

## Supplementary Materials

### Design and synthesis of new modified flexible purine bases as potential inhibitors of Human PNP

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### Content

<sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra (300 MHz, CDCl<sub>3</sub>) of target products.

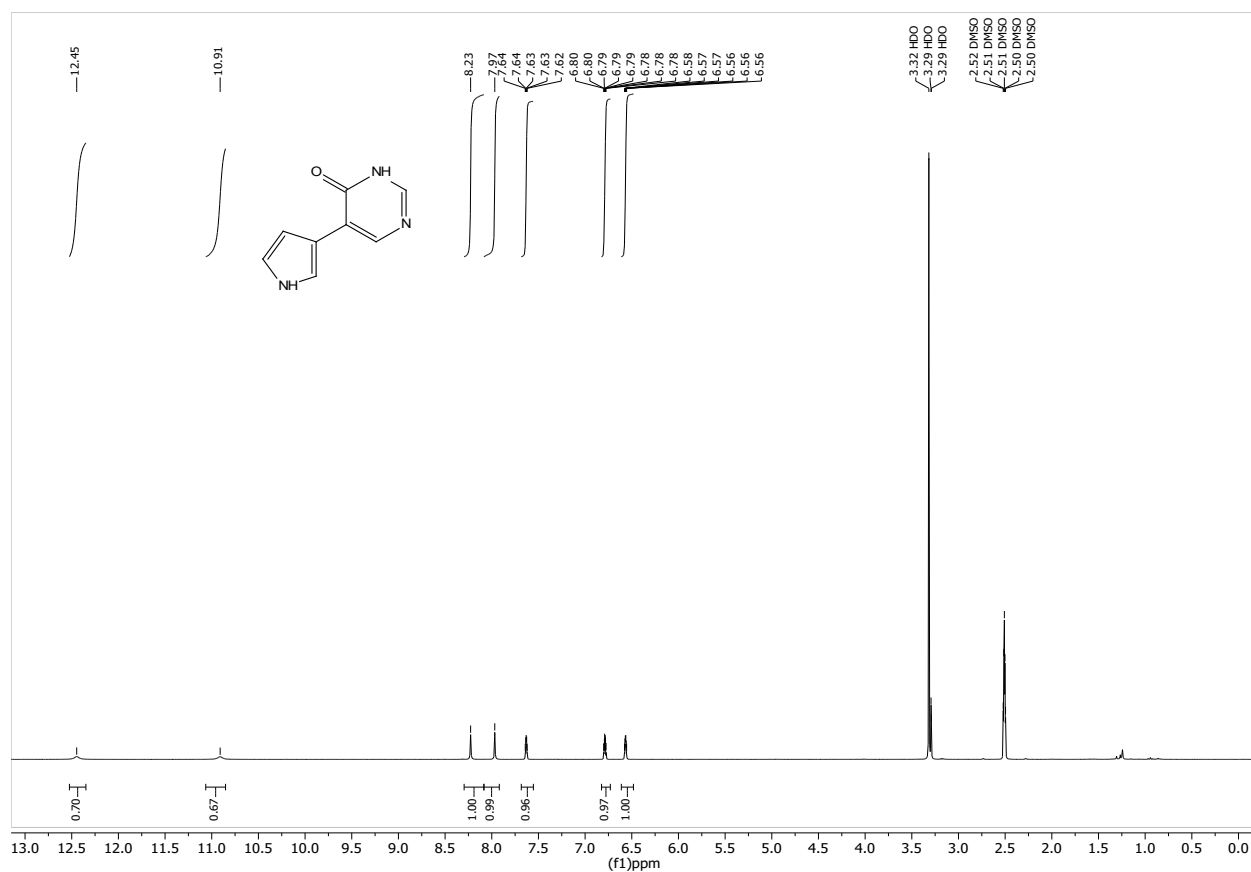
HRMS spectra of compounds target products.

Figure S1: Lineweaver–Burk plots for the inosine phosphorolysis at concentrations of compounds 1, 2, 3 and 4 equal to 0, 0.5, 1 and 2 mM. (A) compound 1, (B) compound 2, (C) compound 3, (D) compound 4.

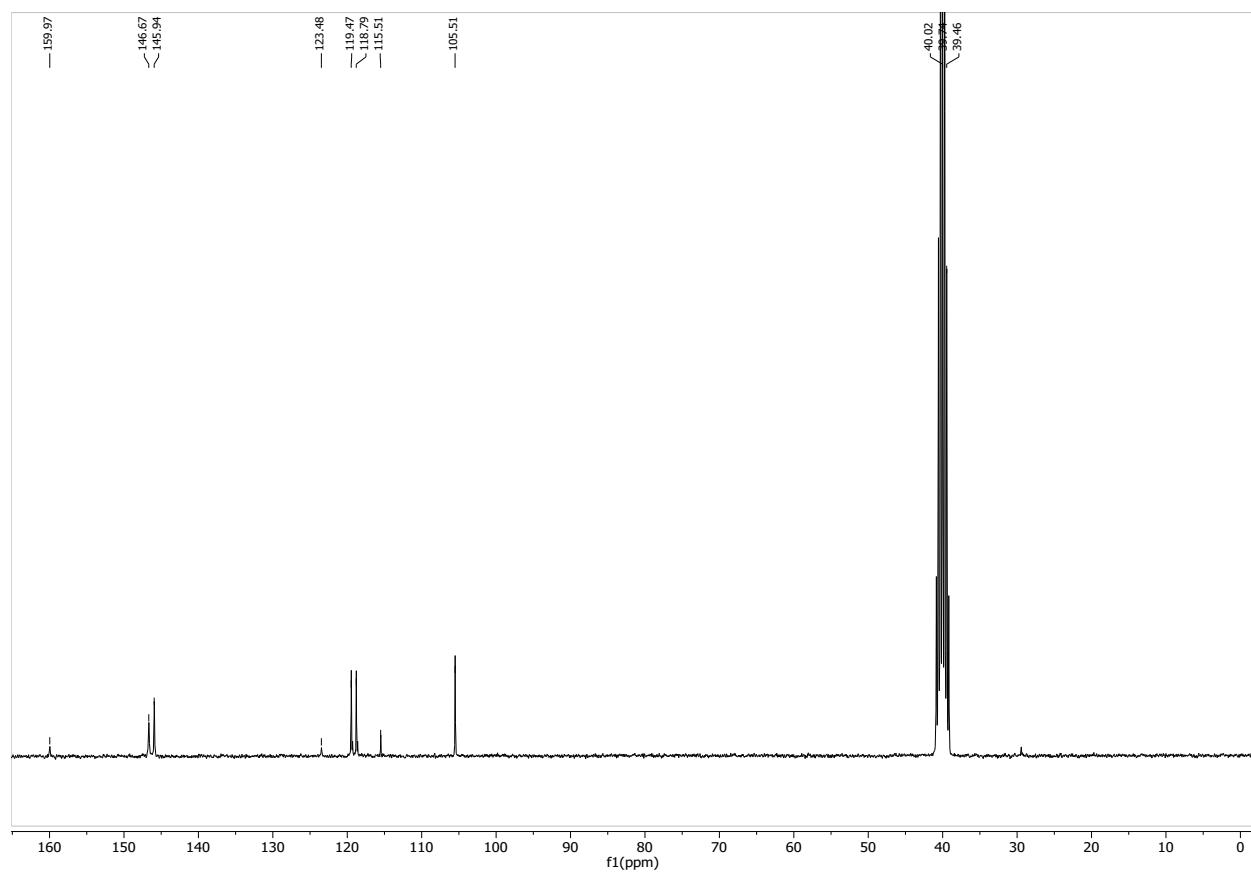
Figure S2: 2D diagrams of complexes PNP with various type of ligands.

Figure S3: Structure of the 3INY with re-docked 7-deazaguanine (An overlap the red wire – native ligand from PDB database; the red stick docked ligand. The box for docking ligands was highlighted in green (12 Å × 10 Å × 10 Å.)

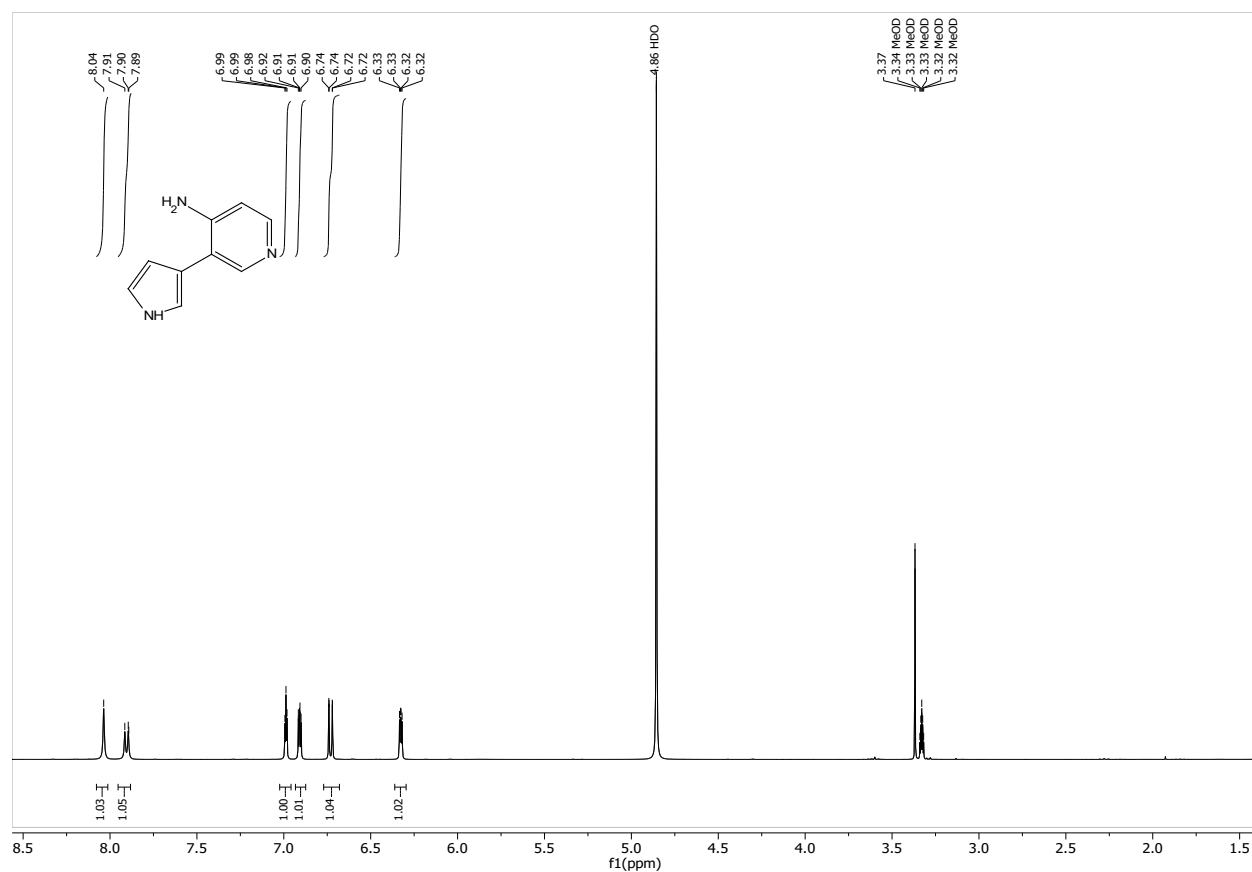
<sup>1</sup>H-NMR spectrum (300 MHz, DMSO-d<sub>6</sub>) of compound **1**



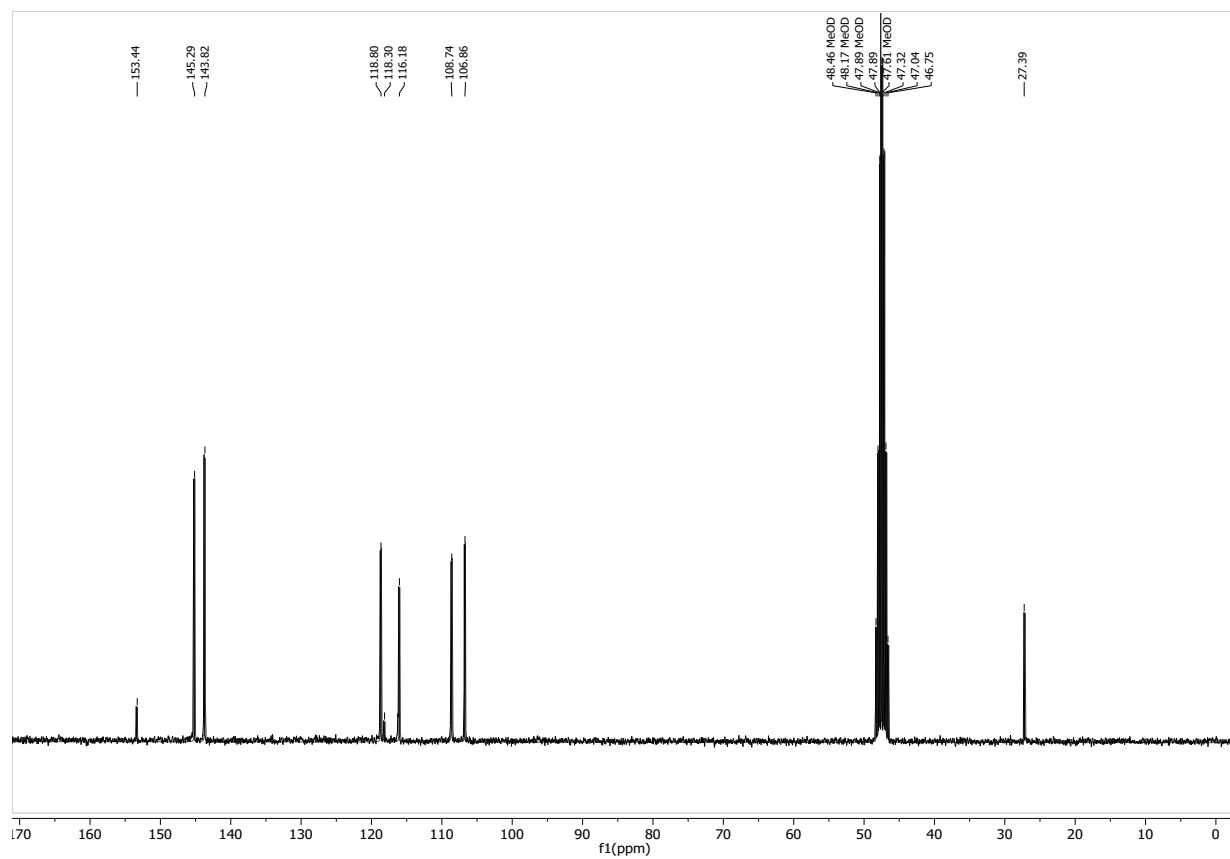
<sup>13</sup>C-NMR spectrum (75.5 MHz, DMSO-d<sub>6</sub>) of compound **1**



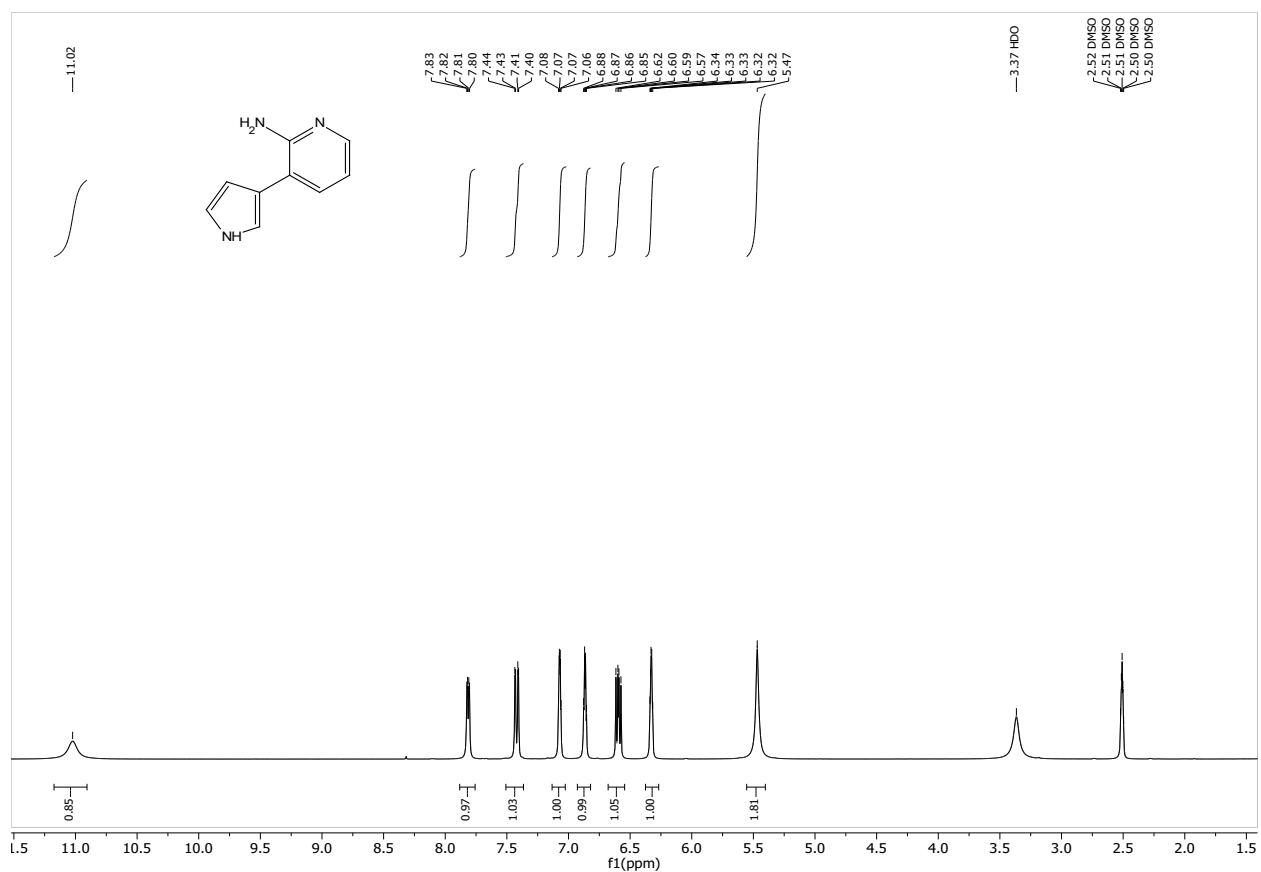
$^1\text{H}$ -NMR spectrum (300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**



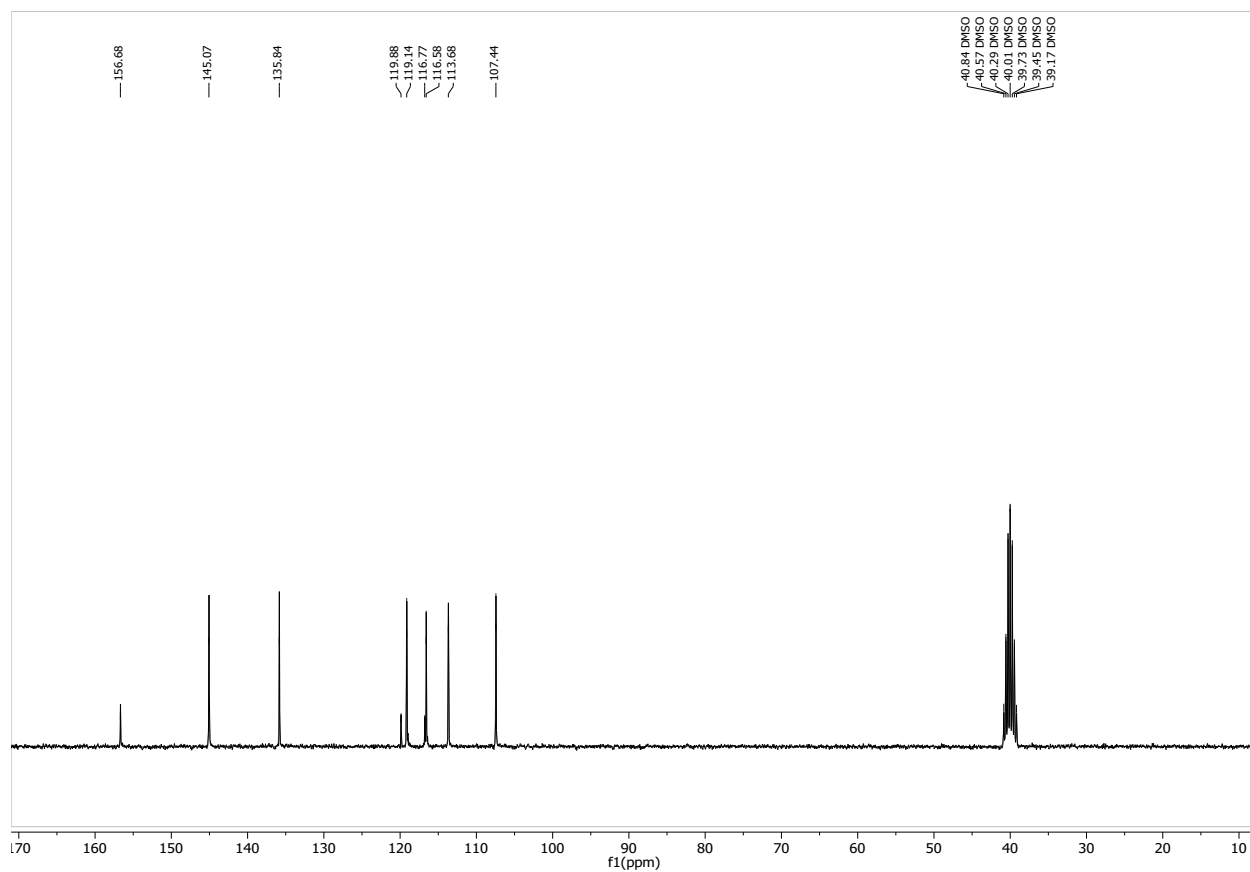
$^{13}\text{C}$ -NMR spectrum (75.5 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**



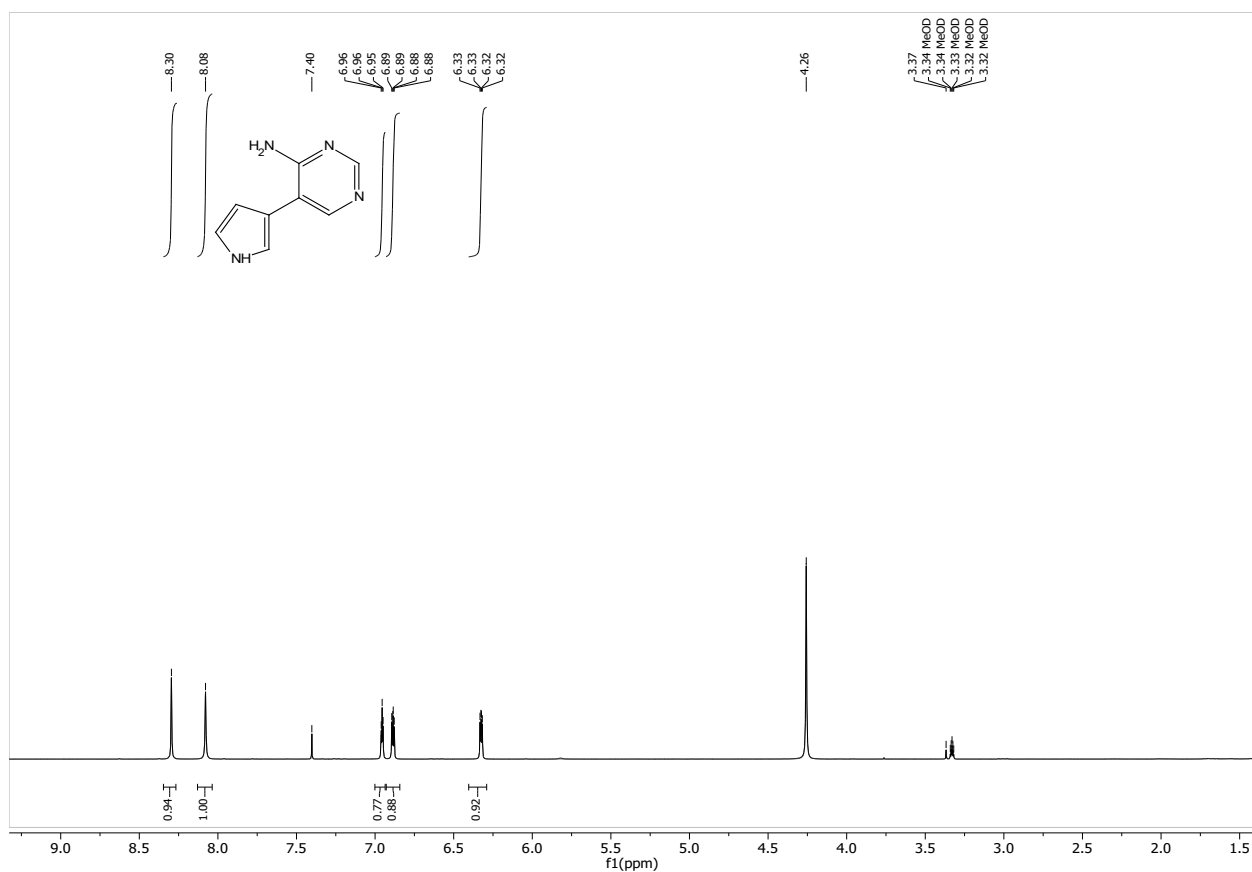
<sup>1</sup>H-NMR spectrum (300 MHz, DMSO-d<sub>6</sub>) of compound **3**



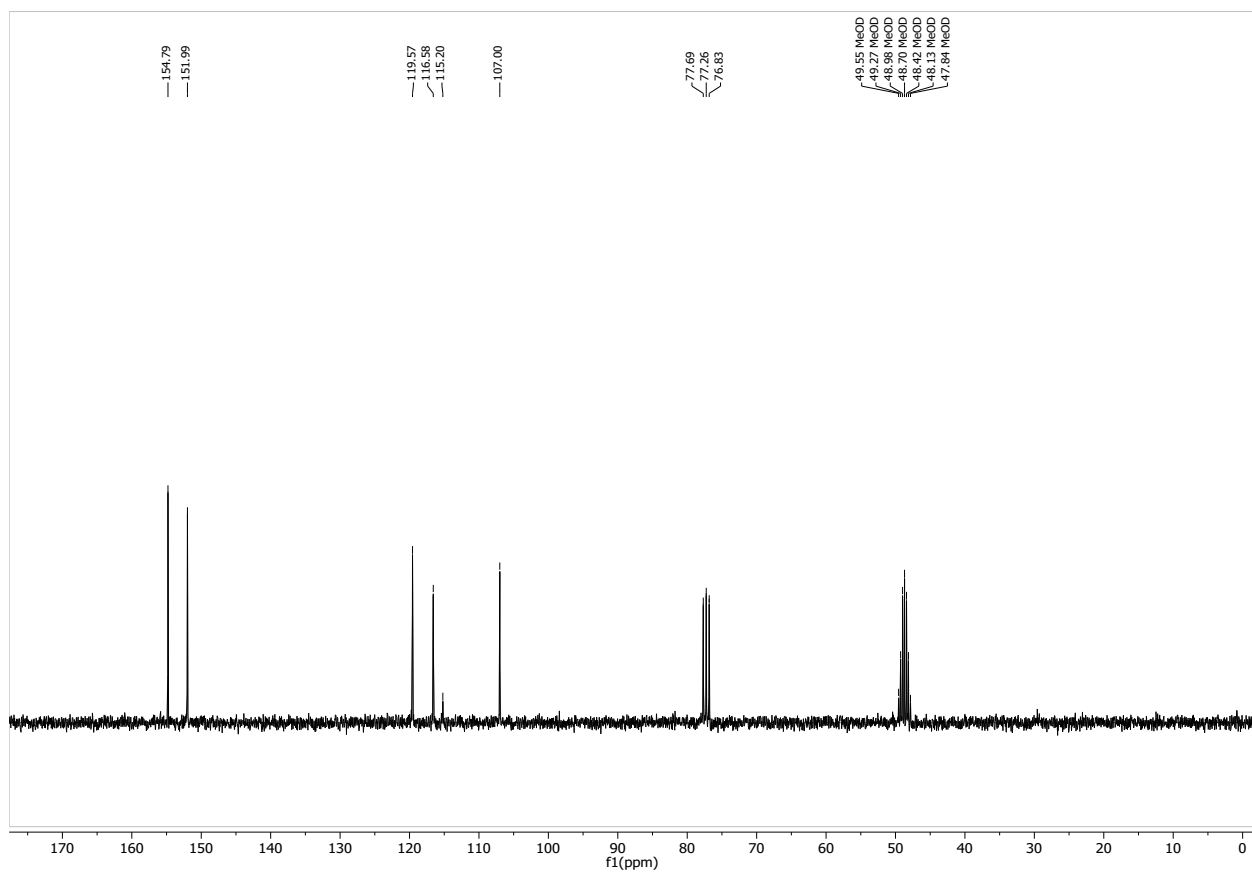
<sup>13</sup>C-NMR spectrum (75.5 MHz, DMSO-d<sub>6</sub>) of compound **3**

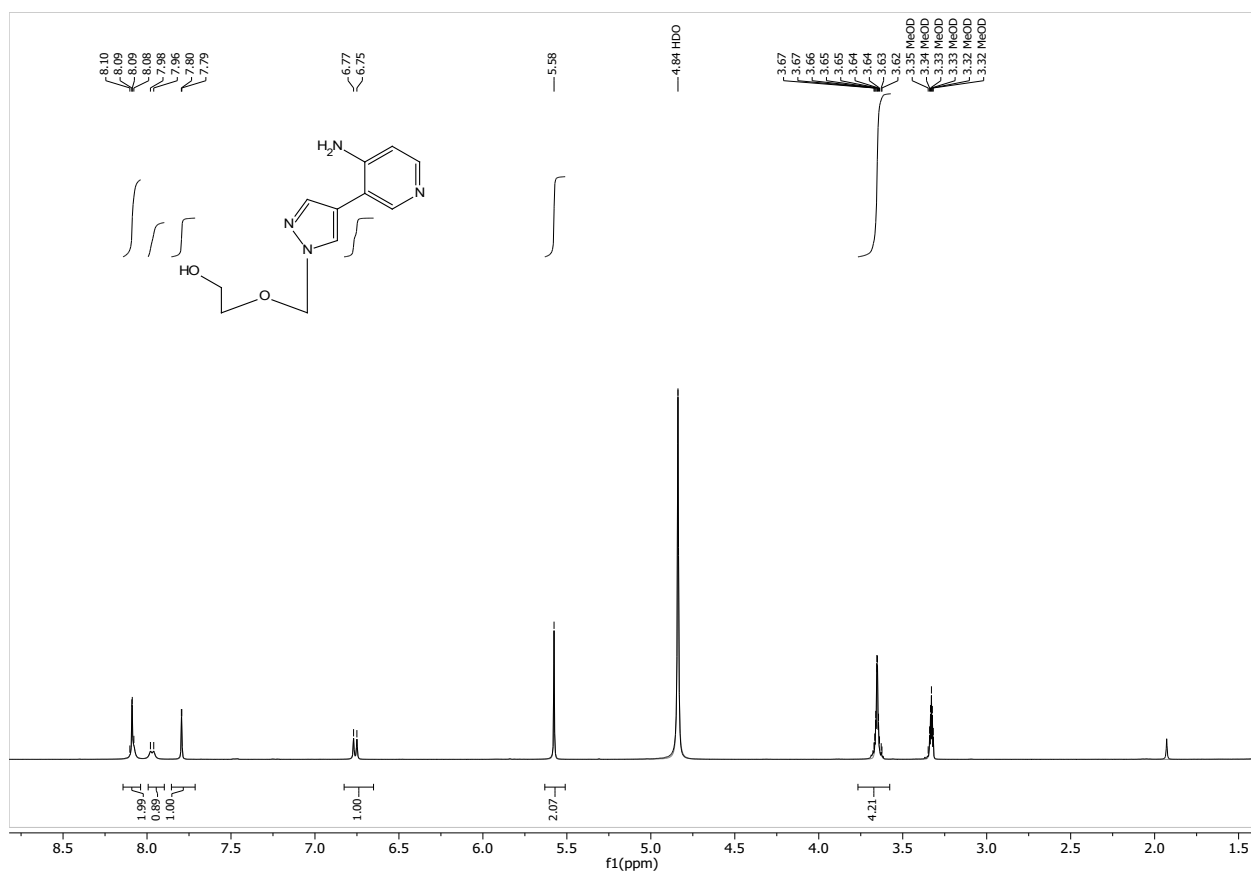


$^1\text{H}$ -NMR spectrum (300 MHz,  $\text{CDCl}_3\text{:CD}_3\text{OD}$ ) of compound **4**

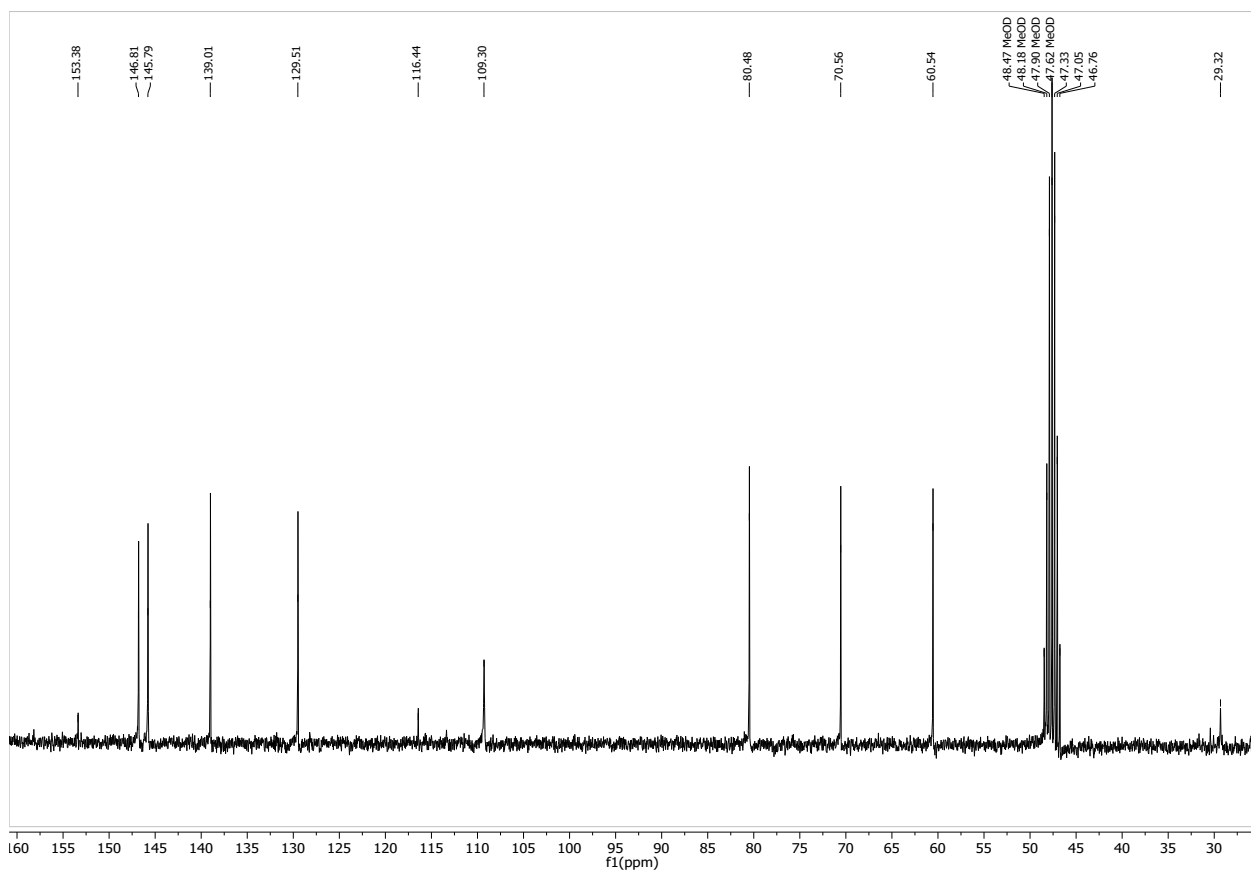


$^{13}\text{C}$ -NMR spectrum (75.5 MHz,  $\text{CDCl}_3\text{:CD}_3\text{OD}$ ) of compound **4**

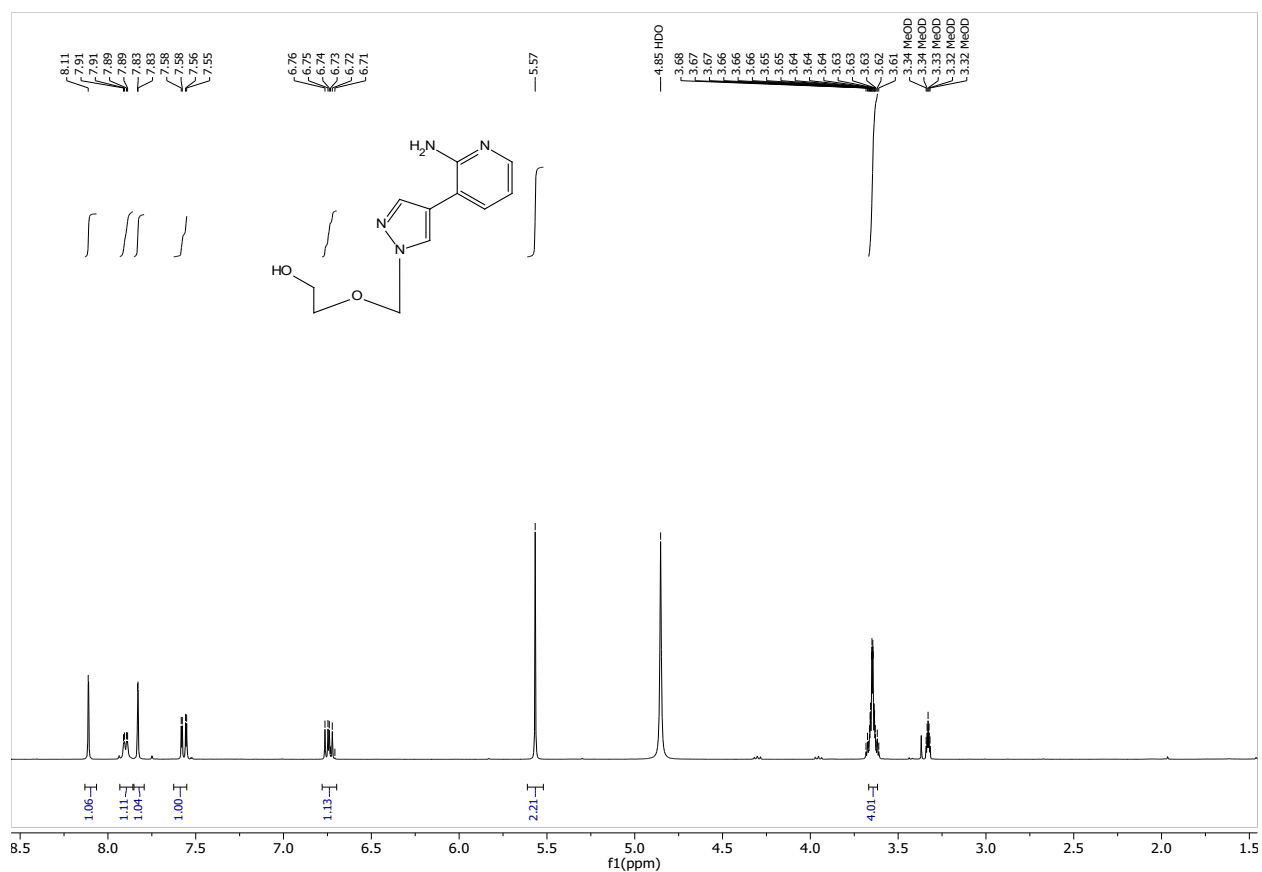


<sup>1</sup>H-NMR spectrum (300 MHz, CD<sub>3</sub>OD) of compound **13**

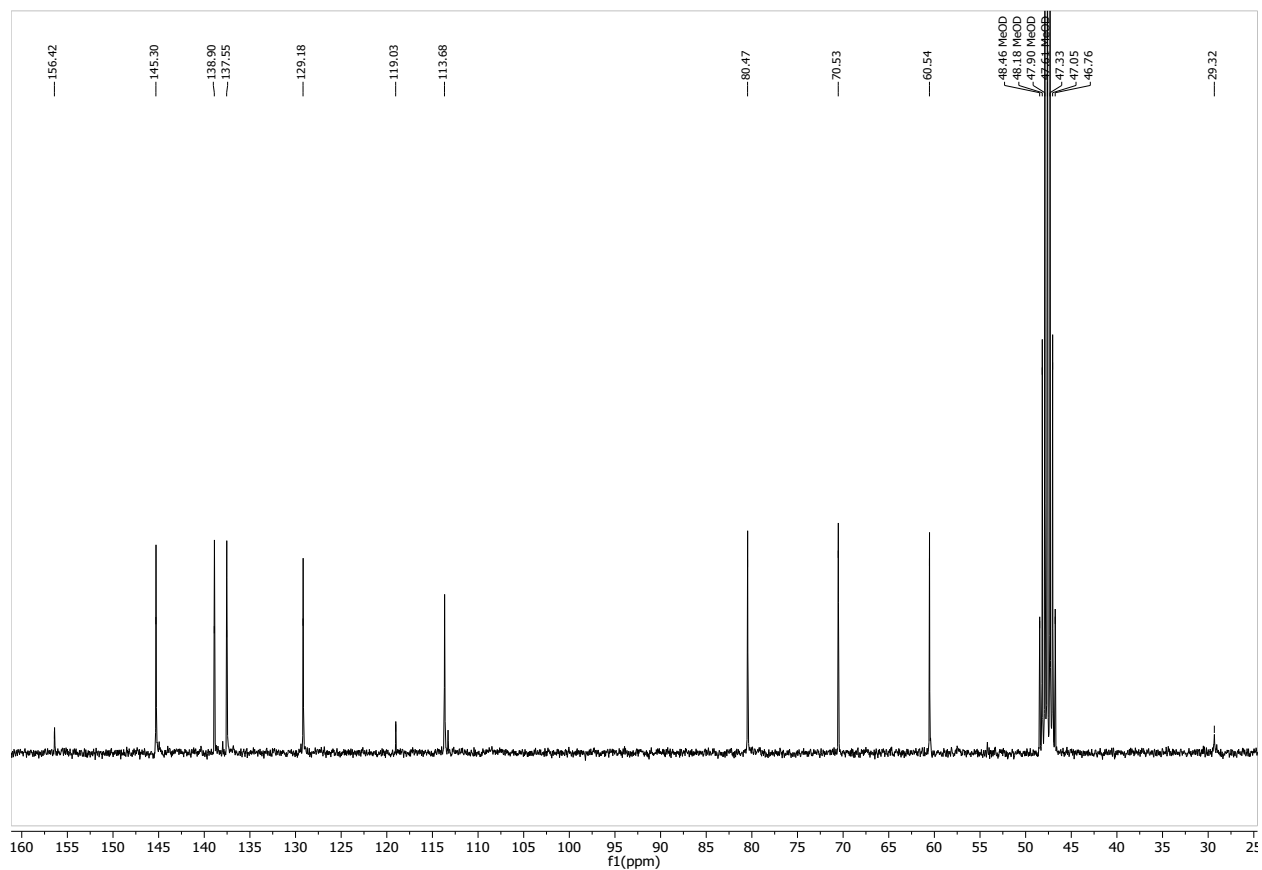
<sup>13</sup>C-NMR spectrum (75.5 MHz, CD<sub>3</sub>OD) of compound **13**



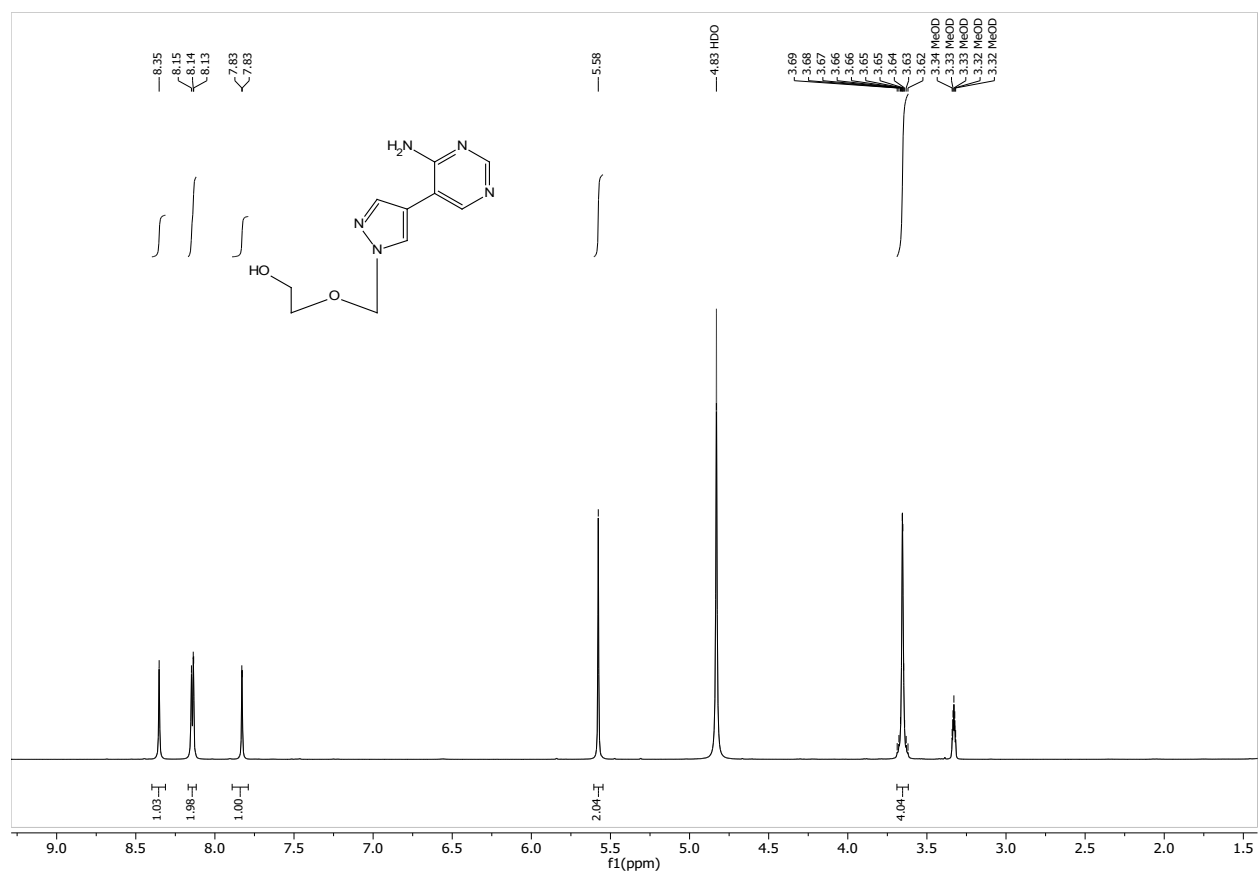
$^1\text{H}$ -NMR spectrum (300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **14**



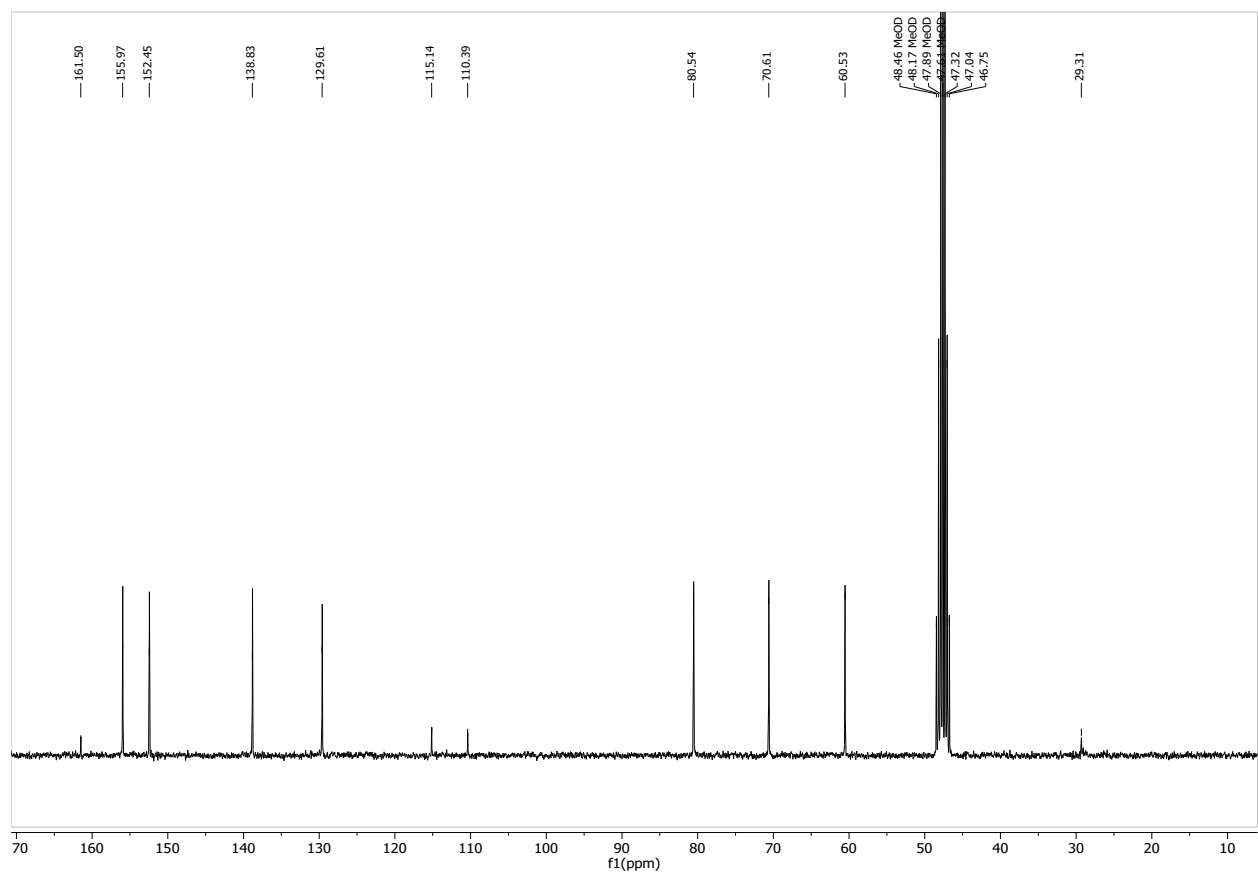
$^{13}\text{C}$ -NMR spectrum (75.5 MHz,  $\text{CD}_3\text{OD}$ ) of compound **14**



$^1\text{H}$ -NMR spectrum (300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **15**

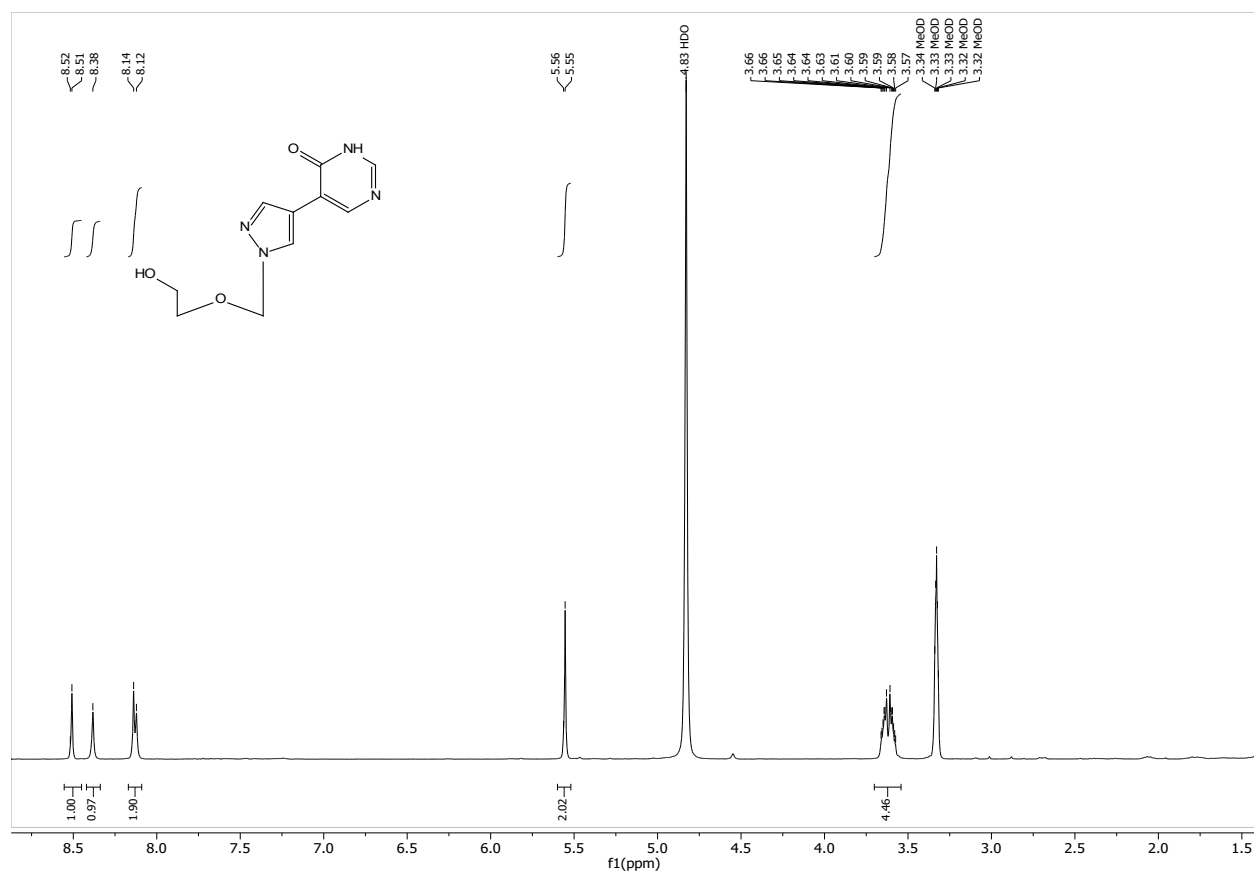


$^{13}\text{C}$ -NMR spectrum (75.5 MHz,  $\text{CD}_3\text{OD}$ ) of compound **15**

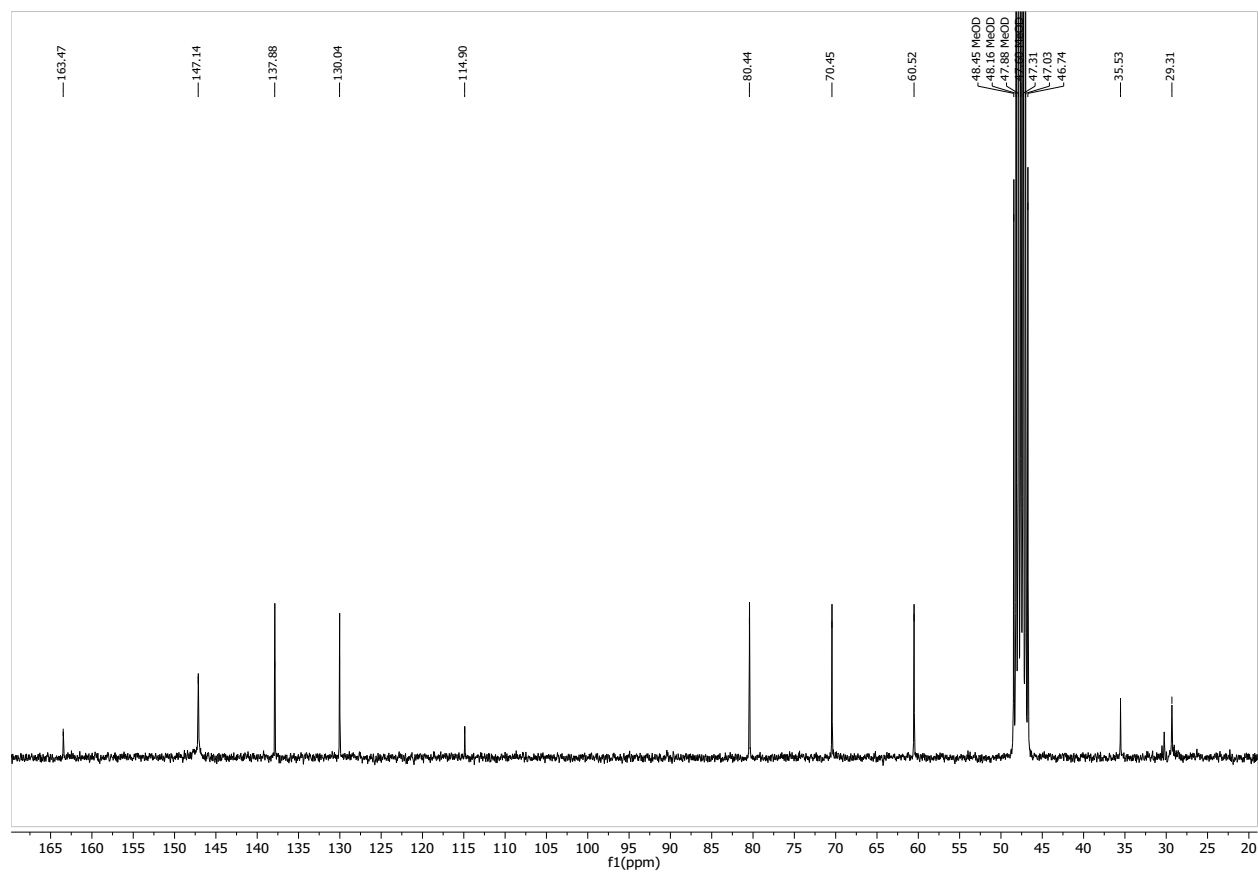




$^1\text{H}$ -NMR spectrum (300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **16**



$^{13}\text{C}$ -NMR spectrum (75.5 MHz,  $\text{CD}_3\text{OD}$ ) of compound **16**



# HRMS spectrum of compound 1

## Display Report

### Analysis Info

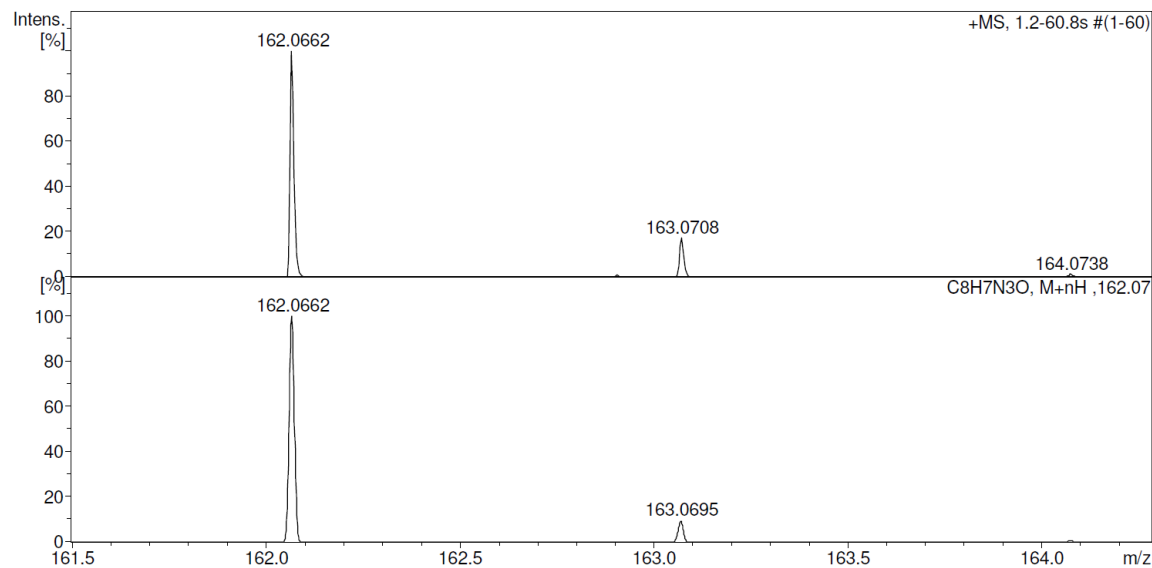
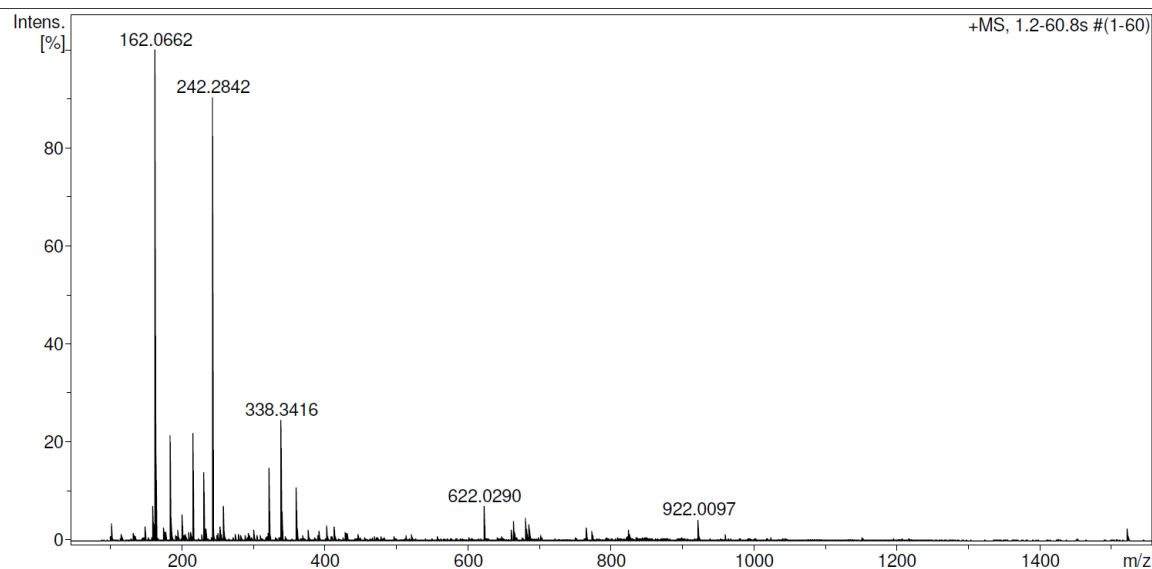
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Method tune\_low\_1550.m  
Sample Name 1  
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Operator BDAL@DE  
Instrument / Ser# maXis 43

### Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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# HRMS spectrum of compound 2

## Display Report

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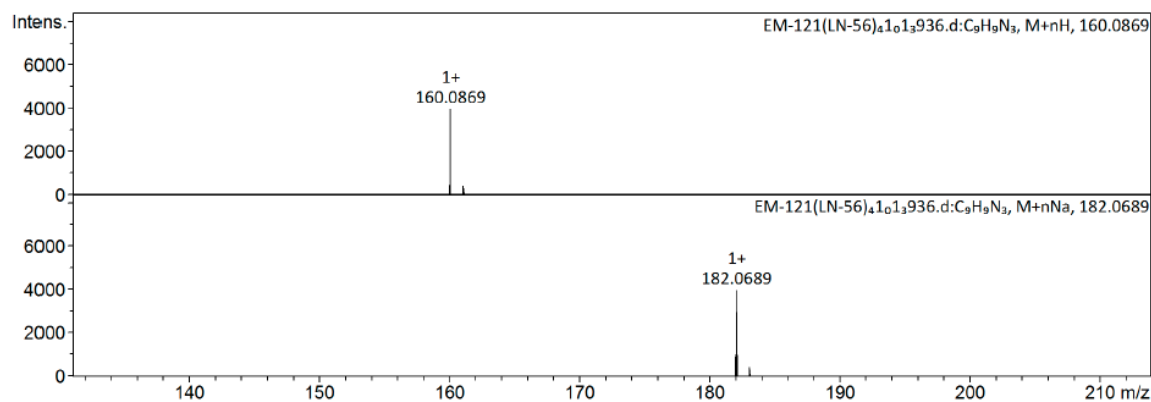
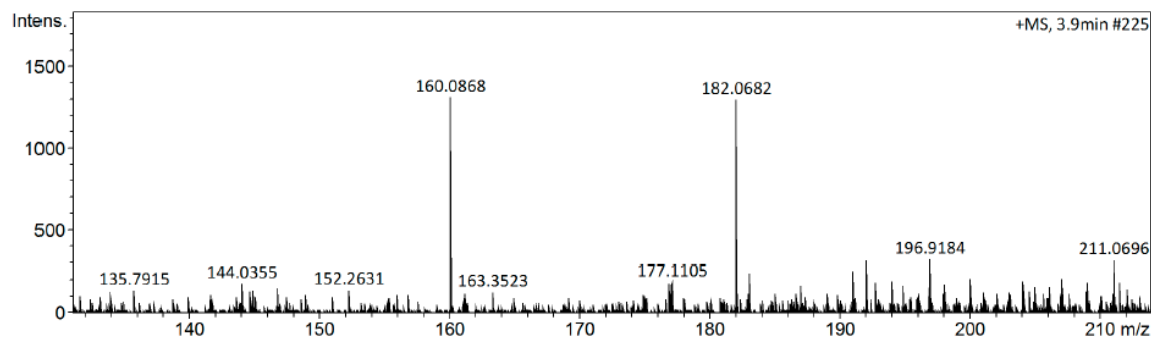
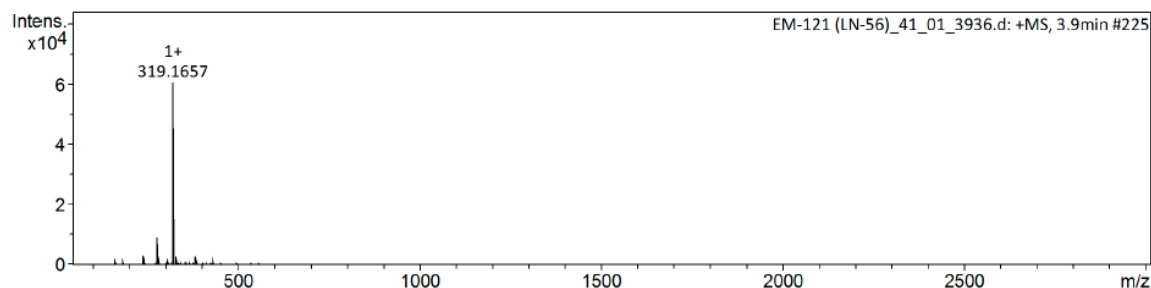
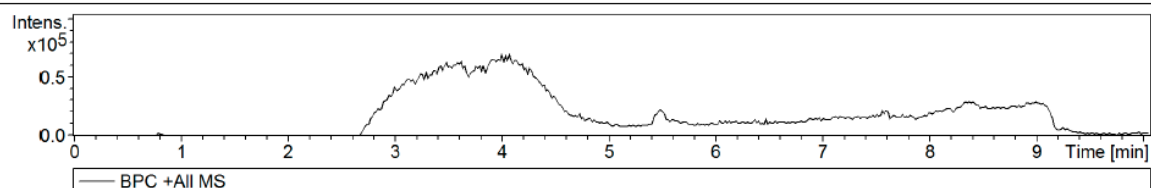
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 Sample Name 2  
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Acquisition Date 12/27/2022 4:59:01 PM

Operator BDAL@DE  
 Instrument compact 8255754.20088

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EM-121 (LN-56)\_41\_01\_3936.d

Bruker Compass DataAnalysis 4.3

printed: 12/27/2022 8:08:31 PM

by: BDAL@DE

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# HRMS spectrum of compound 3

## Display Report

### Analysis Info

Analysis Name D:\Data\Chizhov\IMB\Matyugina\1\ln272\_&clblow.d  
 Method tune\_low\_1550.m  
 Sample Name 3  
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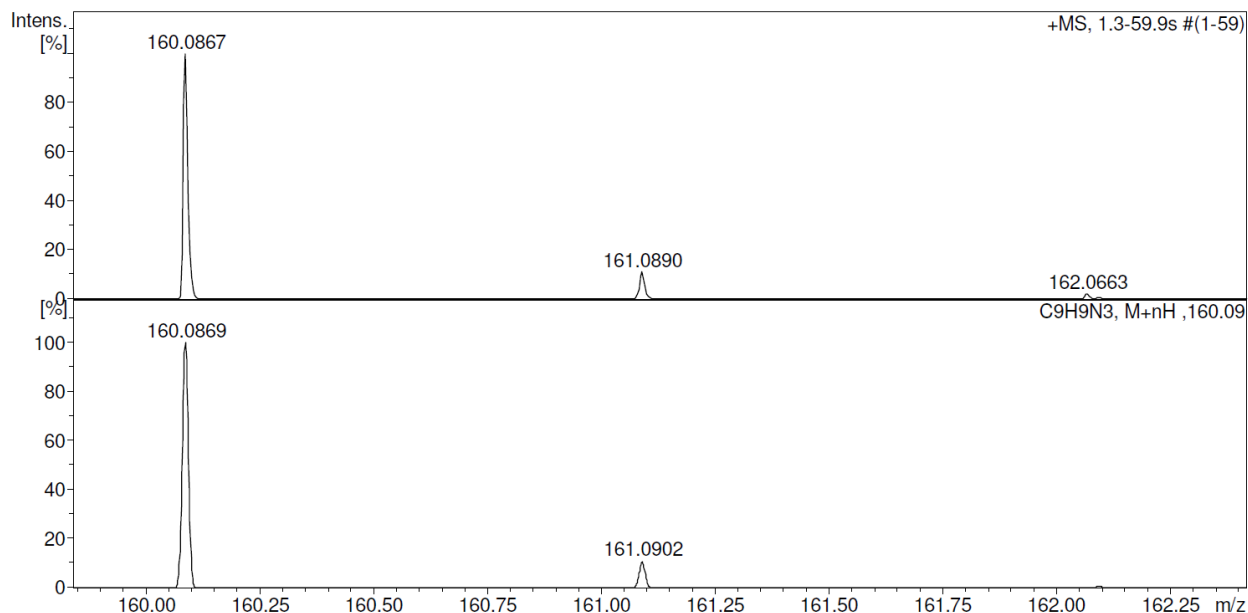
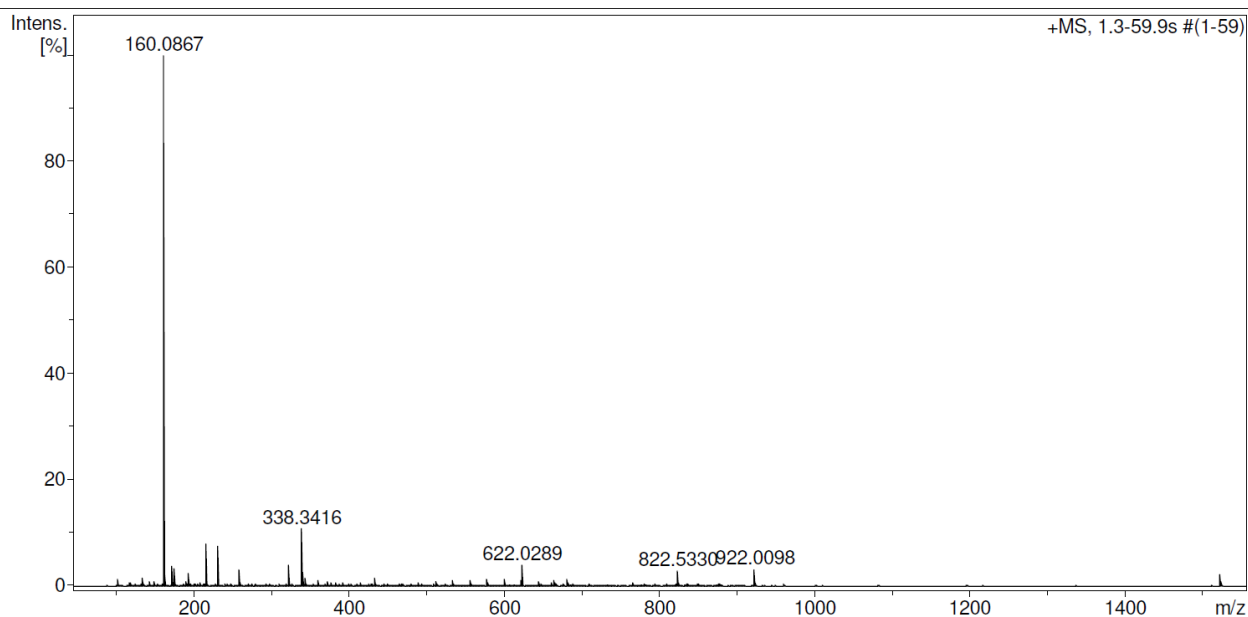
Acquisition Date 25.01.2022 16:05:20

Operator BDAL@DE

Instrument / Ser# maXis 43

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# HRMS spectrum of compound 4

## Display Report

### Analysis Info

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 Method tune\_low\_1550.m  
 Sample Name 4  
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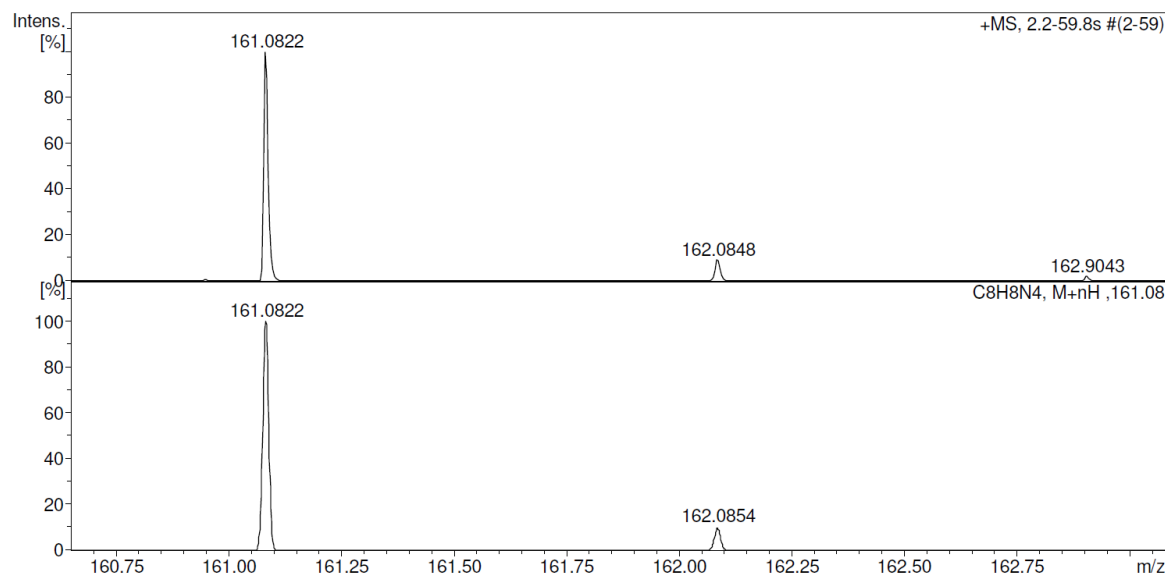
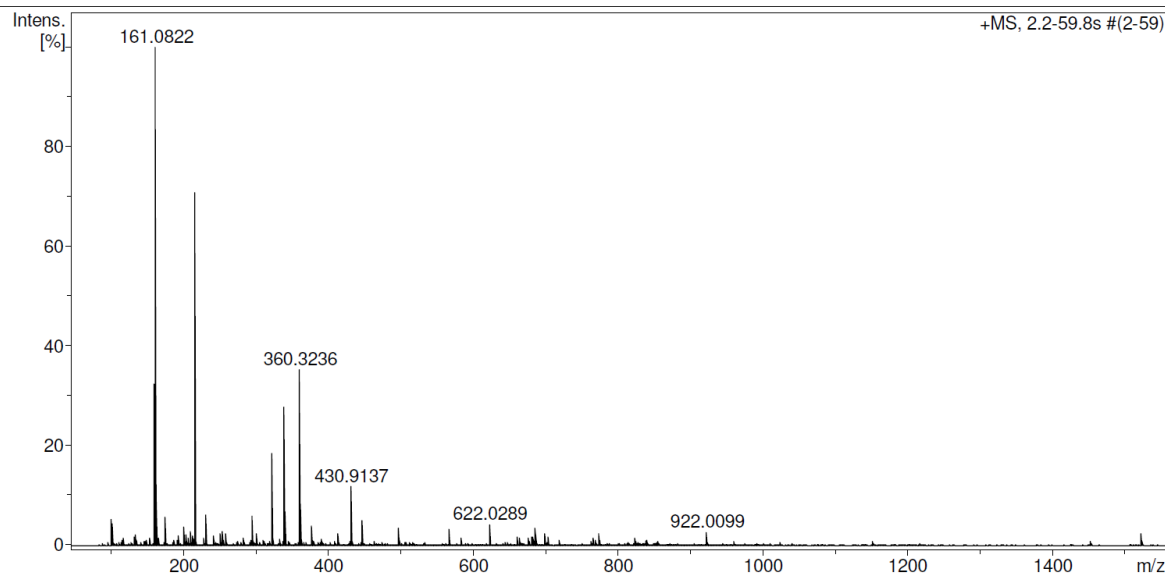
Acquisition Date 25.01.2022 15:51:54

Operator BDAL@DE

Instrument / Ser# maXis 43

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# HRMS spectrum of compound 13

## Display Report

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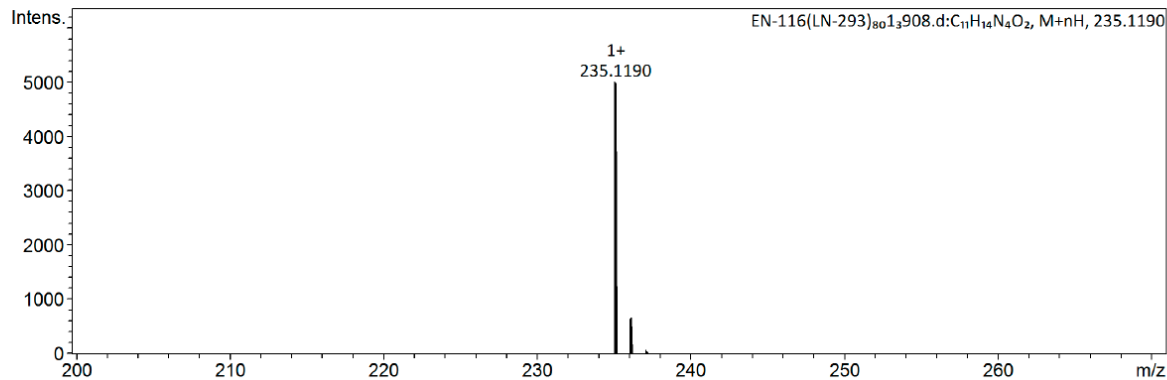
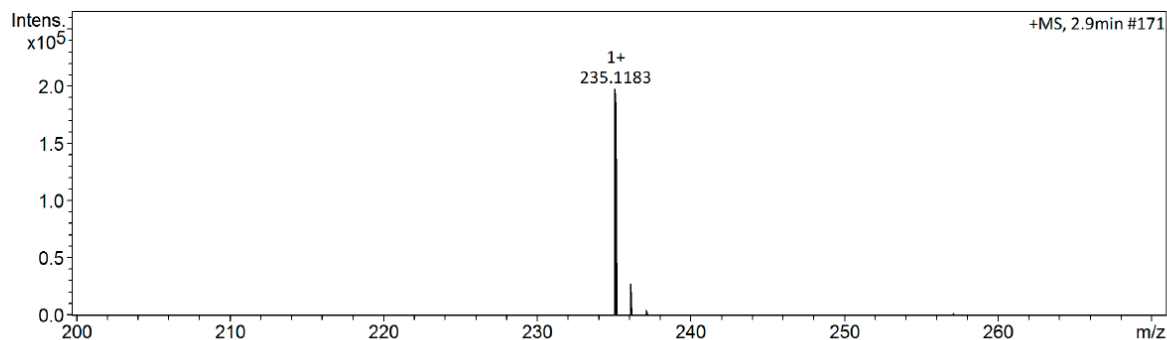
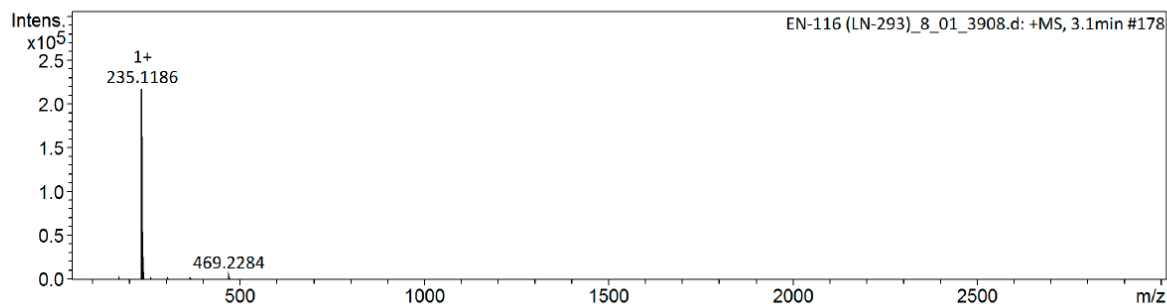
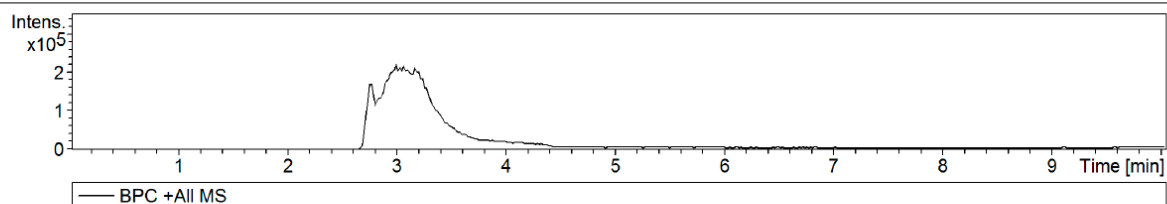
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 Comment

Acquisition Date 11/30/2022 8:25:15 PM

Operator BDAL@DE  
 Instrument compact 8255754.20088

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# HRMS spectrum of compound 14

## Display Report

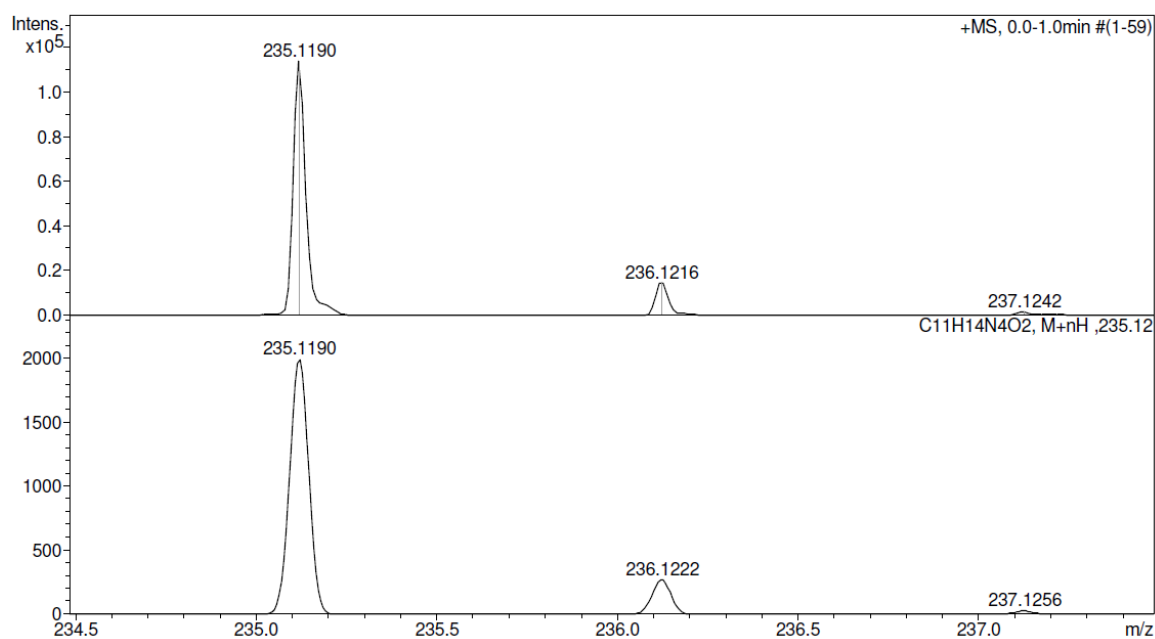
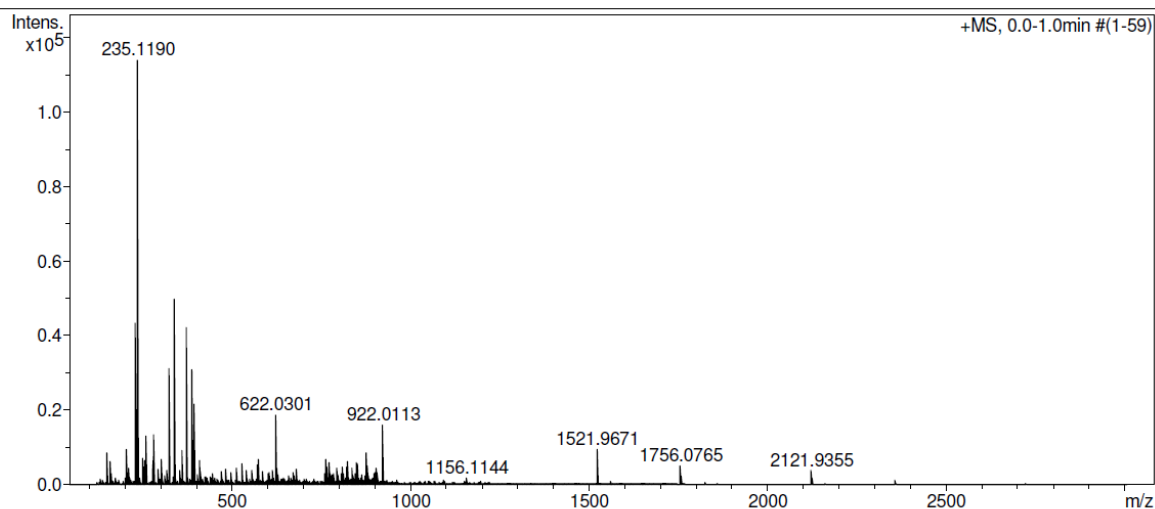
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 Method: tune\_low.m  
 Sample Name: 14  
 Comment: 100 %, dil. 2000, calibrant added

Acquisition Date: 21.10.2022 14:12:12  
 Operator: BDAL@DE  
 Instrument / Ser#: microTOF CH3CN 10248

### Acquisition Parameter

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Focus	Not active			Set Dry Heater	180 °C
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# HRMS spectrum of compound **15**

## Display Report

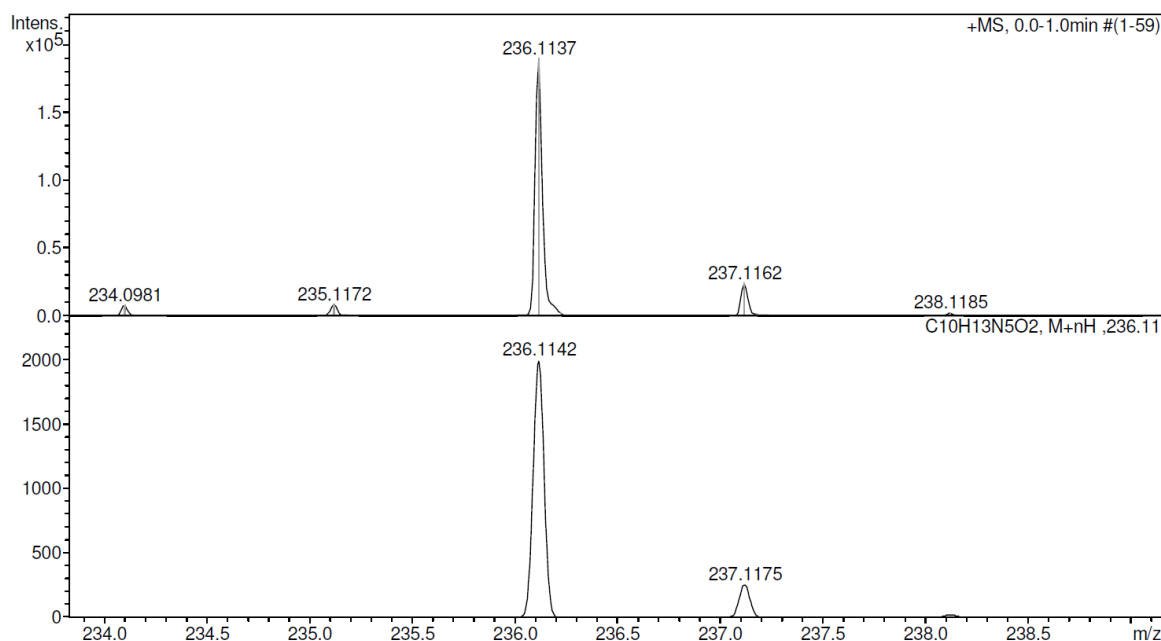
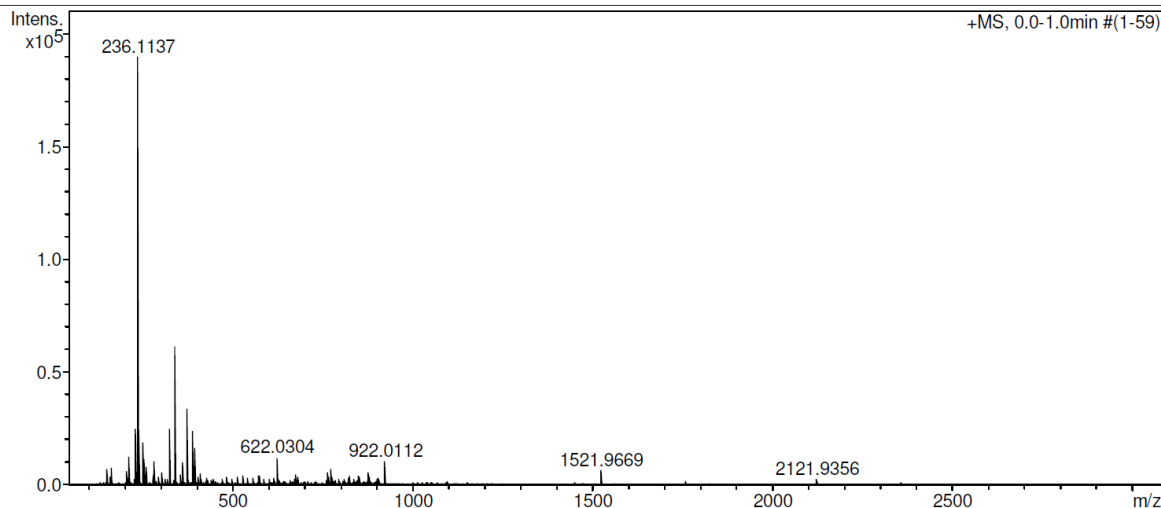
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 Method tune\_low.m  
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 Comment 100 %, dil. 2000, calibrant added

Acquisition Date 21.10.2022 14:16:23  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF CH3CN 10248

### Acquisition Parameter

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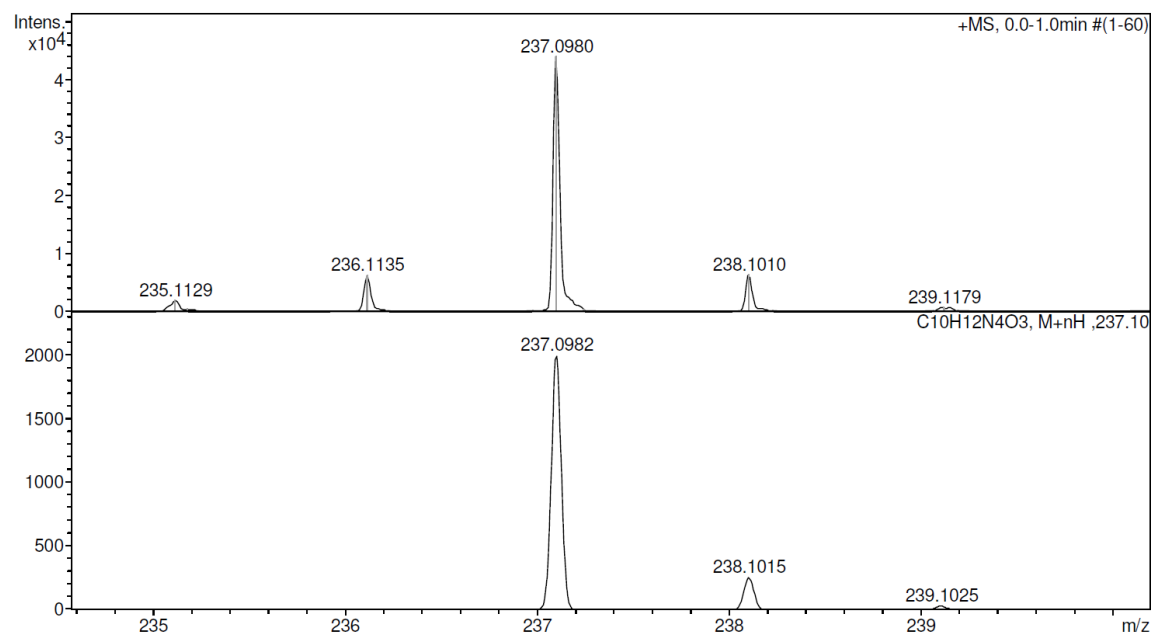
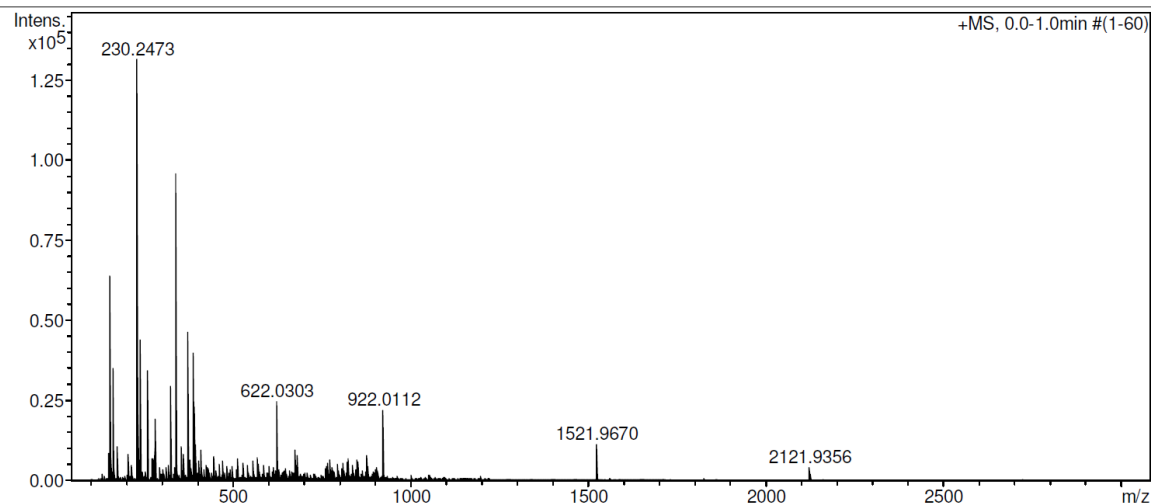
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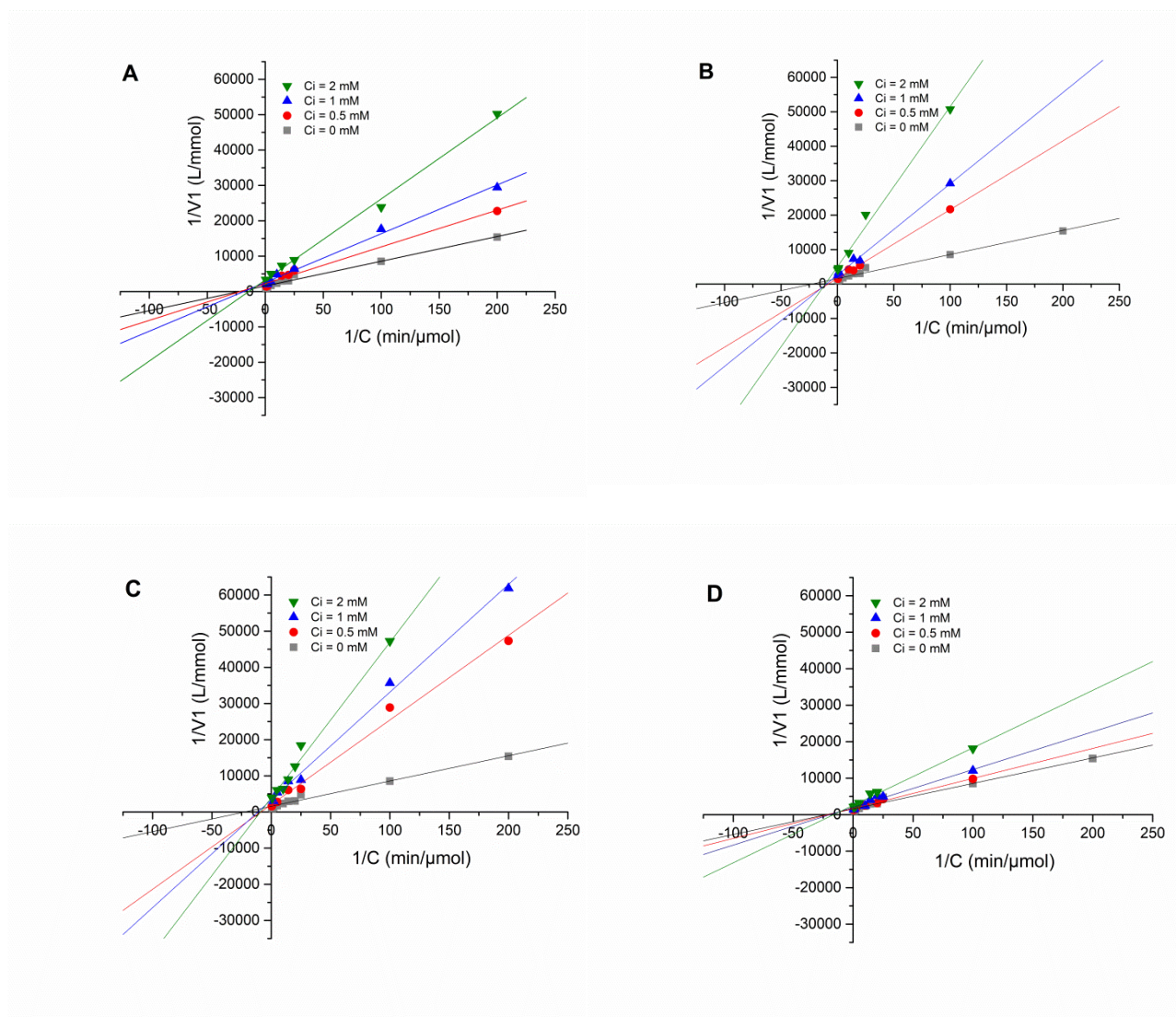
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 Sample Name 16 Instrument / Ser# micrOTOF CH3CN 10248  
 Comment 100 %, dil. 200, calibrant added

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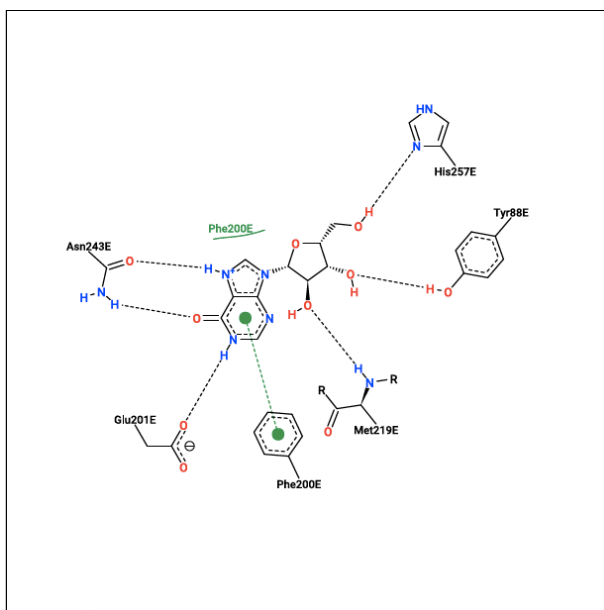
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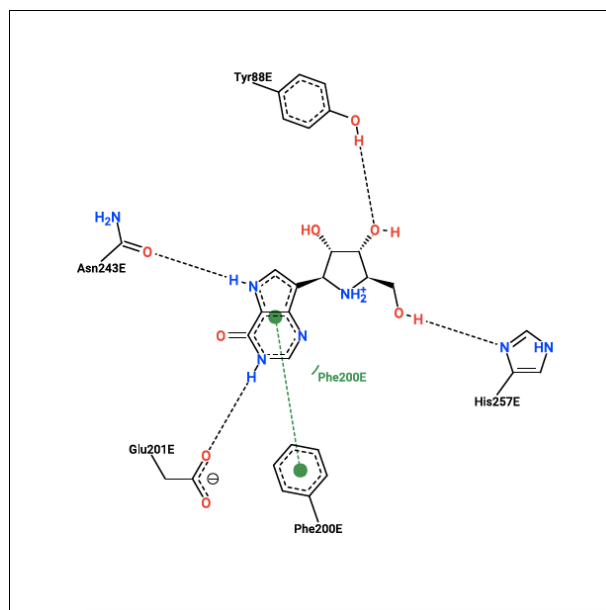
**Figure S1.** Lineweaver–Burk plots for the inosine phosphorolysis at concentrations of compounds 1, 2, 3 and 4 equal to 0, 0.5, 1 and 2 mM. (A) compound 1, (B) compound 2, (C) compound 3, (D) compound 4.



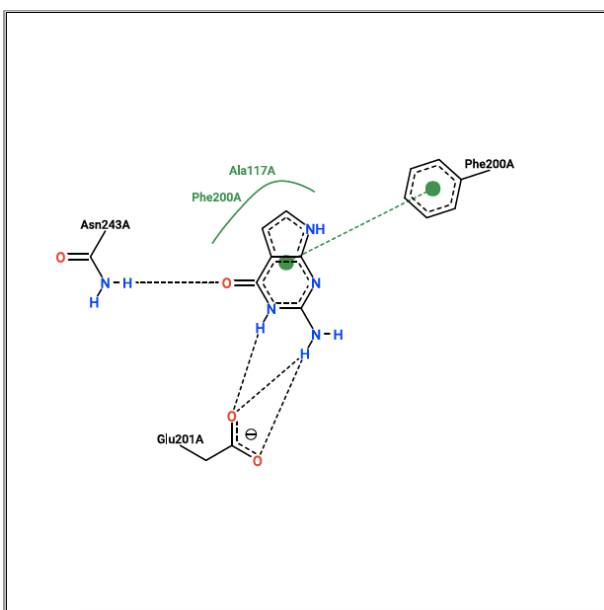
**Figure S2.** 2D diagrams of complexes PNP with various type of ligands.



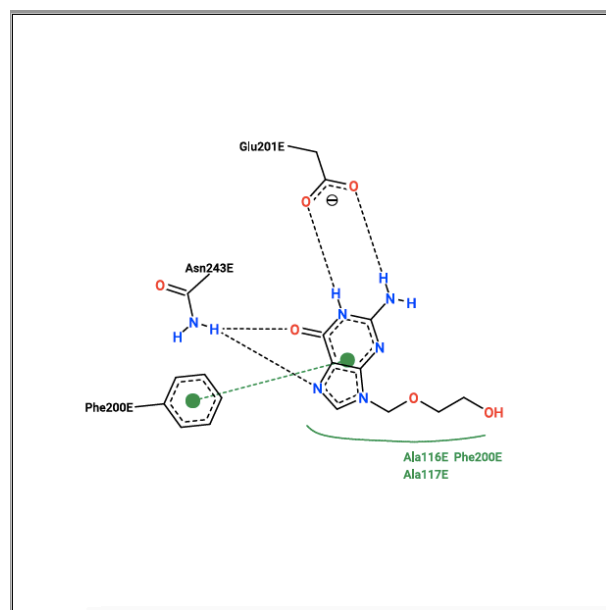
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Complex with Immucillin H (PDB ID code 1PF7)



Complex with 7-deazaguanine. (PDB ID code 3INY)



Complex with acyclovir (PDB ID code 1PWY)

**Figure S3.** Structure of the 3INY with re-docked 7-deazaguanine (An overlap the red wire – native ligand from PDB database; the red stick docked ligand. The box for docking ligands was highlighted in green ( $12 \text{ \AA} \times 10 \text{ \AA} \times 10 \text{ \AA}$ .)

