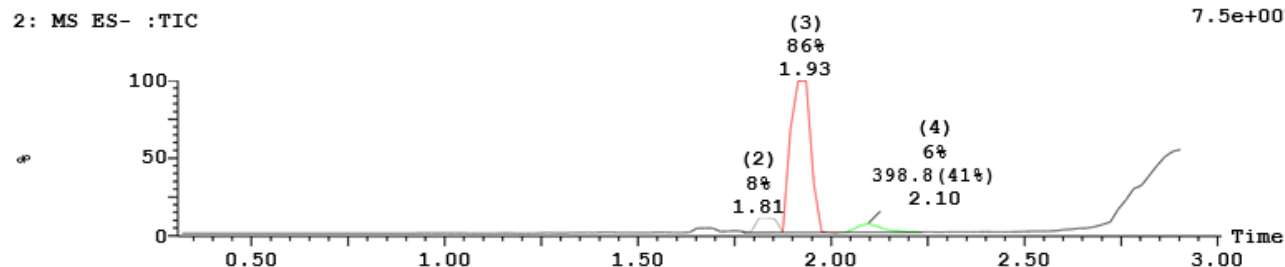
1: MS ES+ :TIC

3.8e+009



2: MS ES- :TIC

7.5e+007



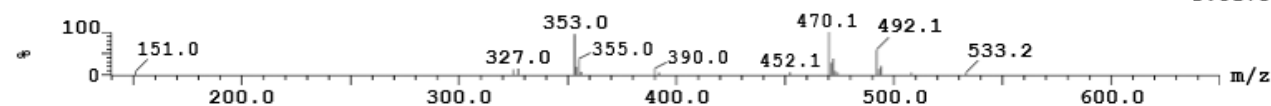
Peak ID Time Mass Found

3 1.92

3: (Time: 1.90)

1:MS ES+

3.8e+006



## Openlynx Report -

Sample: 39

Vial:1:D,10

File:I-0227951-001

Date:18-Jan-2018

Time:18:58:42

Printed: Fri Jan 19 09:28:55 2018

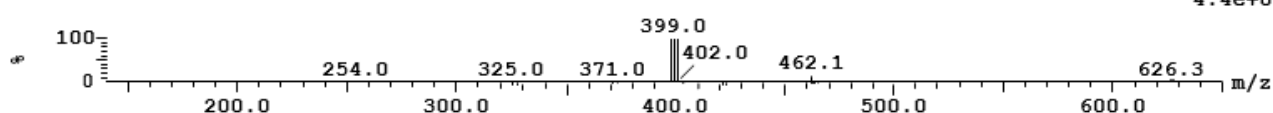
## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 4       | 2.09 | 399.84     |

4: (Time: 2.06)

1:MS ES+

4.4e+007

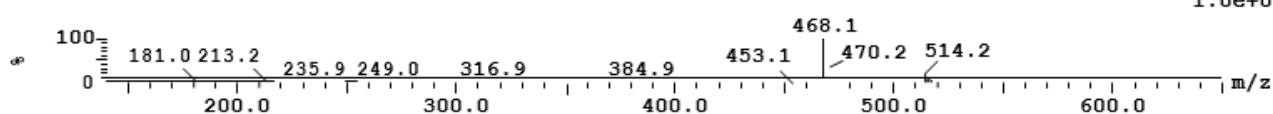


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 1.92 |            |

3: (Time: 1.90)

2:MS ES-

1.0e+006

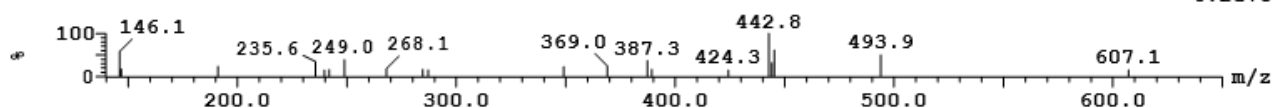


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 4       | 2.09 |            |

4: (Time: 2.06)

2:MS ES-

6.2e+003



## Openlynx Report -

Sample: 44

Vial:1:E,5

File:I-0227956-001

Date:18-Jan-2018

Time:19:19:11

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

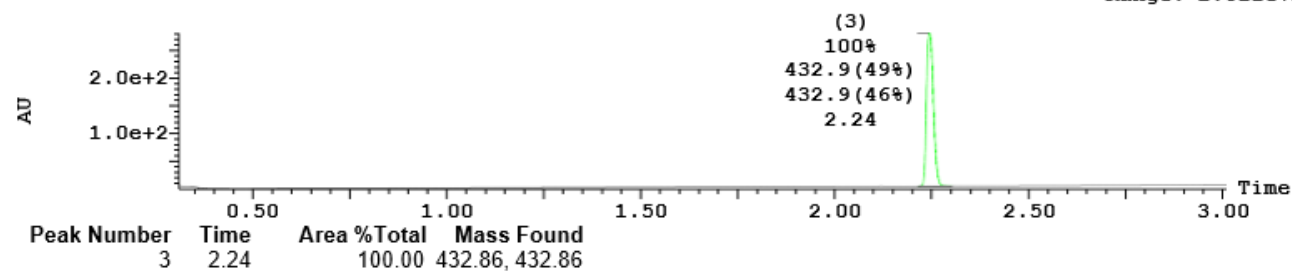
## Compound 2i

Sample 44 Vial 1:E,5 ID File I-0227956-001 Date 18-Jan-2018 Time 19:19:11 Description Met Gen

3: UV Detector: TIC

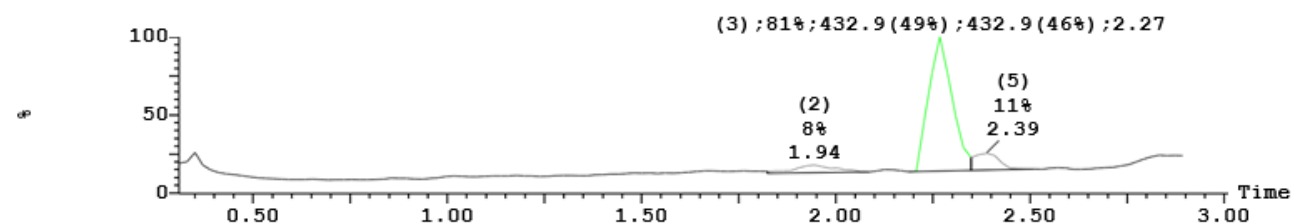
2.815e+2

Range: 2.811e+2



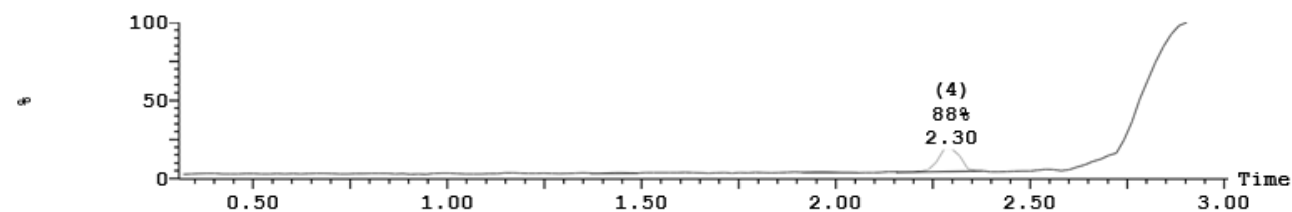
1: MS ES+ :TIC

1.2e+009



2: MS ES- :TIC

3.8e+007

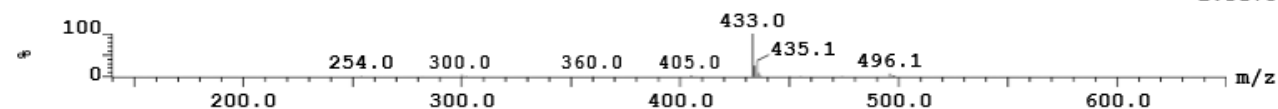


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 2.27 | 433.86     |

3: (Time: 2.24)

1:MS ES+

1.5e+007



## Openlynx Report -

Sample: 44

Date: 18-Jan-2018

Vial: 1:E,5

Time: 19:19:11

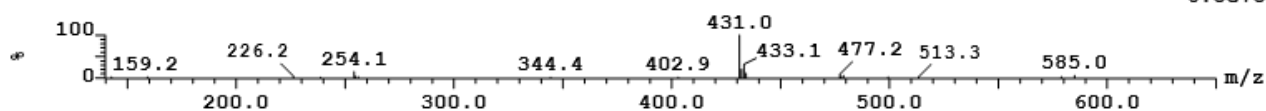
File: I-0227956-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 2.27 | 431.86     |

3: (Time: 2.24)

2: MS ES-  
6.0e+004

## Openlynx Report -

Sample: 7

Date: 18-Jan-2018

Vial: 1:A,8

Time: 16:47:14

File: I-0227919-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

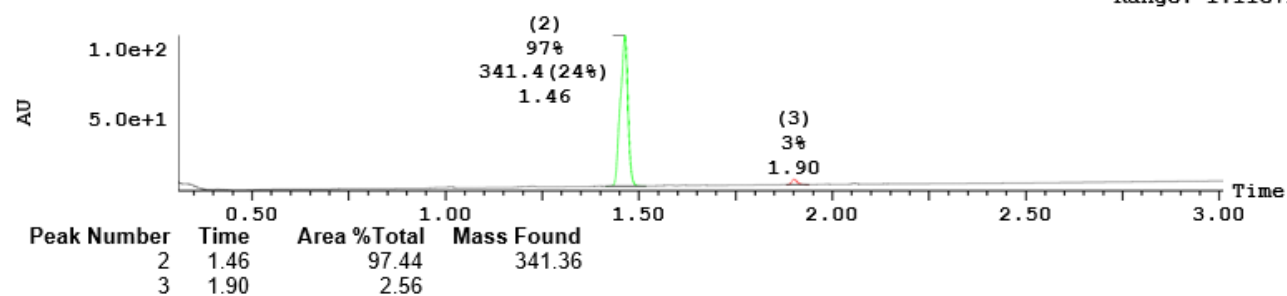
## Compound 3a

Sample 7 Vial 1:A,8 ID File I-0227919-001 Date 18-Jan-2018 Time 16:47:14 Description Met Gen

3: UV Detector: TIC

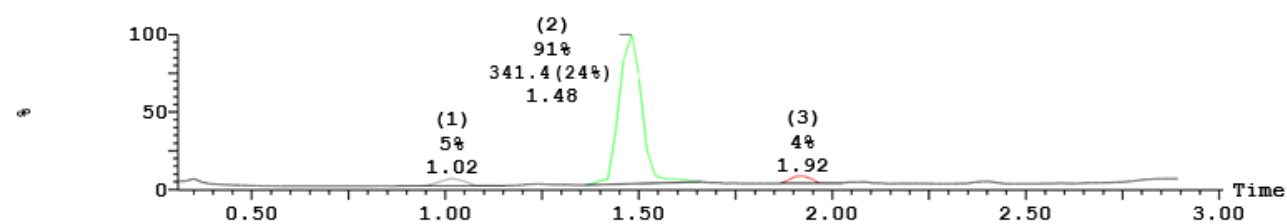
1.114e+2

Range: 1.11e+2



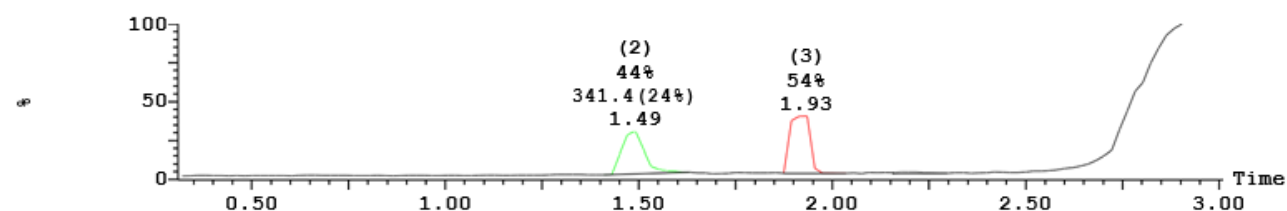
1: MS ES+ :TIC

4.5e+009



2: MS ES- :TIC

4.5e+007

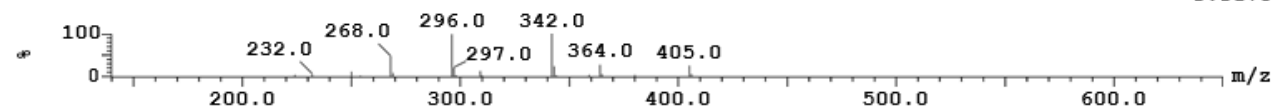


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 2       | 1.48 | 342.36     |

2: (Time: 1.46)

1:MS ES+

3.3e+007



## Openlynx Report -

Sample: 7

Vial:1:A,8

File:I-0227919-001

Date:18-Jan-2018

Time:16:47:14

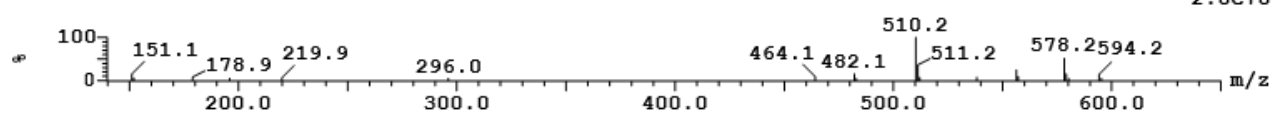
Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

Peak ID Time Mass Found

3 1.92

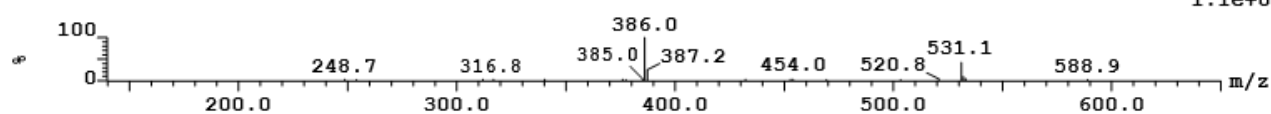
3: (Time: 1.90)

1:MS ES+  
2.0e+006

Peak ID Time Mass Found

2 1.48

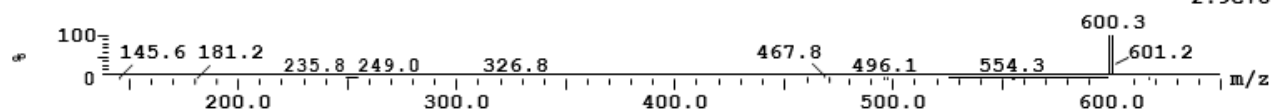
2: (Time: 1.46)

2:MS ES-  
1.1e+005

Peak ID Time Mass Found

3 1.92

3: (Time: 1.90)

2:MS ES-  
2.9e+005

## Compound 3b

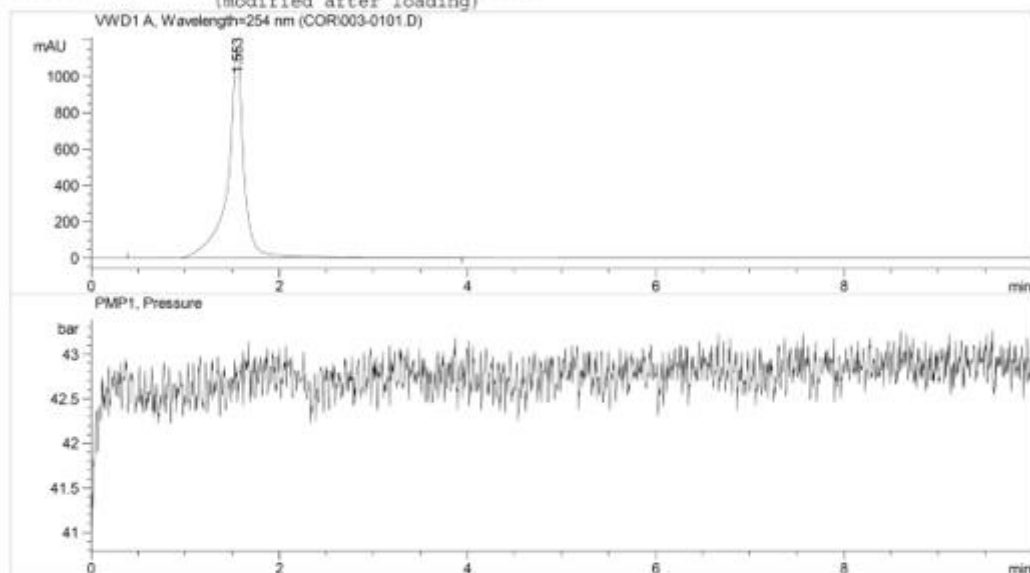
## Compound 3b

Data File C:\HPCHEM\1\DATA\COR\003-0101.D

Sample Name: cor1417

```
=====
Injection Date   : 5/27/2021 4:46:31 PM      Seq. Line :    1
Sample Name      : cor1417                  Location  : Vial 3
Acq. Operator    : MARCO                    Inj       :    1
                                           Inj Volume: 5 µl

Acq. Method      : C:\HPCHEM\1\METHODS\MARGH.M
Last changed     : 5/27/2021 2:22:53 PM by MARCO
Analysis Method  : C:\HPCHEM\1\METHODS\MARGH.M
Last changed     : 5/27/2021 4:35:37 PM by MARCO
                  (modified after loading)
=====
```



=====  
Area Percent Report  
=====

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
```

Signal 1: VWD1 A, Wavelength=254 nm

| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU] | Area %   |
|--------|---------------|------|-------------|-------------|--------------|----------|
| 1      | 1.553         | BB   | 0.1675      | 1.40295e4   | 1158.80127   | 100.0000 |

Totals : 1.40295e4 1158.80127

Results obtained with enhanced integrator!

=====  
\*\*\* End of Report \*\*\*

HPLC 1100 5/27/2021 5:44:56 PM MARCO

## Openlynx Report -

Sample: 5

Date: 18-Jan-2018

Vial: 1:A,6

Time: 16:39:00

File: I-0227917-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

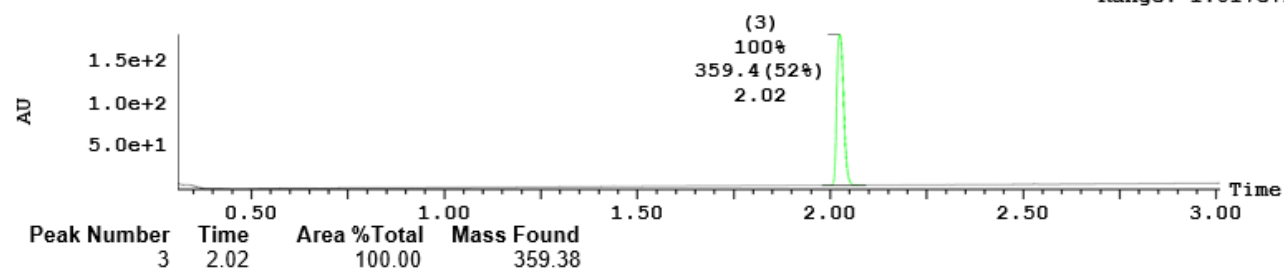
## Compound 3c

Sample 5 Vial 1:A,6 ID File I-0227917-001 Date 18-Jan-2018 Time 16:39:00 Description Met Gen

3: UV Detector: TIC

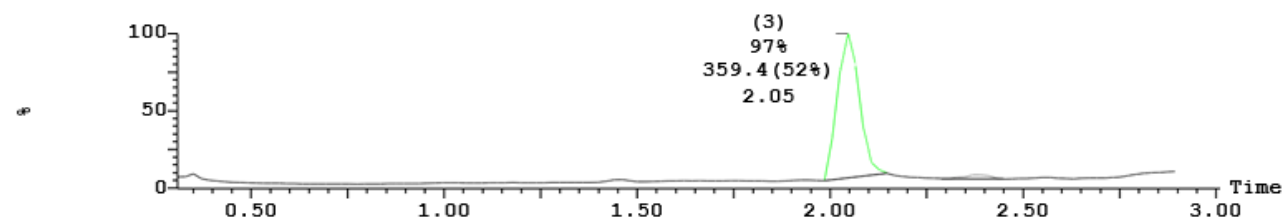
1.821e+2

Range: 1.817e+2



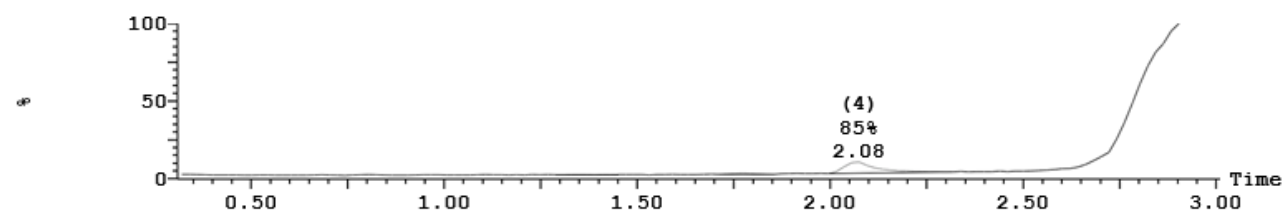
1: MS ES+ :TIC

3.3e+009



2: MS ES- :TIC

4.6e+007

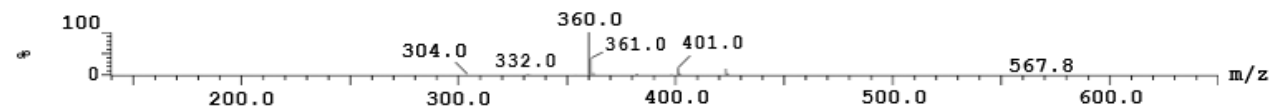


| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 2.05 | 360.38     |

3: (Time: 2.02)

1:MS ES+

5.1e+007



## Openlynx Report -

Sample: 5

Vial:1:A,6

File:I-0227917-001

Date:18-Jan-2018

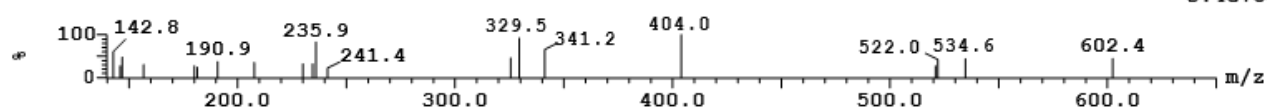
Time:16:39:00

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 3       | 2.05 |            |

3: (Time: 2.02)

2:MS ES-  
3.4e+003

## Openlynx Report -

Sample: 40

Date: 18-Jan-2018

Vial: 1:D,11

Time: 19:02:50

File: I-0227952-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

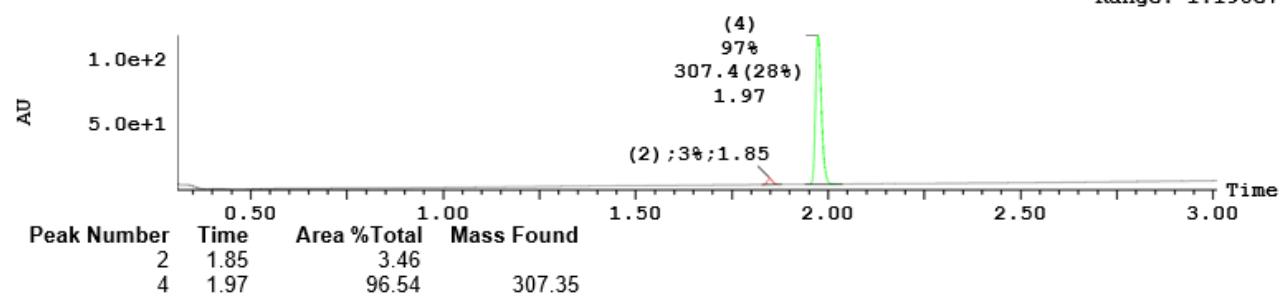
## Compound 3d

Sample 40 Vial 1:D,11 ID File I-0227952-001 Date 18-Jan-2018 Time 19:02:50 Description Met Gen

3: UV Detector: TIC

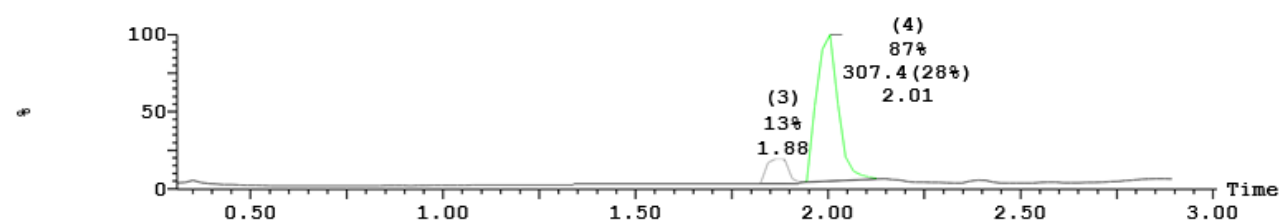
1.202e+2

Range: 1.198e+2



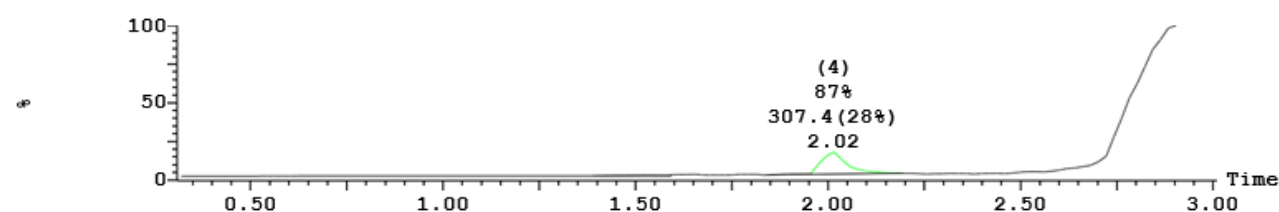
1: MS ES+ :TIC

5.2e+009



2: MS ES- :TIC

4.1e+007



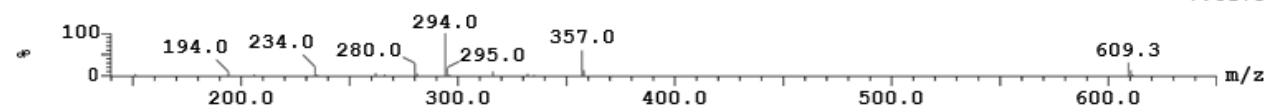
Peak ID Time Mass Found

2 1.85

2: (Time: 1.85)

1: MS ES+

7.6e+006



## Openlynx Report -

Sample: 40

Date: 18-Jan-2018

Vial: 1:D,11

Time: 19:02:50

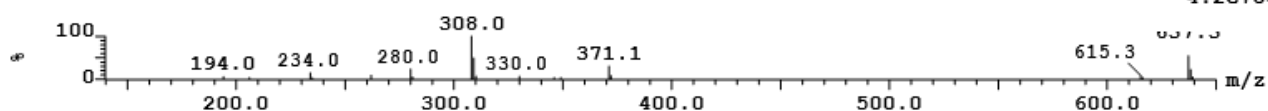
File: I-0227952-001

Printed: Fri Jan 19 09:28:55 2018

## Sample Report (continued):

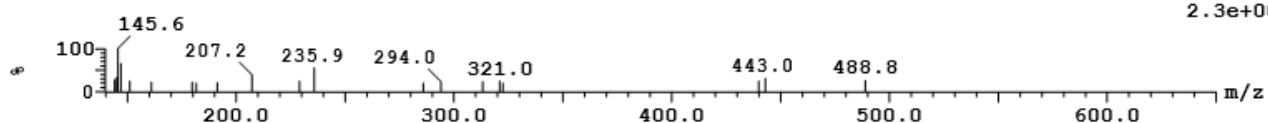
| Peak ID | Time | Mass Found |
|---------|------|------------|
| 4       | 2.01 | 308.35     |

4: (Time: 1.97)

1: MS ES+  
4.2e+007

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 2       | 1.85 |            |

2: (Time: 1.85)

2: MS ES-  
2.3e+003

| Peak ID | Time | Mass Found |
|---------|------|------------|
| 4       | 2.01 |            |

4: (Time: 1.97)

2: MS ES-  
2.5e+003