

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

Claudia Mugnaini, Livia Pasculini, Carlotta Pagli, Antonella Brizzi, Marco Paolino, Beatrice Gianibbi, and Federico Corelli*

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

Email: federico.corelli@unisi.it

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HPLC/MS traces for compounds **2a-f**

Compound 2a	S2
Compound 2b	S4
Compound 2c	S6
Compound 2d	S8
Compound 2e	S10
Compound 2f	S12

¹³C NMR spectra of compounds **4,5** and **2a-f**

Compound 4	S14
Compound 5	S15
Compound 2a	S16
Compound 2b	S17
Compound 2c	S18
Compound 2d	S19
Compound 2e	S20
Compound 2f	S21

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

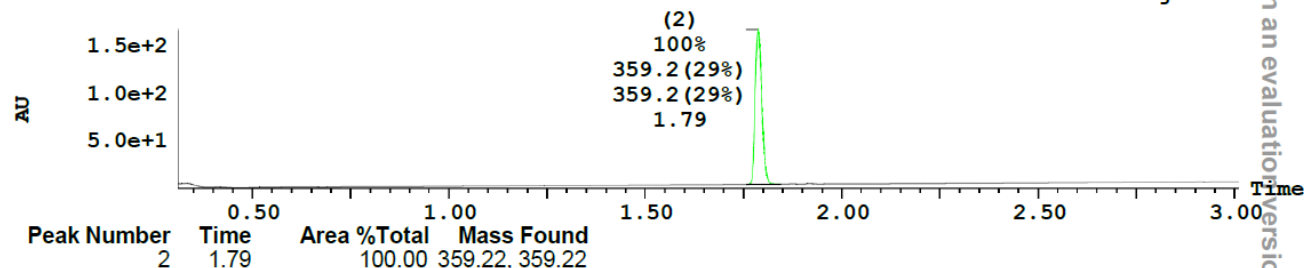
Sample Report (continued):

Compound 2a

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

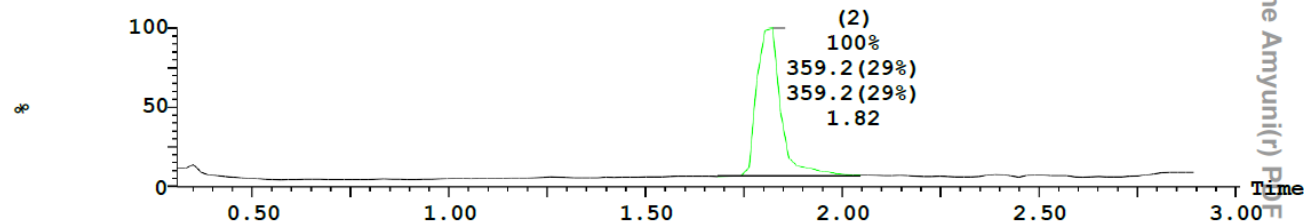
3: UV Detector: TIC

1.684e+2
Range: 1.679e+2



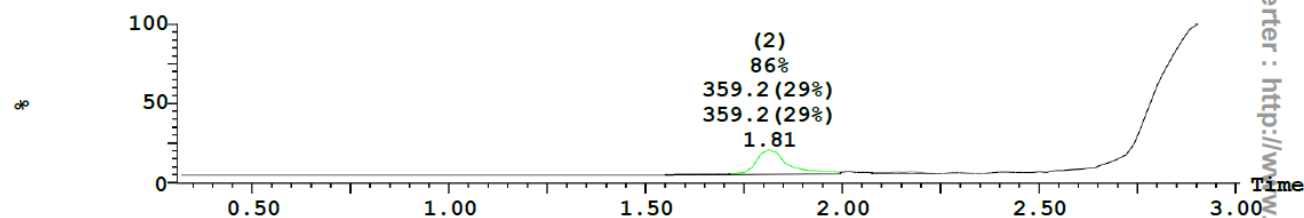
1: MS ES+ :TIC

3.1e+009



2: MS ES- :TIC

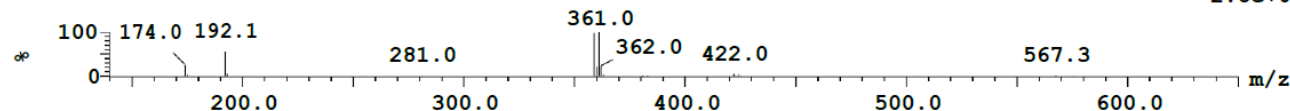
3.5e+007



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) P/F 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

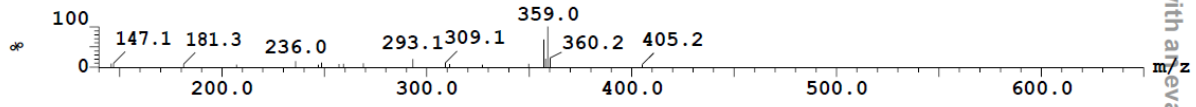
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Sample Report (continued):

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

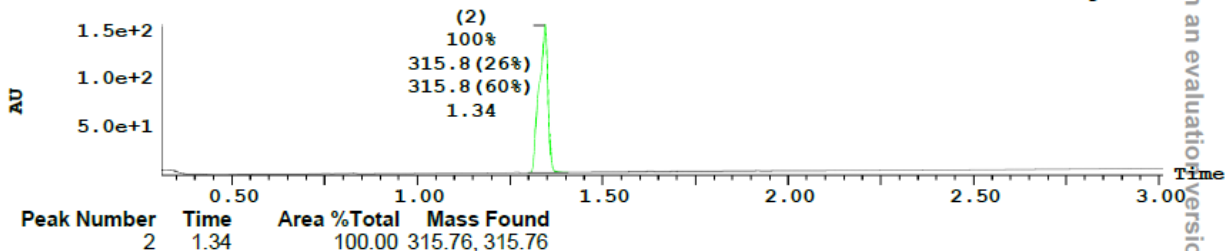
Sample Report (continued):

Compound 2b

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

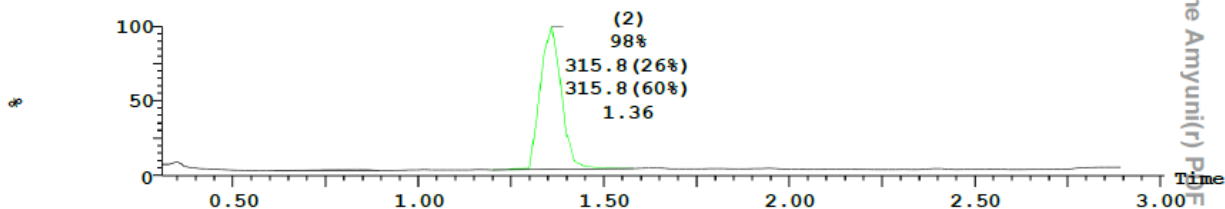
3: UV Detector: TIC

1.552e+2
Range: 1.546e+2



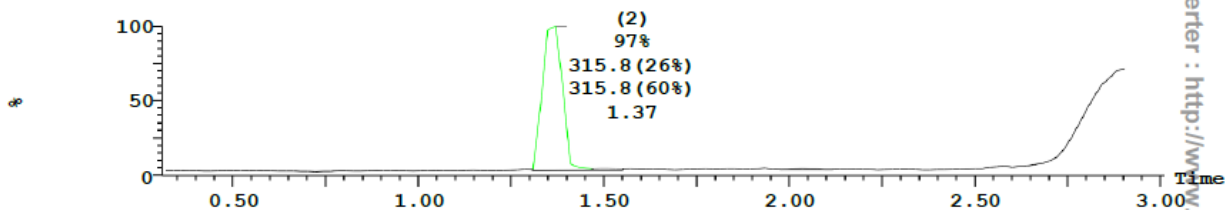
1: MS ES+ :TIC

4.8e+009



2: MS ES- :TIC

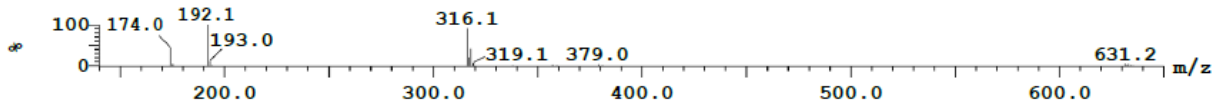
4.7e+007



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

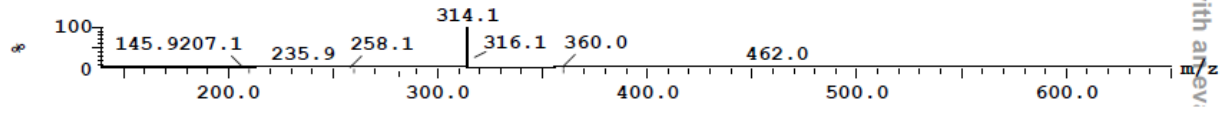
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Sample Report (continued):

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

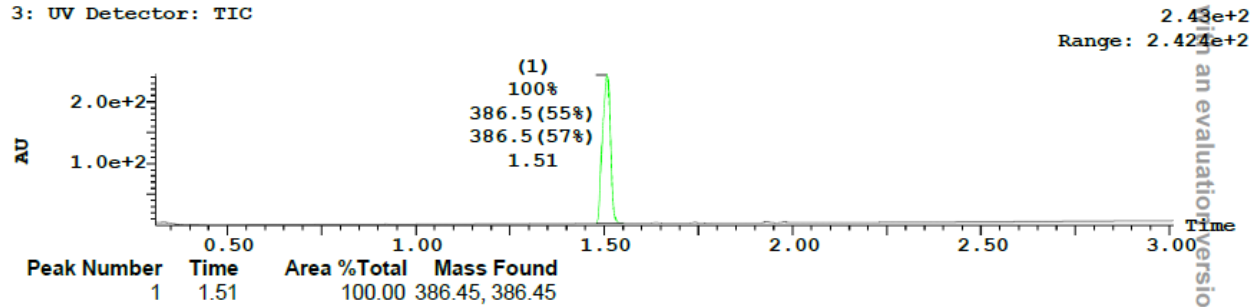
Printed: Mon Jan 15 12:57:57 2018

Sample Report (continued):

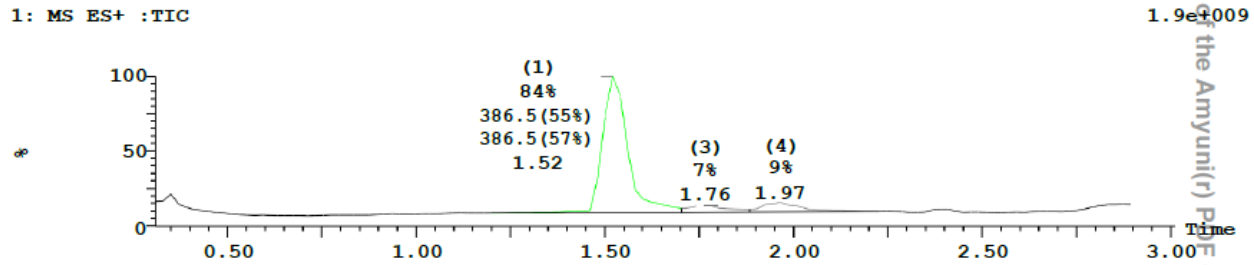
Compound 2c

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

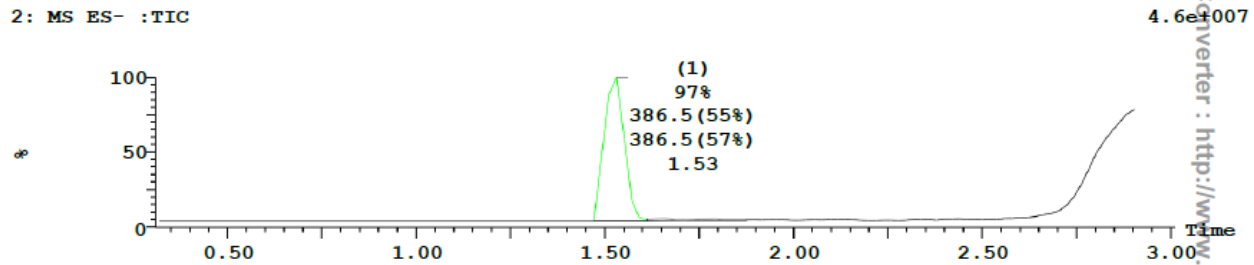
3: UV Detector: TIC



1: MS ES+ :TIC

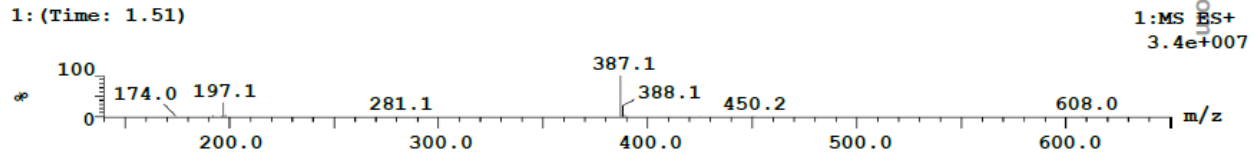


2: MS ES- :TIC



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

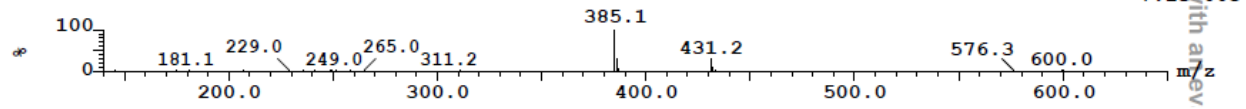
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Sample Report (continued):

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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Printed: Mon Jan 15 12:57:57 2018

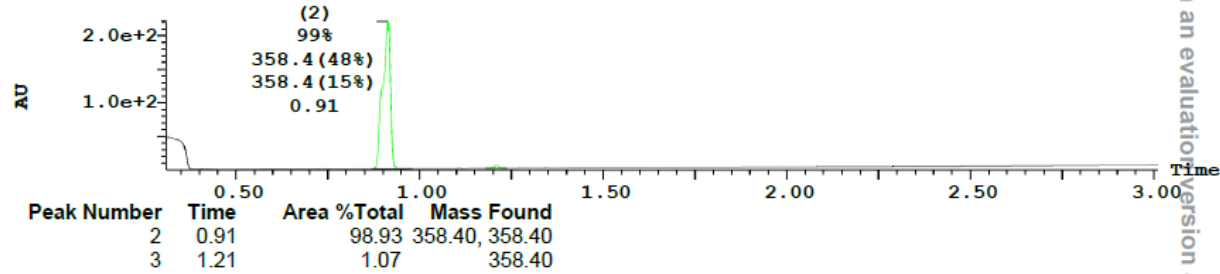
Sample Report (continued):

Compound 2d

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

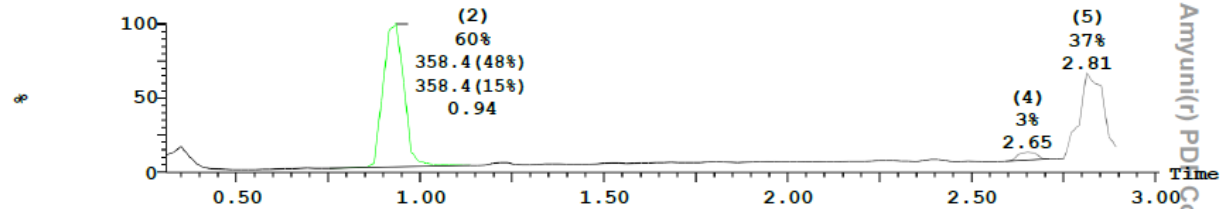
3: UV Detector: TIC

2.207e+2
Range: 2.2e+2



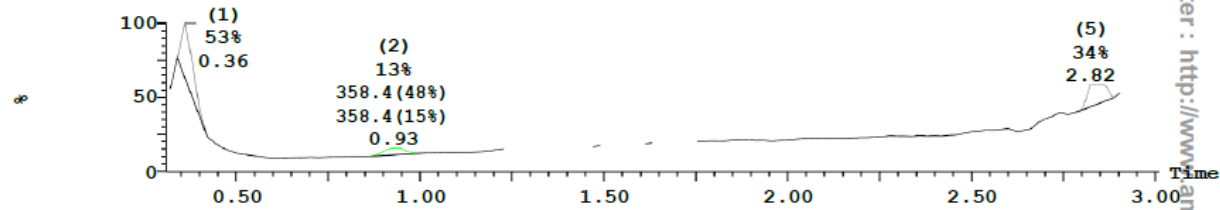
1: MS ES+ :TIC

2.9e+009



2: MS ES- :TIC

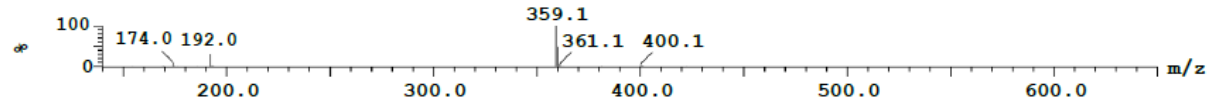
3.3e+008



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

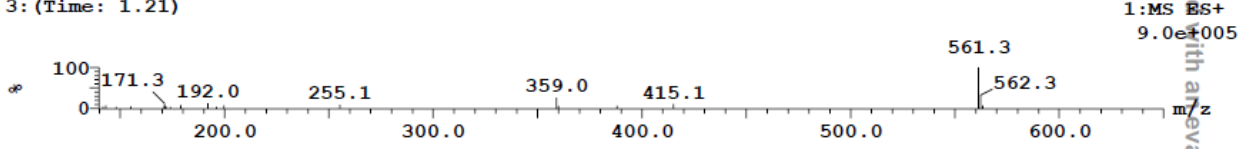
File: I-0226557-001_

Printed: Mon Jan 15 12:57:57 2018

Sample Report (continued):

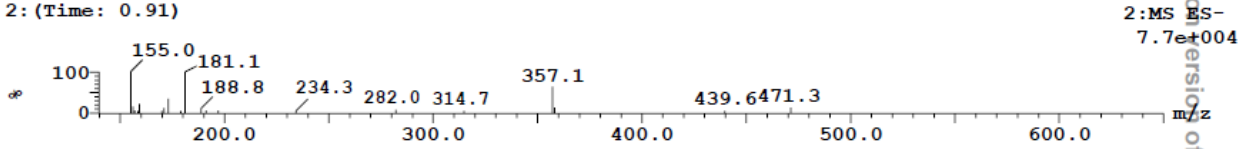
Peak ID	Time	Mass Found
3	1.21	359.40

3: (Time: 1.21)



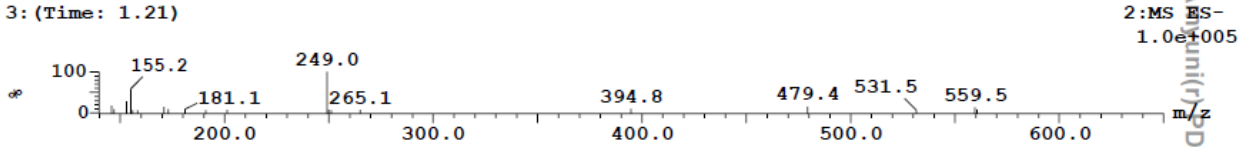
Peak ID	Time	Mass Found
2	0.94	357.40

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.1.0)

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

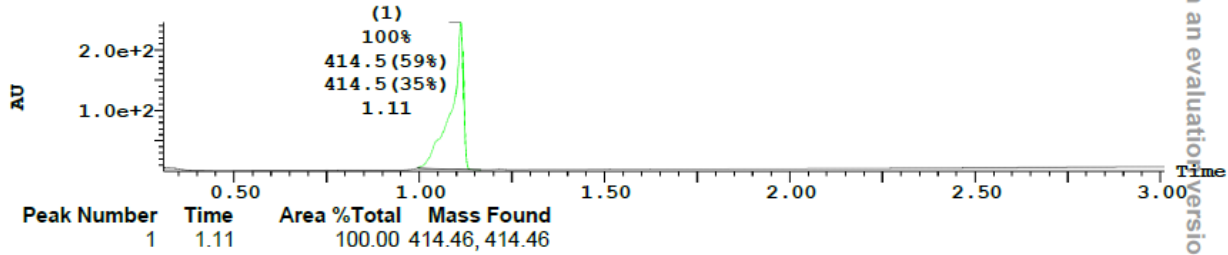
Sample Report (continued):

Compound 2e

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

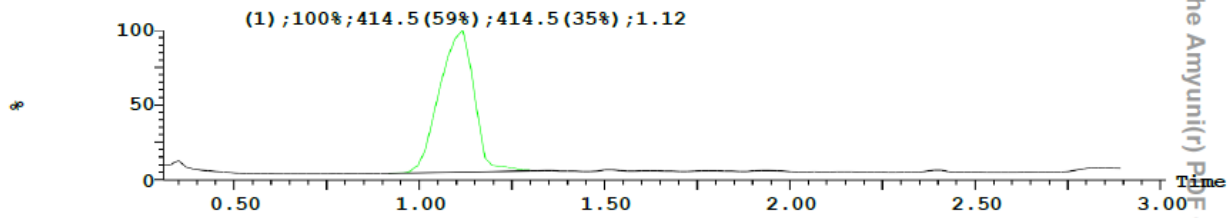
3: UV Detector: TIC

2.463e+2
Range: 2.458e+2



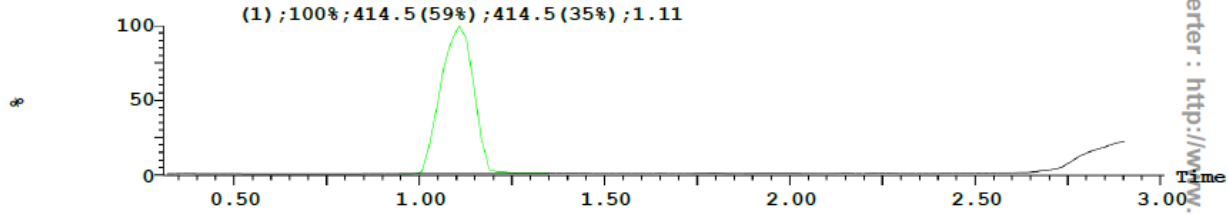
1: MS ES+ :TIC

3.5e+009



2: MS ES- :TIC

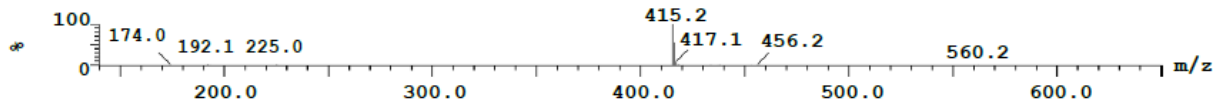
1.6e+008



Peak ID	Time	Mass Found
1	1.12	415.46

1: (Time: 1.11)

1:MS ES+
1.0e+008



Openlynx Report -

Sample: 47
Date: 09-Jan-2018

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

File: I-0226559-001

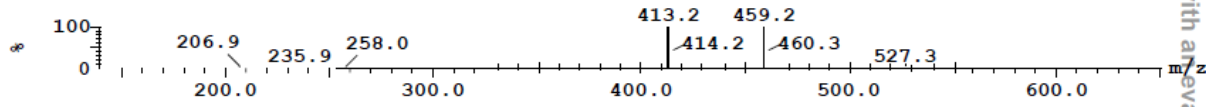
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Sample Report (continued):

Peak ID	Time	Mass Found
1	1.12	413.46

1: (Time: 1.11)



Openlynx Report -

Sample: 31
Date: 18-Jan-2018

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

File: I-0227943-001

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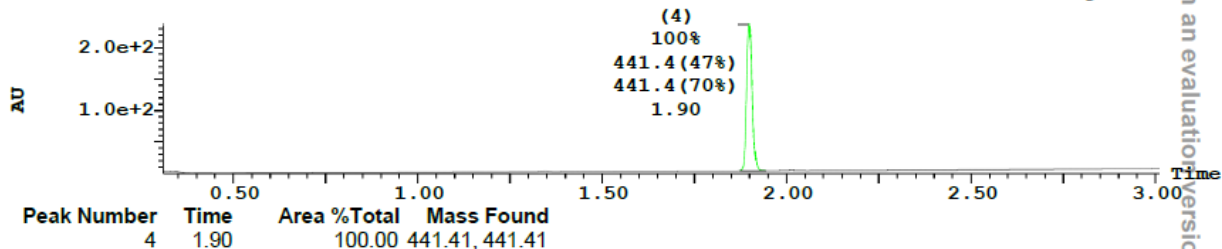
Sample Report (continued):

Compound 2f

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

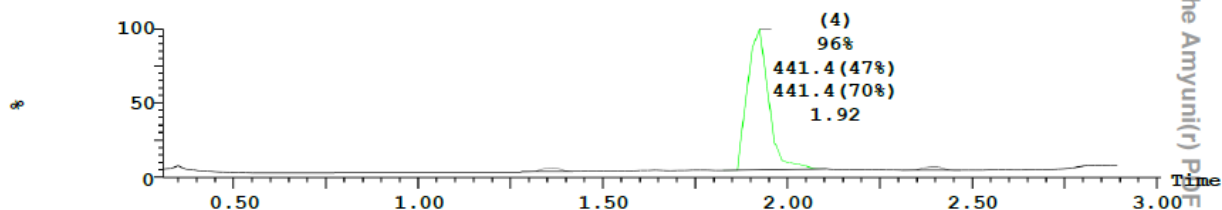
3: UV Detector: TIC

2.36e+2
Range: 2.36e+2



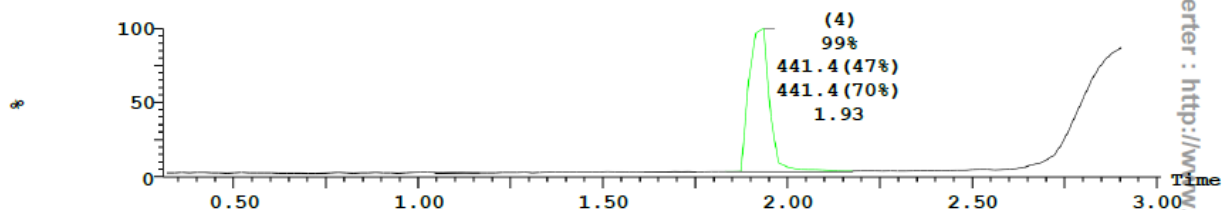
1: MS ES+ :TIC

3.7e+009



2: MS ES- :TIC

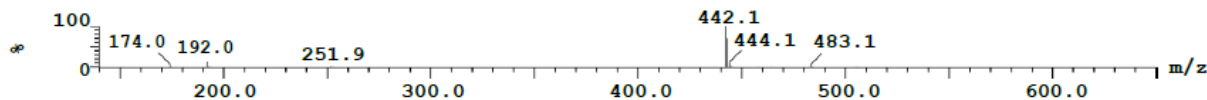
4.9e+007



Peak ID	Time	Mass Found
4	1.92	442.41

4: (Time: 1.90)

1:MS ES+
5.4e+007



Openlynx Report -

Sample: 31
Date: 18-Jan-2018

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

File: I-0227943-001

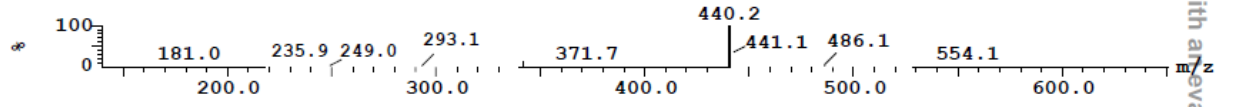
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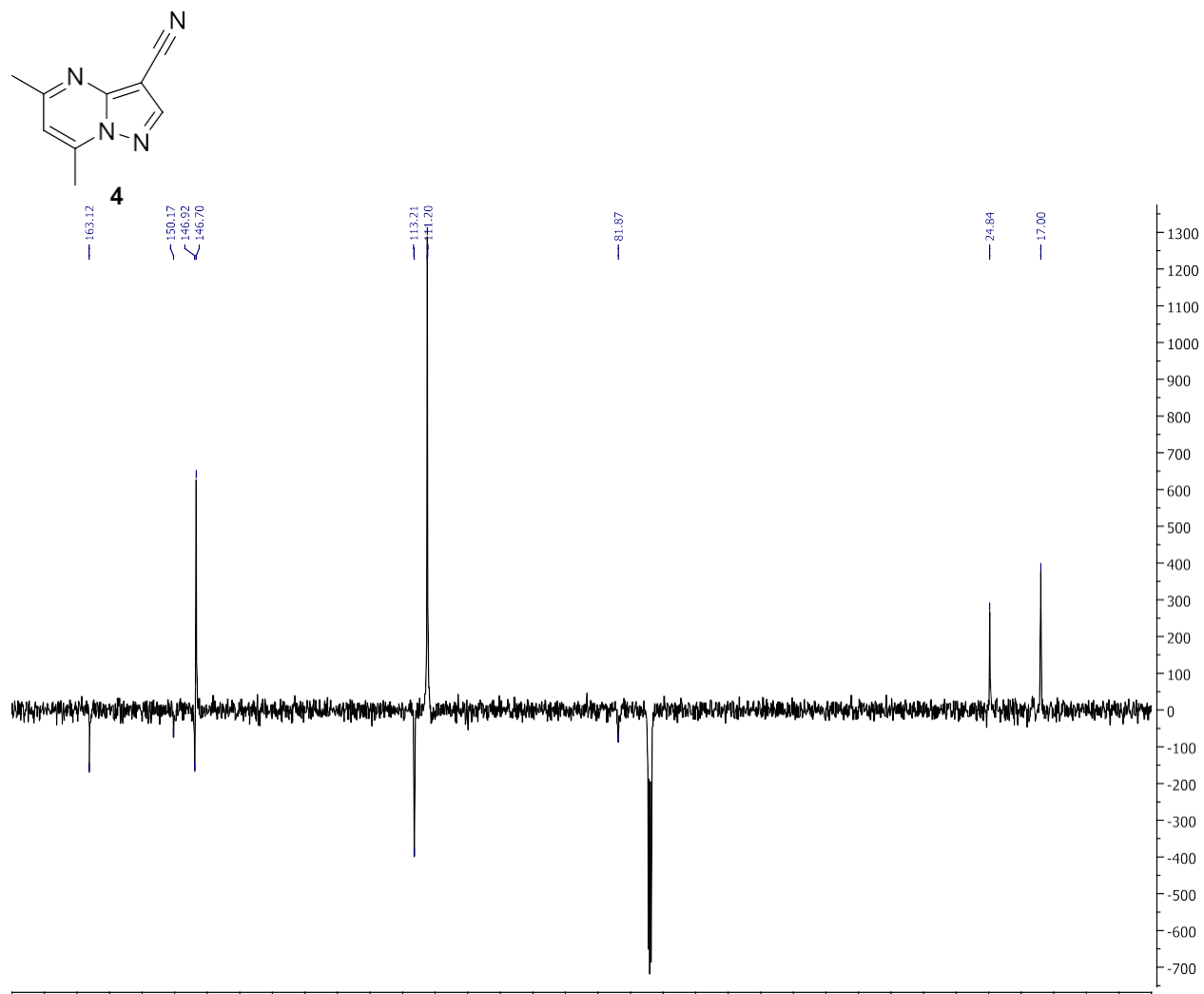
Printed: Fri Jan 19 09:28:55 2018

Sample Report (continued):

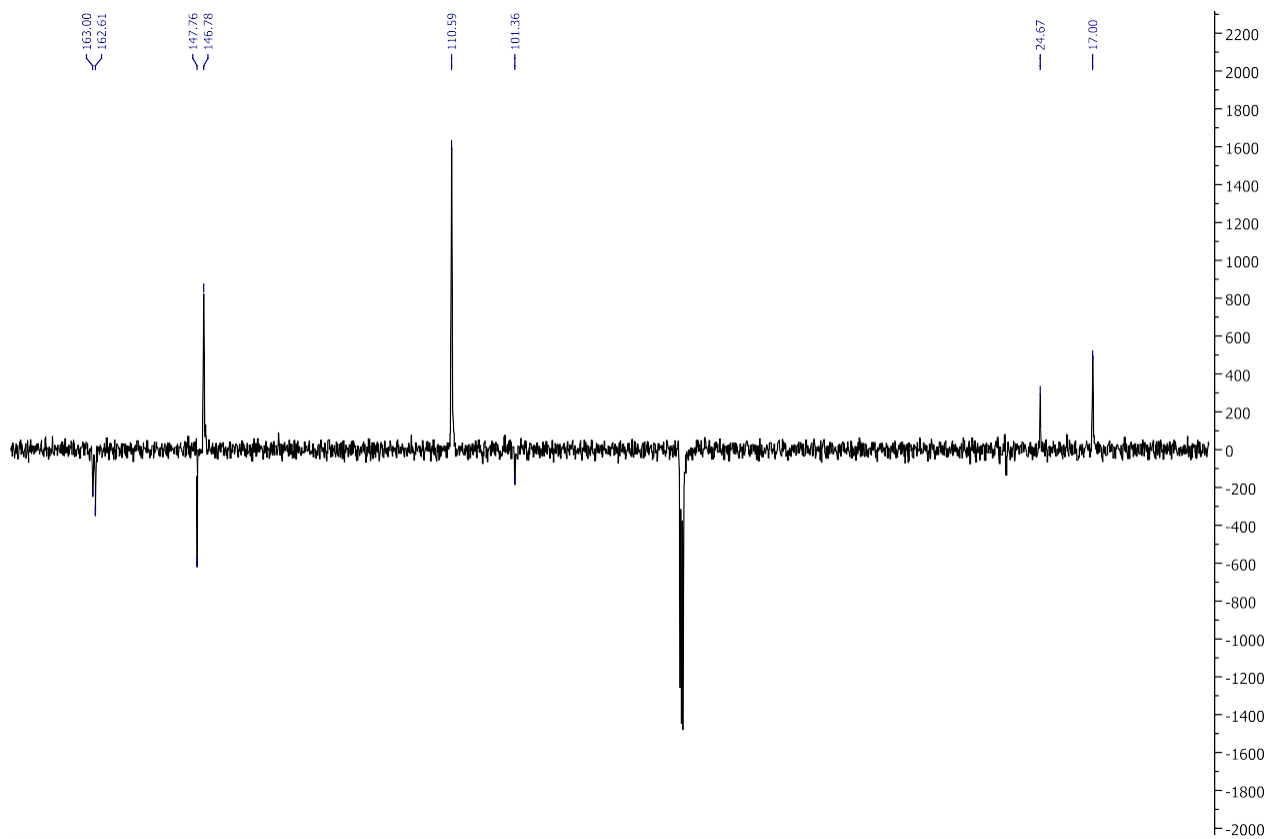
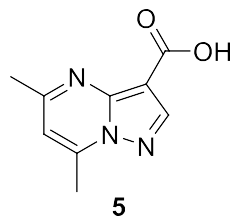
Peak ID	Time	Mass Found
4	1.92	440.41

4: (Time: 1.90)

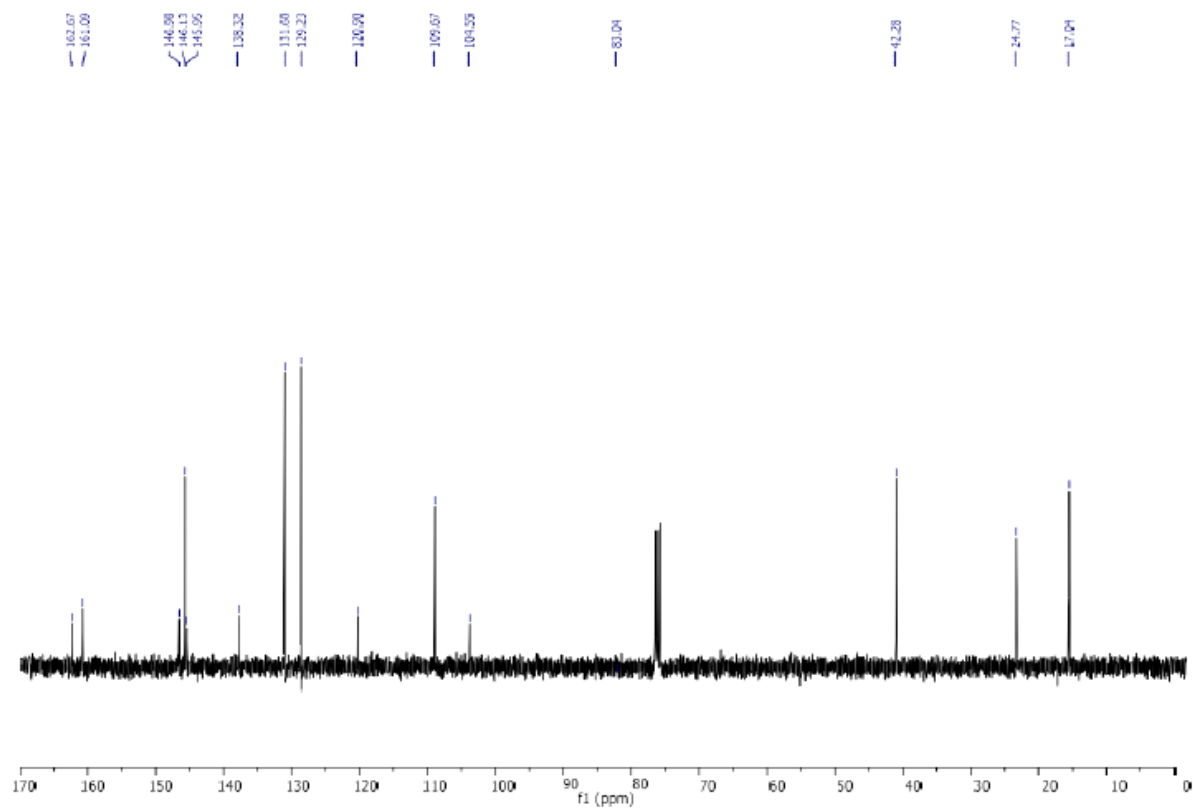
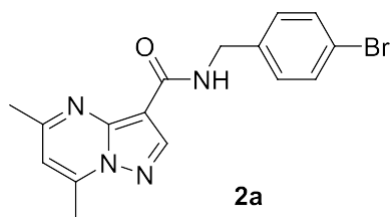




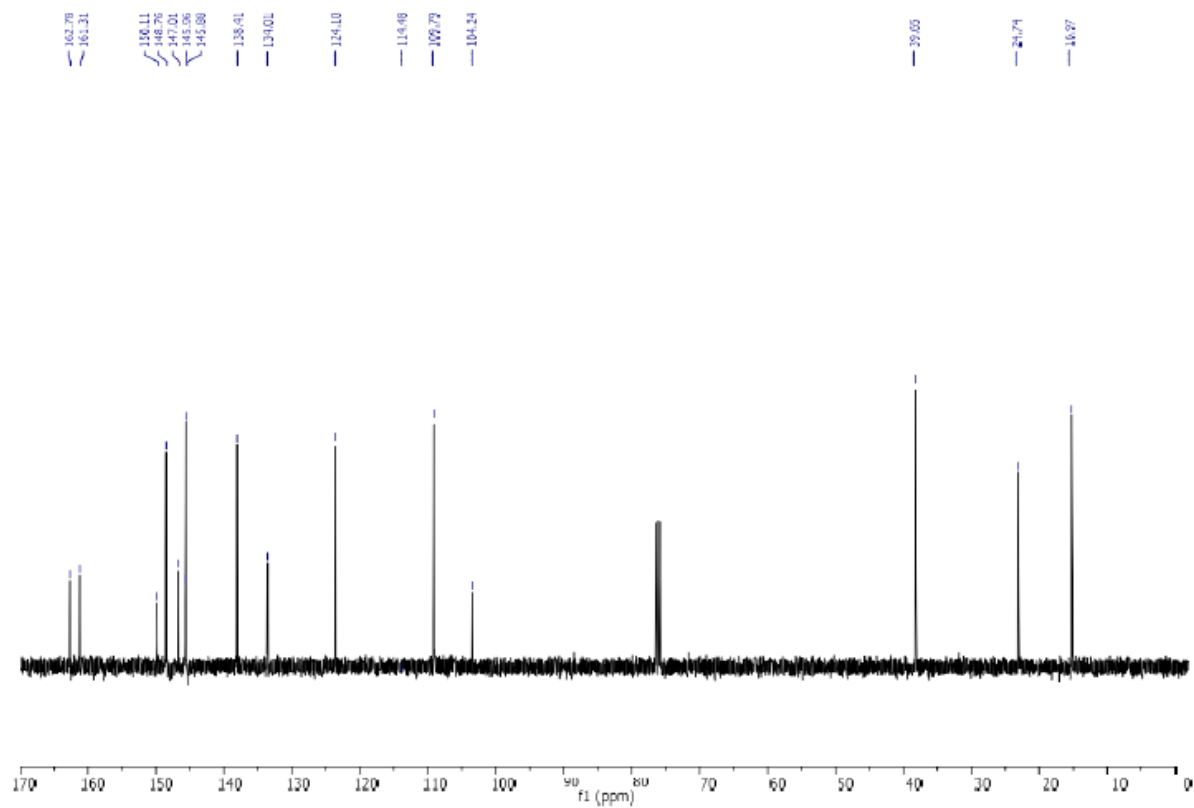
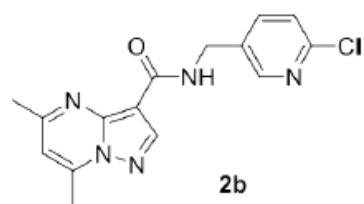
¹³C DEPT (CDCl₃, 600 MHz) of compound **4**.



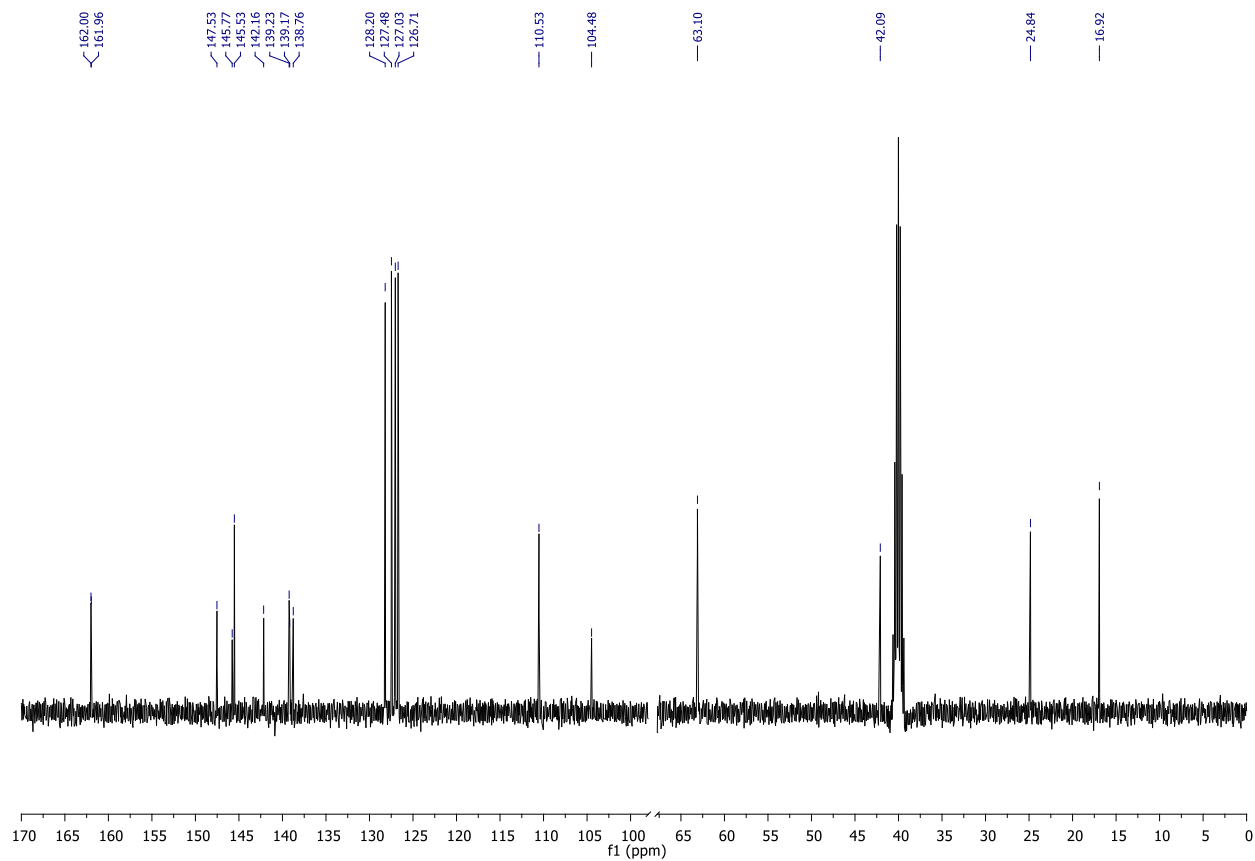
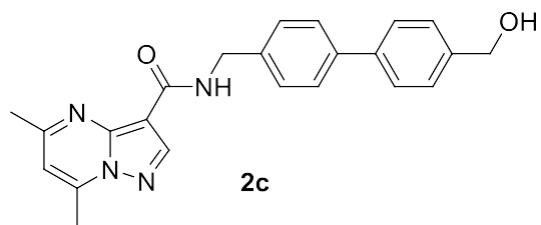
^{13}C DEPT (CDCl_3 , 600 MHz) of compound 5.



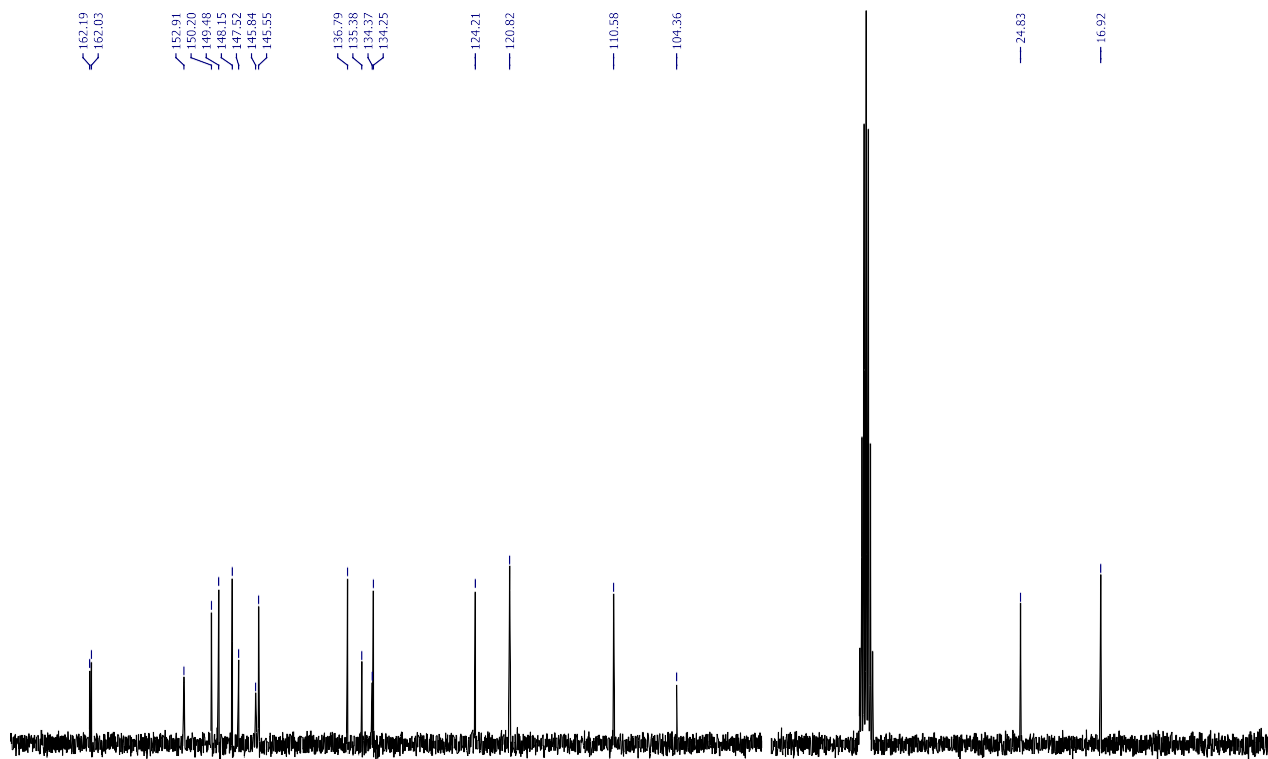
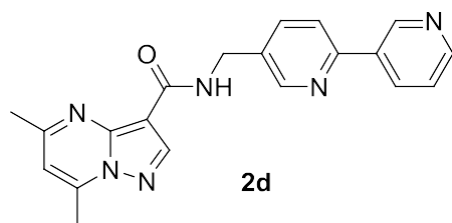
¹³C NMR (CDCl₃, 400 MHz) of compound **2a**.



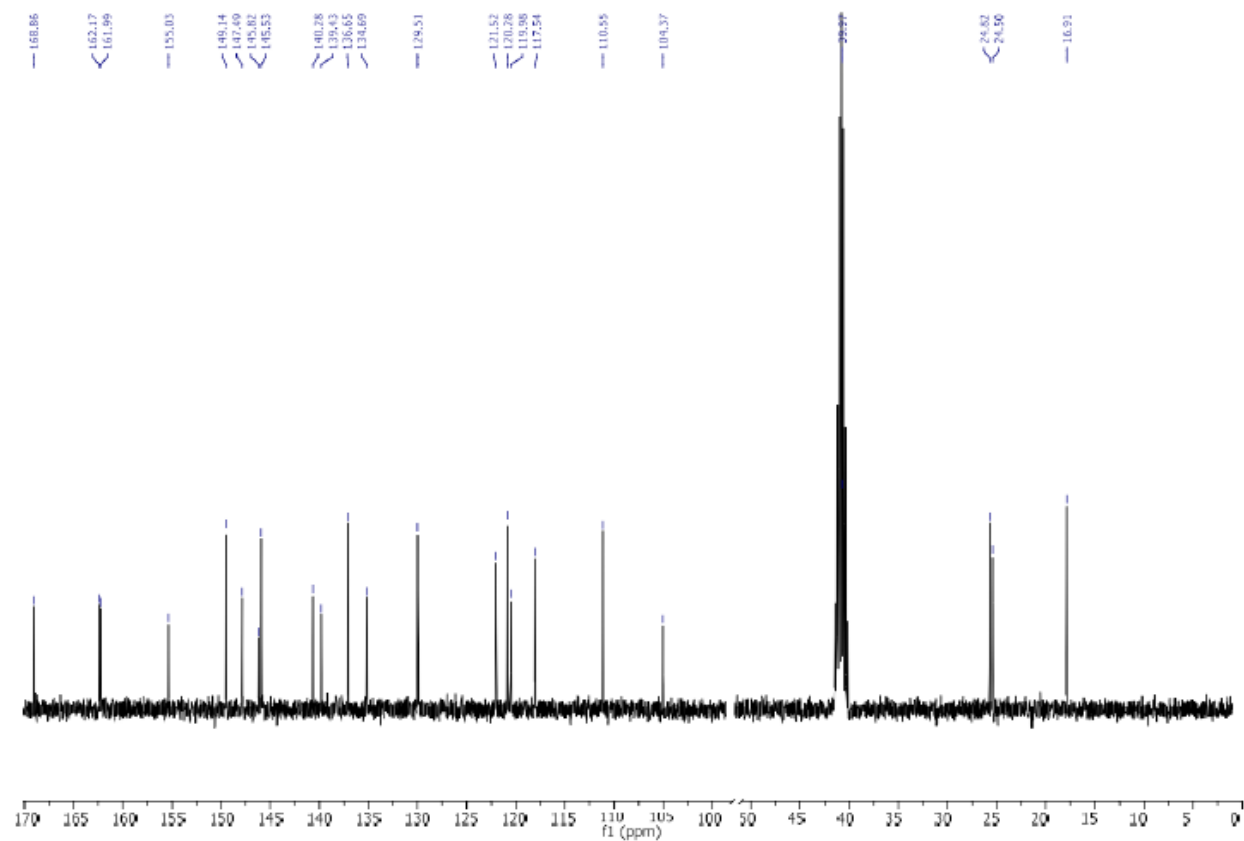
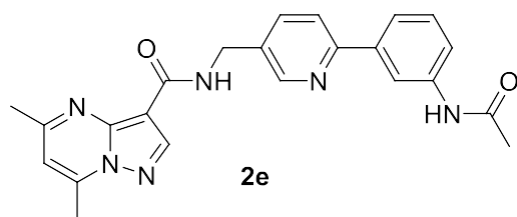
¹³C NMR (CDCl₃, 400 MHz) of compound **2b**



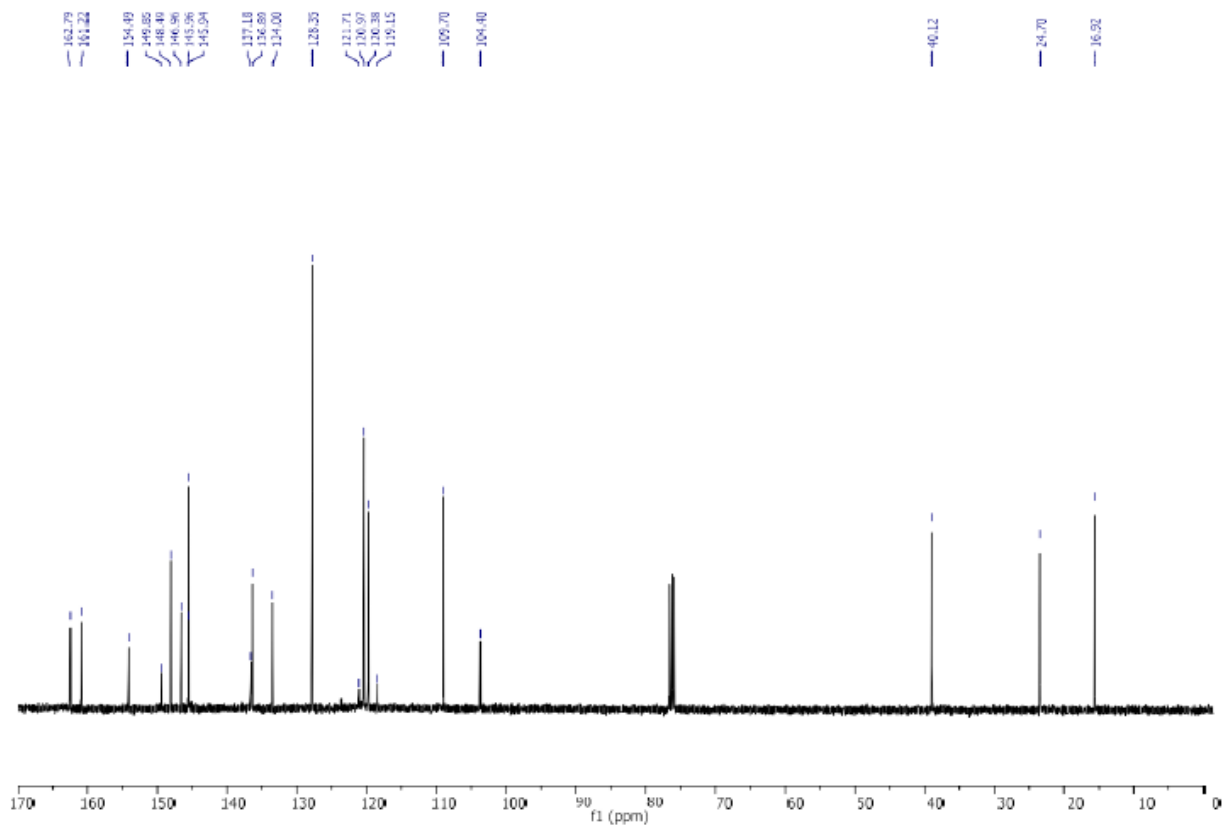
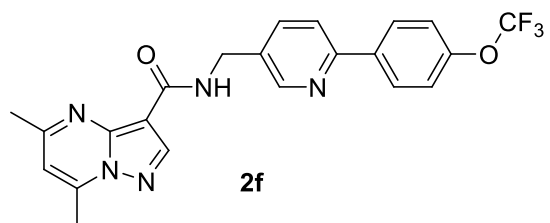
¹³C NMR (DMSO-d₆, 400 MHz) of compound **2c**.



¹³C NMR (DMSO-d₆, 400 MHz) of compound **2d**.



¹³C NMR (DMSO-d₆, 400 MHz) of compound **2e**.



¹³C NMR (CDCl₃, 400 MHz) of compound **2f**.