

## Supplementary Material

### Synthesis of pyrazolo[1,5-*a*]pyrimidine ring as a possible bioisosteric replacement of the 5-(1*H*-pyrrol-1-yl)pyrazole scaffold

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Openlynx Report -

Sample: 43  
Date:09-Jan-2018

Vial:1:E,4  
Time:14:48:35

File:I-0226555-001

Printed: Mon Jan 15 12:57:57 2018

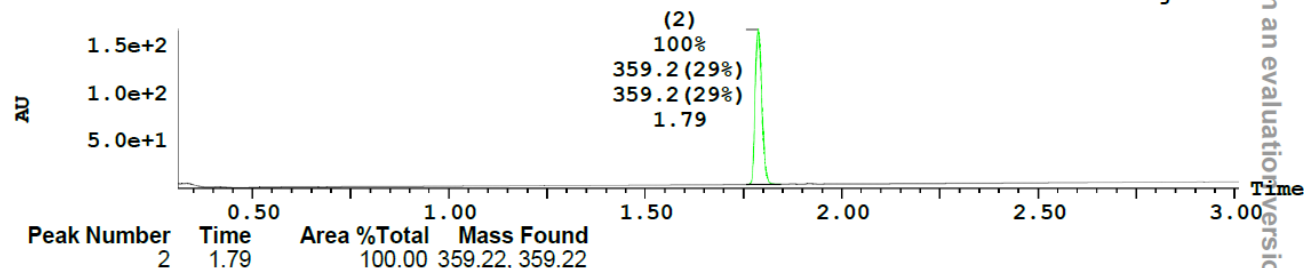
Sample Report (continued):

**Compound 2a**

Sample 43 Vial 1:E,4 ID File I-0226555-001 Date 09-Jan-2018 Time 14:48:35 Description Met Gen

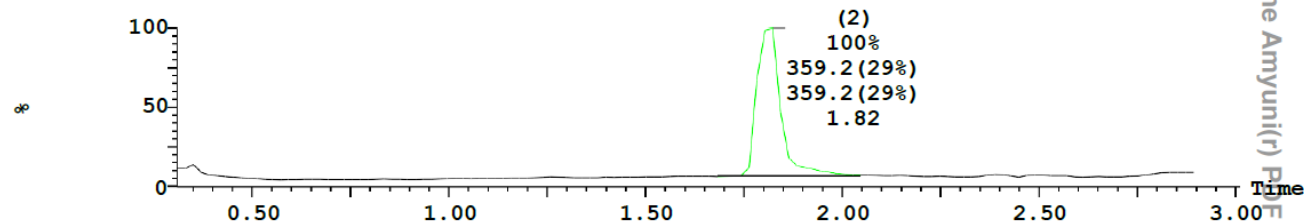
3: UV Detector: TIC

1.684e+2  
Range: 1.679e+2



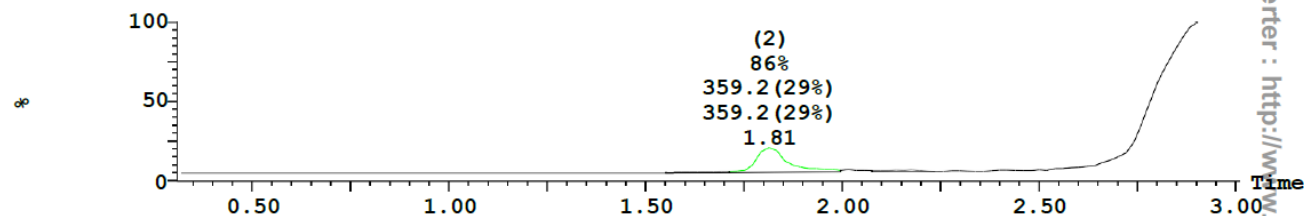
1: MS ES+ :TIC

3.1e+009



2: MS ES- :TIC

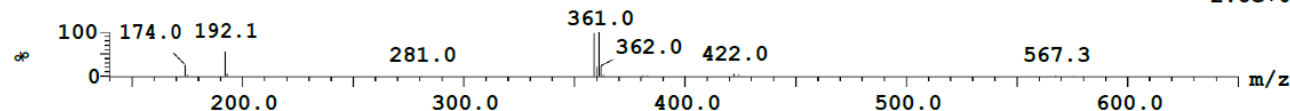
3.5e+007



Peak ID	Time	Mass Found
2	1.82	360.22

2: (Time: 1.79)

1:MS ES+  
2.8e+007



This file was generated in an evaluation version of the Amyuni(r) PDF Converter : http://www.amyuni.com

Openlynx Report -

Sample: 43  
Date:09-Jan-2018

Vial:1:E.4  
Time:14:48:35

File:I-0226555-001

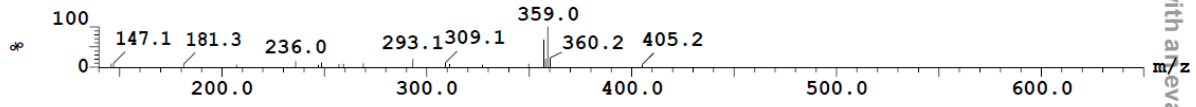
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Sample Report (continued):

Peak ID	Time	Mass Found
2	1.82	358.22

2: (Time: 1.79)



This file was generated with a Hewlett-Packard 1100 series GC/MSD.

Openlynx Report -

Sample: 44  
Date: 09-Jan-2018

Vial: 1:E,5  
Time: 14:52:39

File: I-0226556-001

Printed: Mon Jan 15 12:57:57 2018

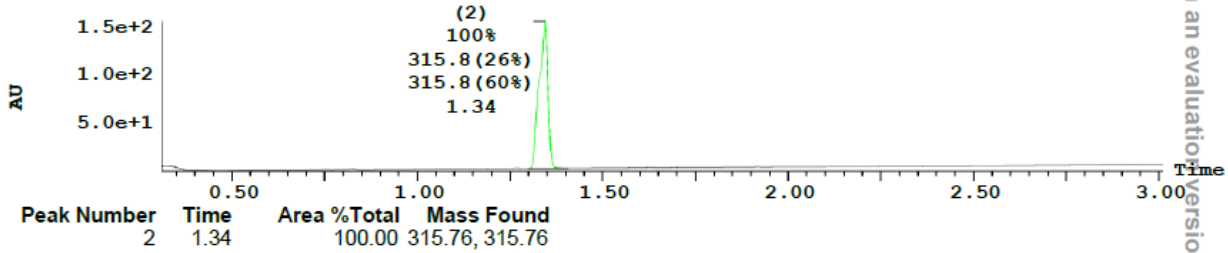
Sample Report (continued):

**Compound 2b**

Sample 44 Vial 1:E,5 ID File I-0226556-001 Date 09-Jan-2018 Time 14:52:39 Description Met Gen

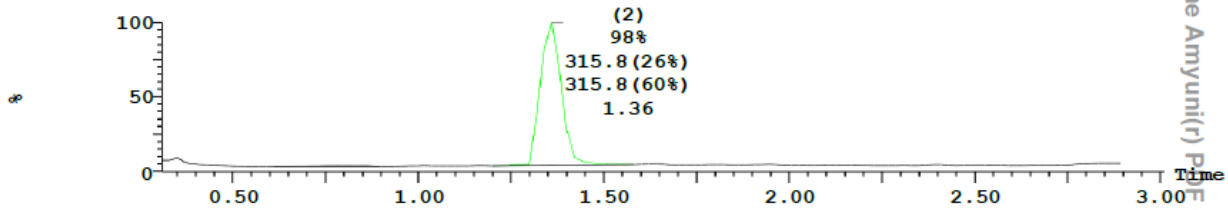
3: UV Detector: TIC

1.552e+2  
Range: 1.546e+2



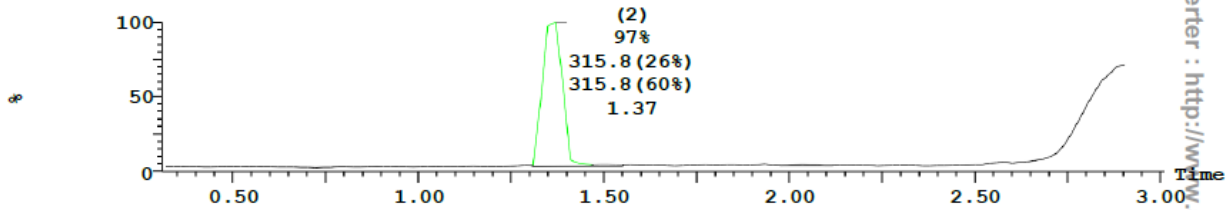
1: MS ES+ :TIC

4.8e+009



2: MS ES- :TIC

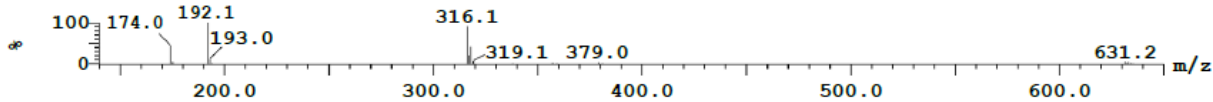
4.7e+007



Peak ID	Time	Mass Found
2	1.36	316.76

2: (Time: 1.34)

1:MS ES+  
4.4e+007



Openlynx Report -

Sample: 44  
Date: 09-Jan-2018

Vial: 1:E,5  
Time: 14:52:39

File: I-0226556-001

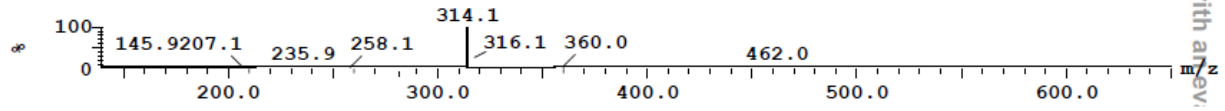
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Sample Report (continued):

Peak ID	Time	Mass Found
2	1.36	314.76

2: (Time: 1.34)



Openlynx Report -

Sample: 46  
Date:09-Jan-2018

Vial:1:E,7  
Time:15:00:50

File:I-0226558-001

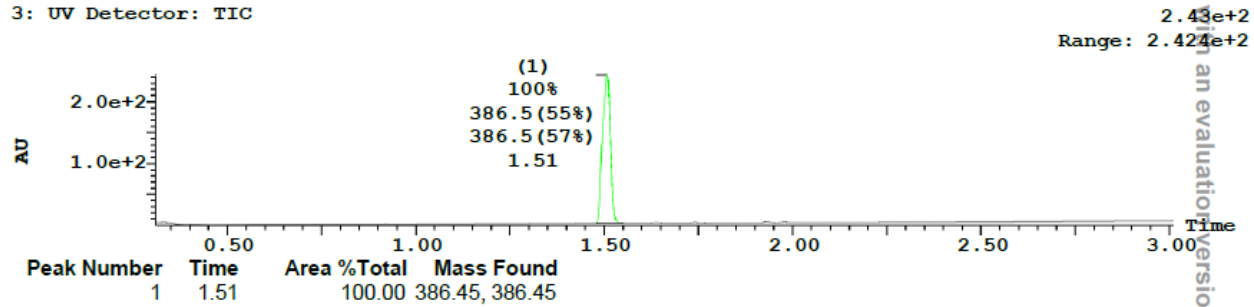
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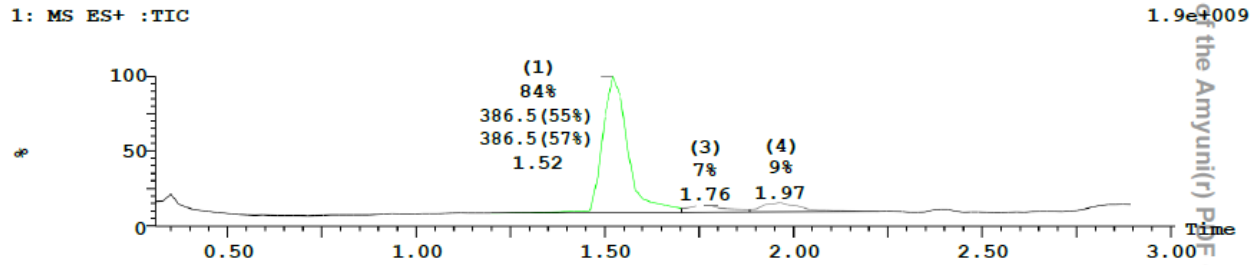
**Compound 2c**

Sample 46 Vial 1:E,7 ID File I-0226558-001 Date 09-Jan-2018 Time 15:00:50 Description Met Gen

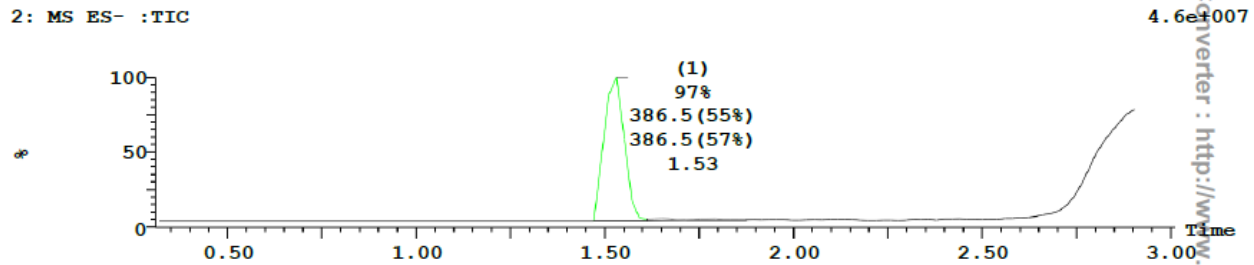
3: UV Detector: TIC



1: MS ES+ :TIC

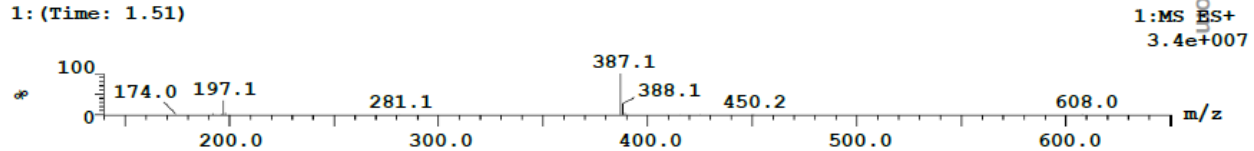


2: MS ES- :TIC



Peak ID	Time	Mass Found
1	1.52	387.45

1: (Time: 1.51)



Openlynx Report -

Sample: 46  
Date: 09-Jan-2018

Vial: 1:E,7  
Time: 15:00:50

File: I-0226558-001

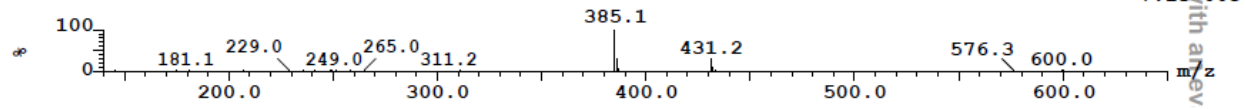
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Sample Report (continued):

Peak ID	Time	Mass Found
1	1.52	385.45

1: (Time: 1.51)



Openlynx Report -

Sample: 45  
Date: 10-Jan-2018

Vial: 1:E,6  
Time: 16:28:09

File: I-0226557-001\_

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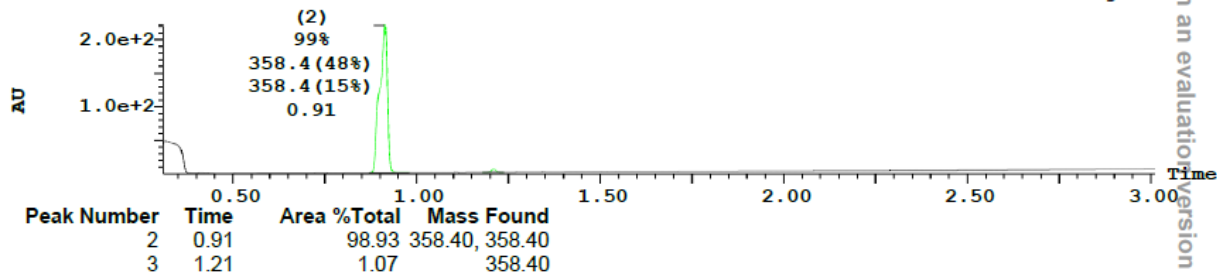
Sample Report (continued):

**Compound 2d**

Sample 45 Vial 1:E,6 ID File I-0226557-001\_ Date 10-Jan-2018 Time 16:28:09 Description Met Gen

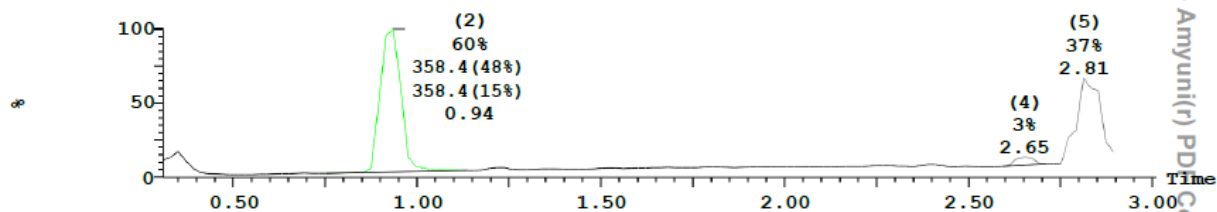
3: UV Detector: TIC

2.207e+2  
Range: 2.2e+2



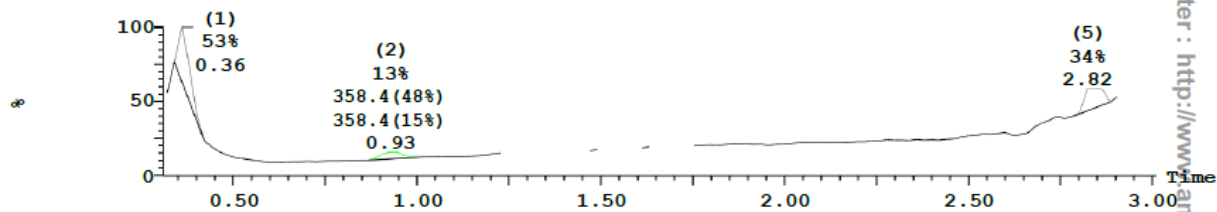
1: MS ES+ :TIC

2.9e+009



2: MS ES- :TIC

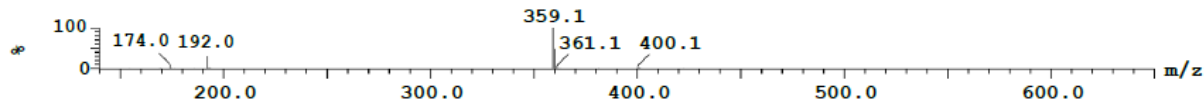
3.3e+008



Peak ID	Time	Mass Found
2	0.94	359.40

2: (Time: 0.91)

1: MS ES+  
4.5e+007





Openlynx Report -

Sample: 45  
Date: 10-Jan-2018

Vial: 1:E,6  
Time: 16:28:09

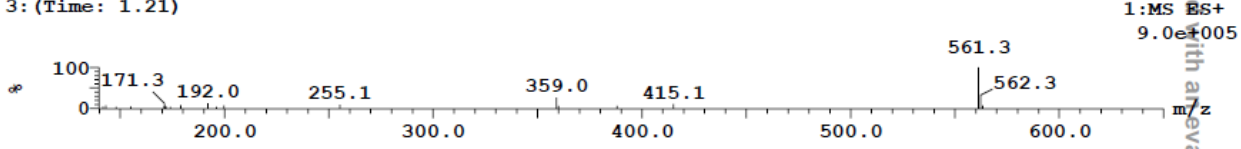
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Printed: Mon Jan 15 12:57:57 2018

Sample Report (continued):

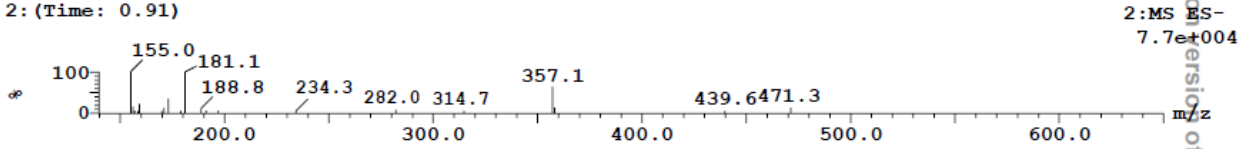
Peak ID	Time	Mass Found
3	1.21	359.40

3: (Time: 1.21)



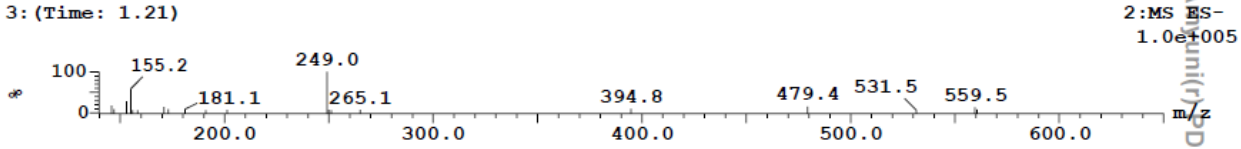
Peak ID	Time	Mass Found
2	0.94	357.40

2: (Time: 0.91)



Peak ID	Time	Mass Found
3	1.21	

3: (Time: 1.21)



This file was generated with a new version of the Analytic (v.10.1)

Openlynx Report -

Sample: 47

Date:09-Jan-2018

Vial:1:E,8

Time:15:04:56

File:I-0226559-001

Printed: Mon Jan 15 12:57:57 2018

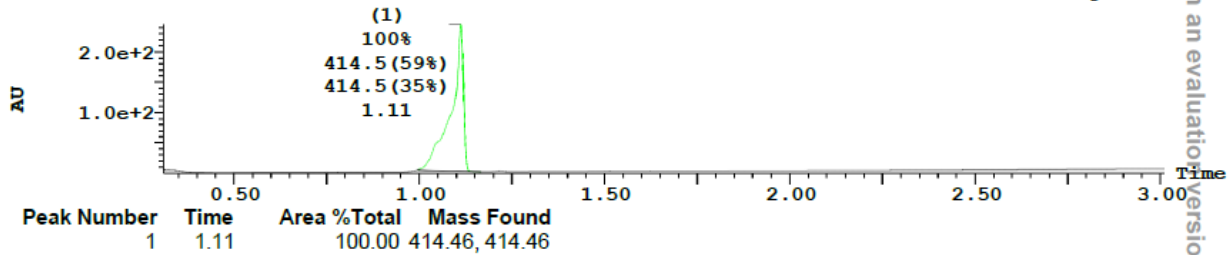
Sample Report (continued):

Compound 2e

Sample 47 Vial 1:E,8 ID File I-0226559-001 Date 09-Jan-2018 Time 15:04:56 Description Met Gen

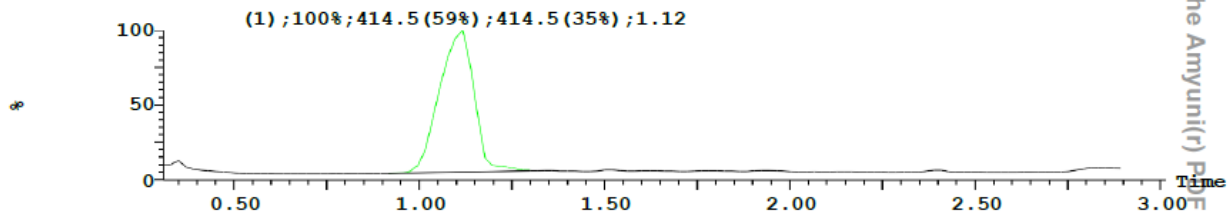
3: UV Detector: TIC

2.463e+2  
Range: 2.458e+2



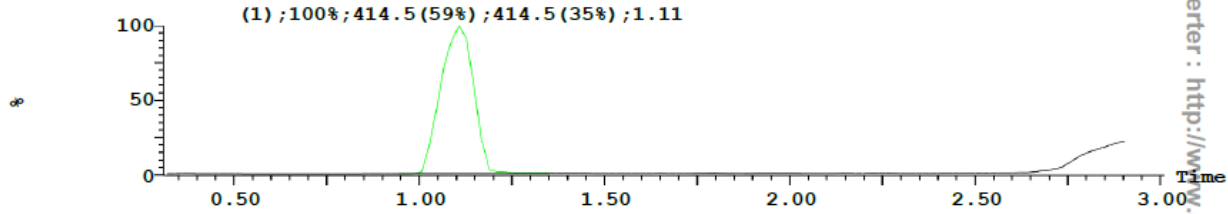
1: MS ES+ :TIC

3.5e+009



2: MS ES- :TIC

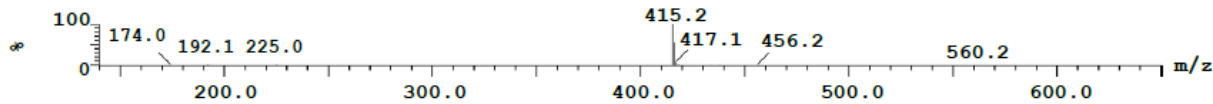
1.6e+008



Peak ID	Time	Mass Found
1	1.12	415.46

1: (Time: 1.11)

1:MS ES+  
1.0e+008



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Openlynx Report -

Sample: 47  
Date: 09-Jan-2018

Vial: 1:E,8  
Time: 15:04:56

File: I-0226559-001

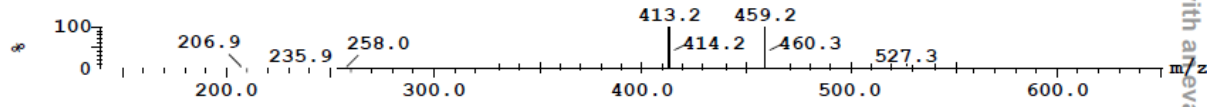
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Printed: Mon Jan 15 12:57:57 2018

Sample Report (continued):

Peak ID	Time	Mass Found
1	1.12	413.46

1: (Time: 1.11)



2:MS ES-  
2.2e+006

This file was generated with anova

Openlynx Report -

Sample: 31  
Date: 18-Jan-2018

Vial: 1:D,2  
Time: 18:25:54

File: I-0227943-001

Printed: Fri Jan 19 09:28:55 2018

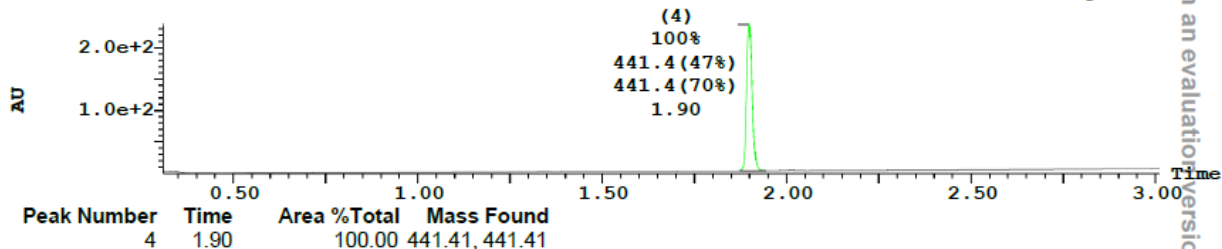
Sample Report (continued):

**Compound 2f**

Sample 31 Vial 1:D,2 ID File I-0227943-001 Date 18-Jan-2018 Time 18:25:54 Description Met Gen

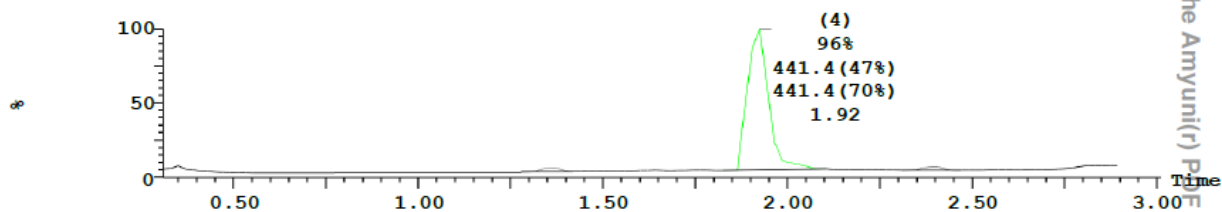
3: UV Detector: TIC

2.36e+2  
Range: 2.36e+2



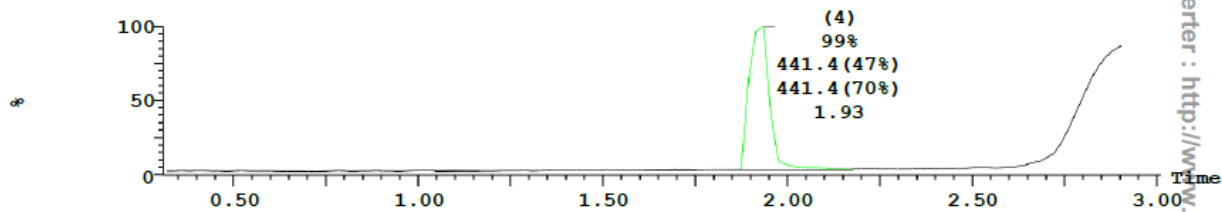
1: MS ES+ :TIC

3.7e+009



2: MS ES- :TIC

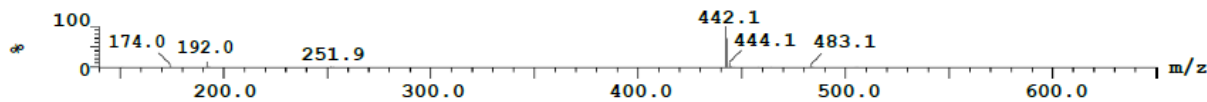
4.9e+007



Peak ID	Time	Mass Found
4	1.92	442.41

4: (Time: 1.90)

1:MS ES+  
5.4e+007



This file was generated by an evaluation version of the Amyuni(r) PDF Converter : http://www.amyuni.com

Openlynx Report -

Sample: 31  
Date: 18-Jan-2018

Vial: 1:D,2  
Time: 18:25:54

File: I-0227943-001

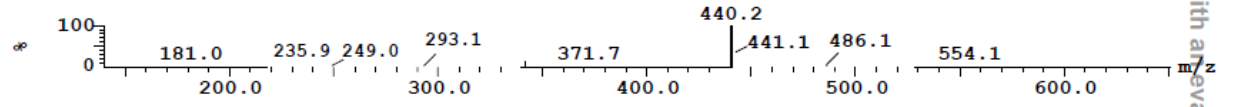
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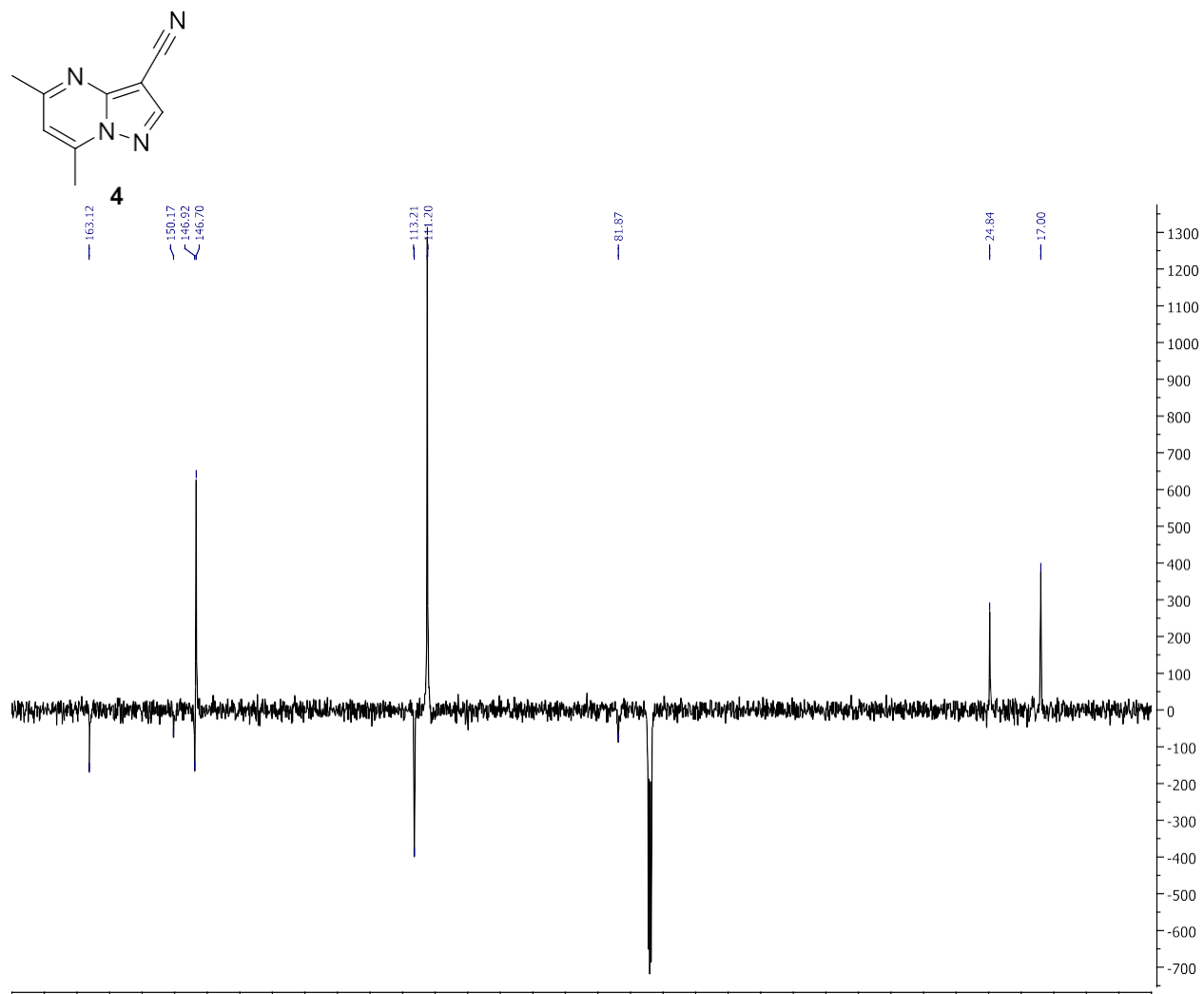
Printed: Fri Jan 19 09:28:55 2018

Sample Report (continued):

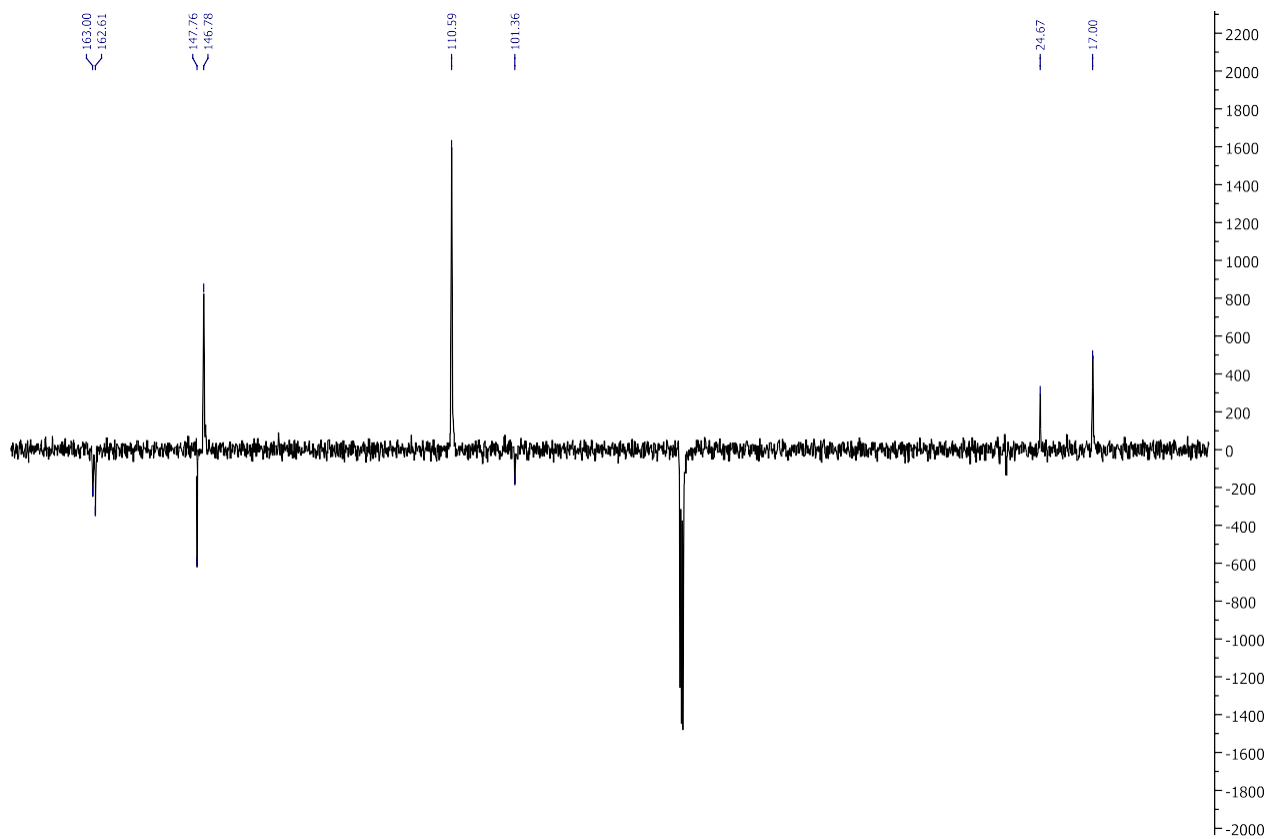
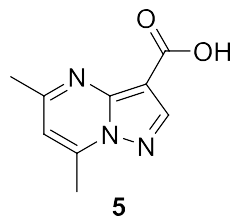
Peak ID	Time	Mass Found
4	1.92	440.41

4: (Time: 1.90)

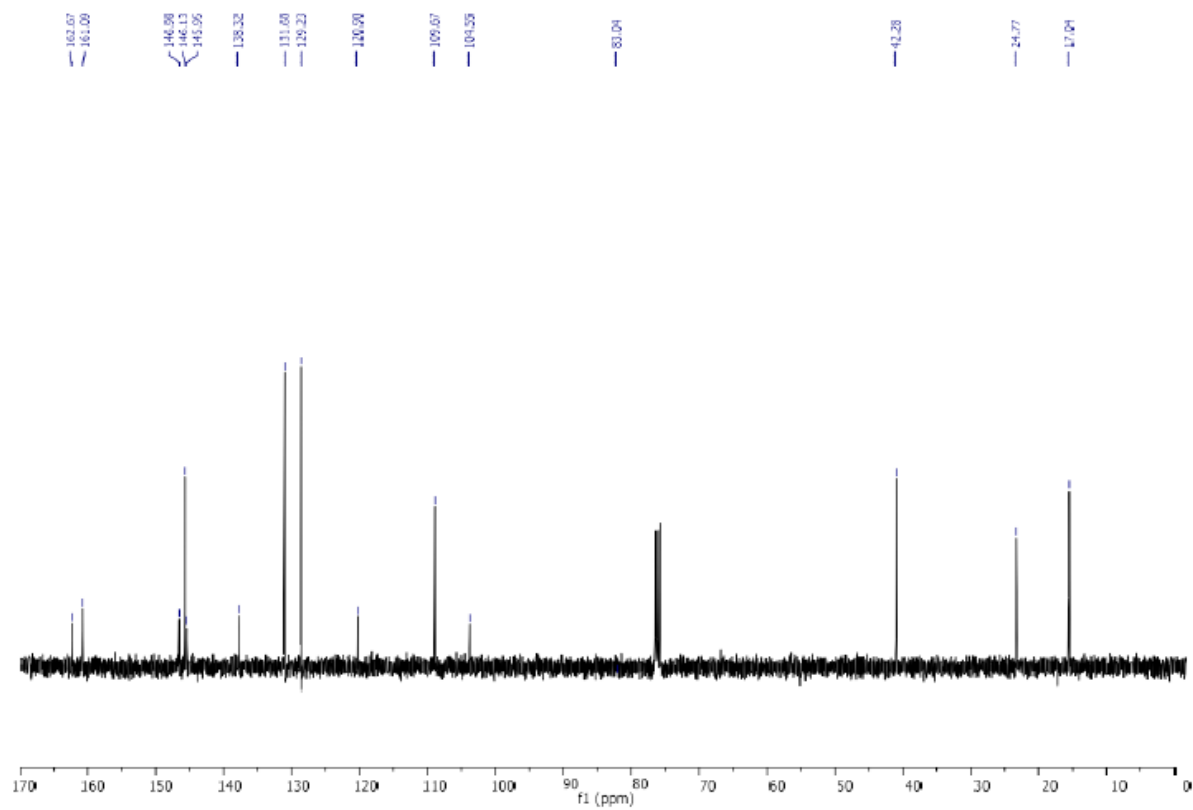
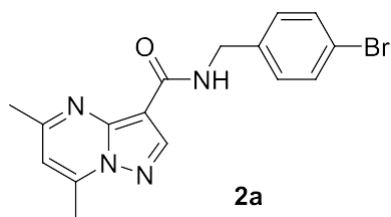




<sup>13</sup>C DEPT (CDCl<sub>3</sub>, 600 MHz) of compound **4**.

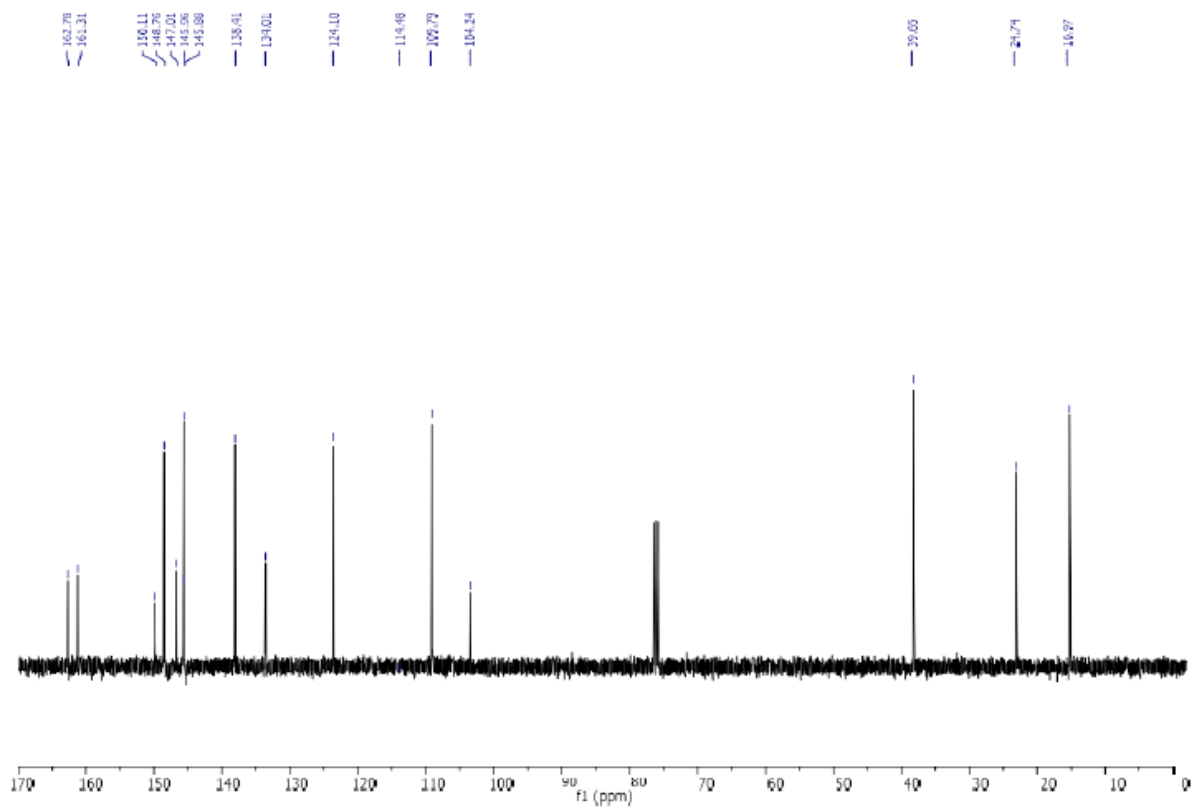
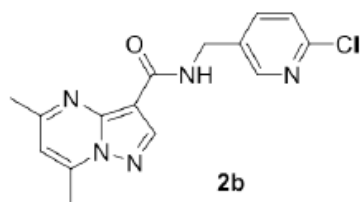


$^{13}\text{C}$  DEPT ( $\text{CDCl}_3$ , 600 MHz) of compound 5.

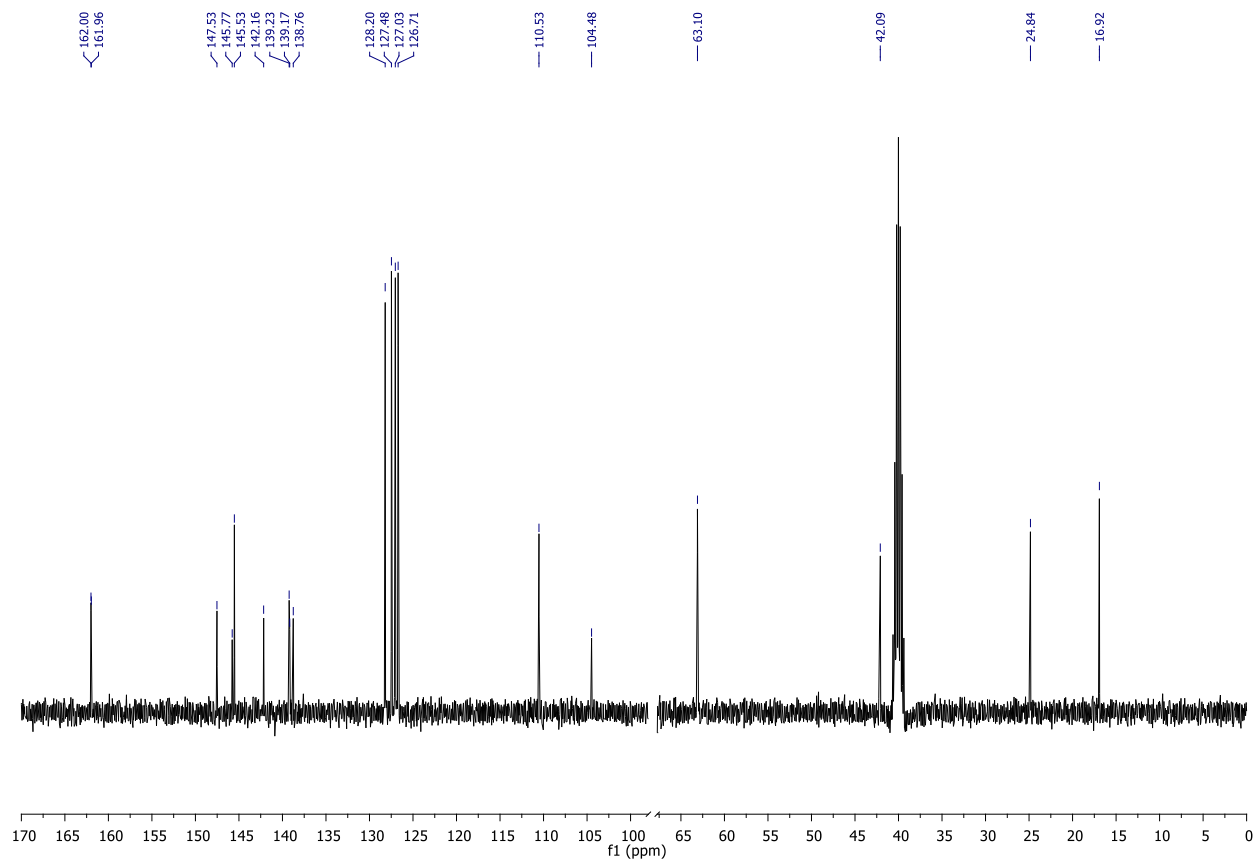
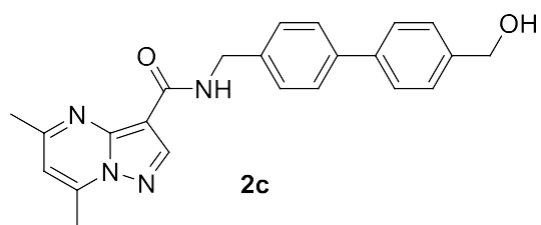


<sup>13</sup>C NMR (CDCl<sub>3</sub>, 400 MHz) of compound **2a**.

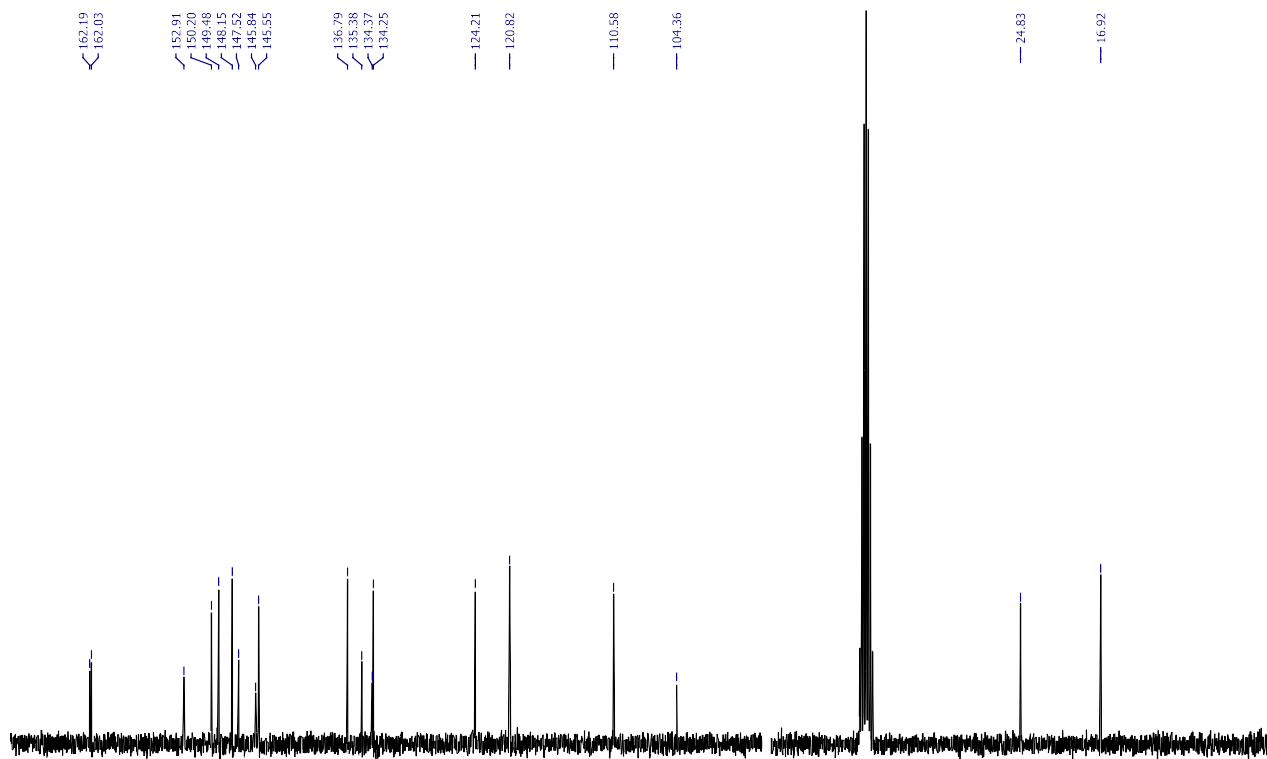
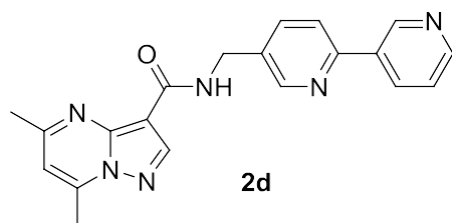




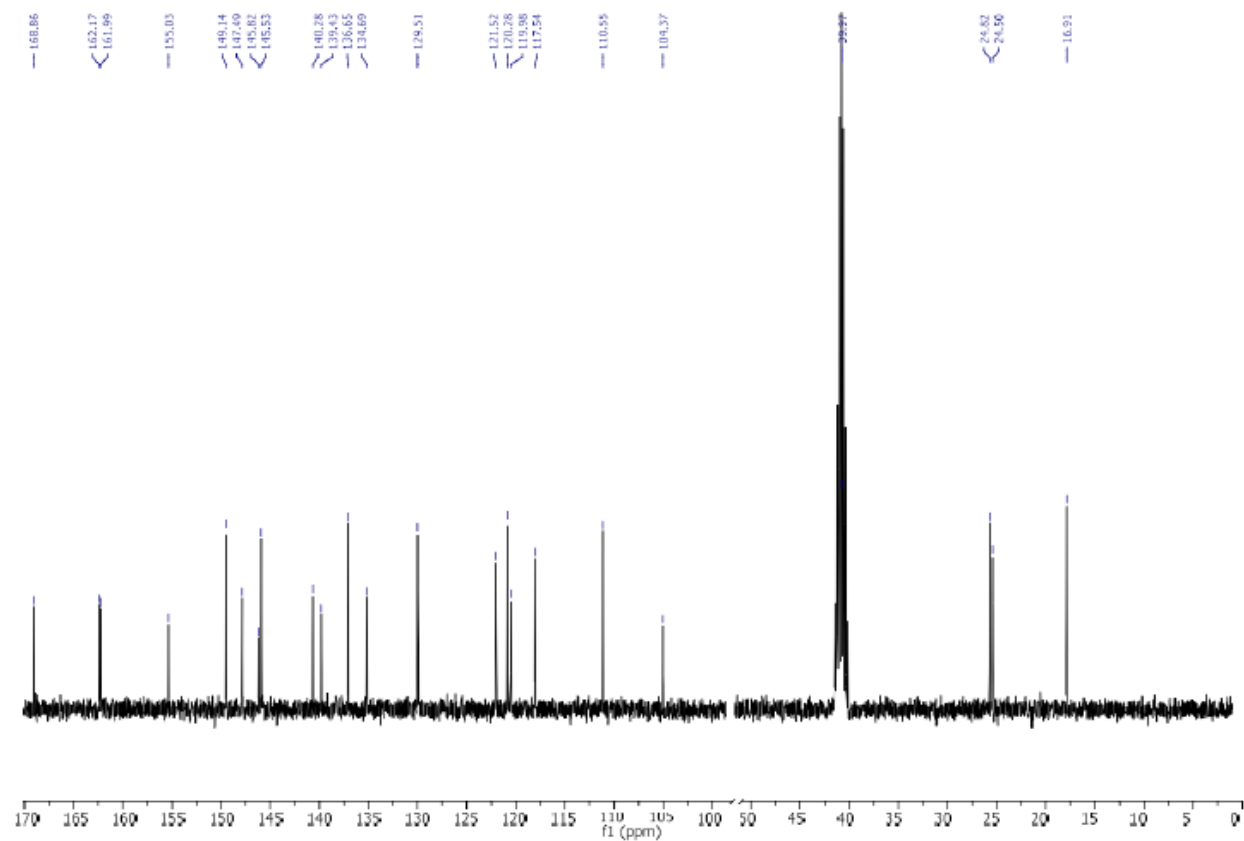
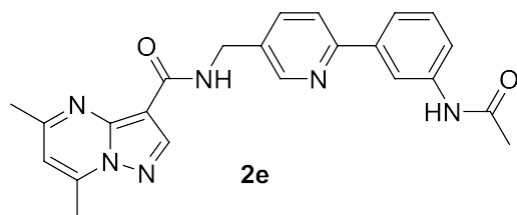
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 400 MHz) of compound **2b**



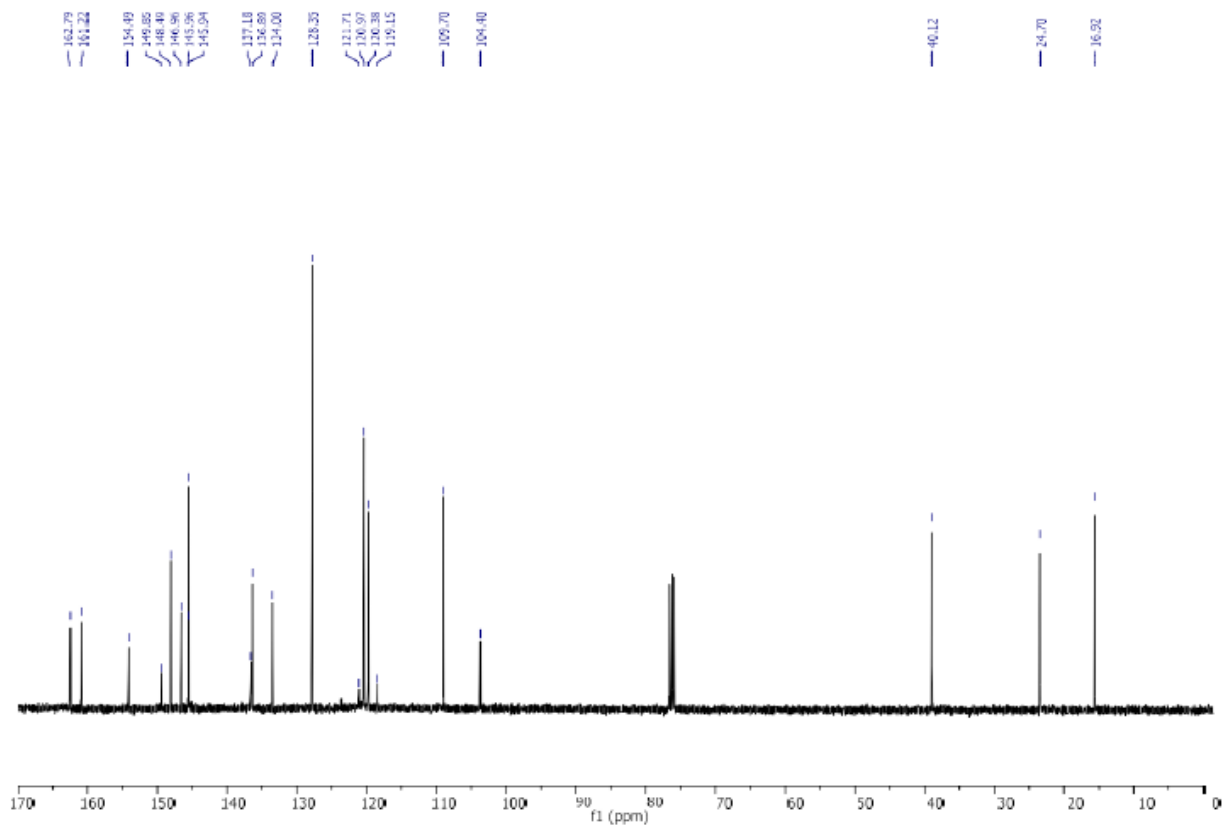
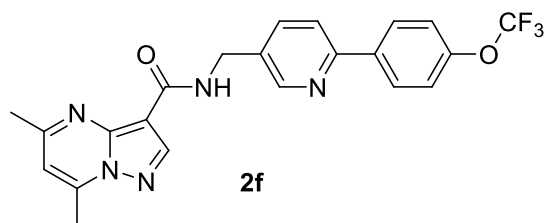
<sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 400 MHz) of compound **2c**.



<sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 400 MHz) of compound **2d**.



<sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 400 MHz) of compound **2e**.



<sup>13</sup>C NMR (CDCl<sub>3</sub>, 400 MHz) of compound **2f**.