

## Supplementary Material

### New flexible analogues of 8-aza-7-deazapurine nucleosides as potential antibacterial agents

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# HPLC and mass spectrometry data

IBCH RAS

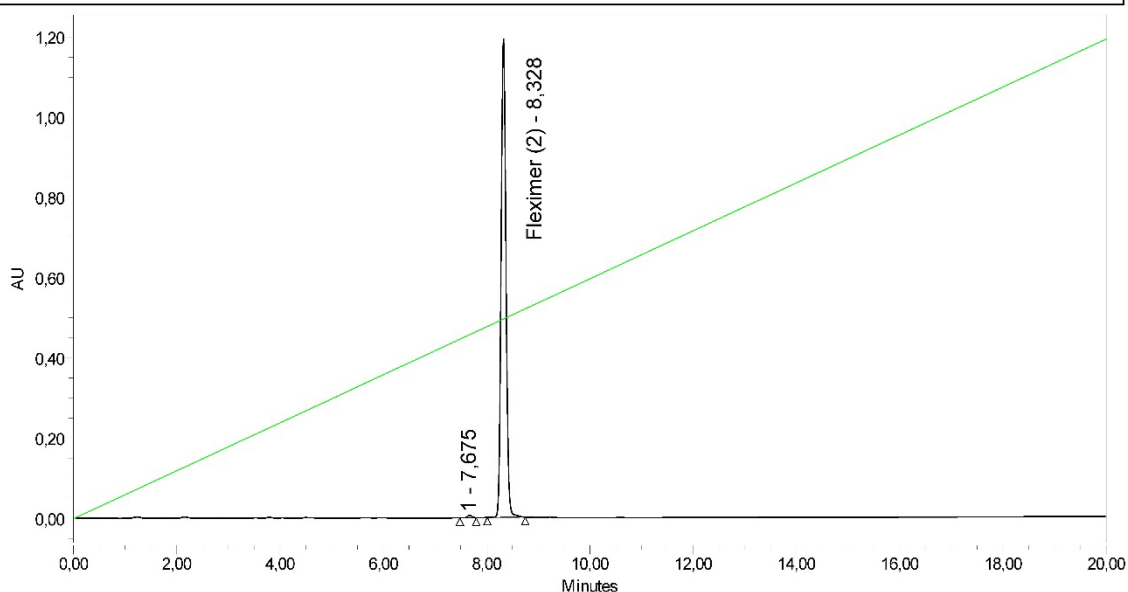
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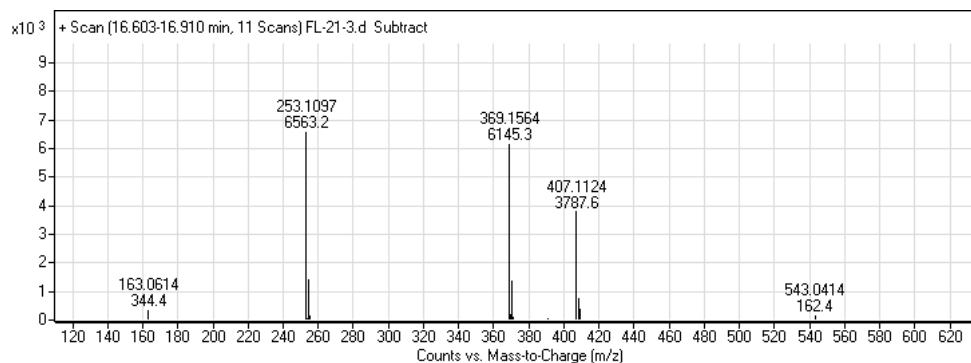


## SAMPLE INFORMATION

Sample Name:	Fleximer (2)	Acquired By:	Breeze
Sample Type:	Unknown	Date Acquired:	20.03.2023 18:54:10 GMT-4
Vial:	1	Acq. Method:	100B_dual_230nm_05ml
Injection #:	2	Date Processed:	20.03.2023 19:15:34 GMT-4
Injection Volume:	20,00 ul	Channel Name:	W2489 ChB
Run Time:	20,00 Minutes	Channel Desc.:	W2489 ChB 254nm
Column Type:		Sample Set Name:	



	Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	Peak 1	7,675	35388	0,46	5740	0,48
2	Fleximer (2)	8,328	7637798	99,54	1194687	99,52

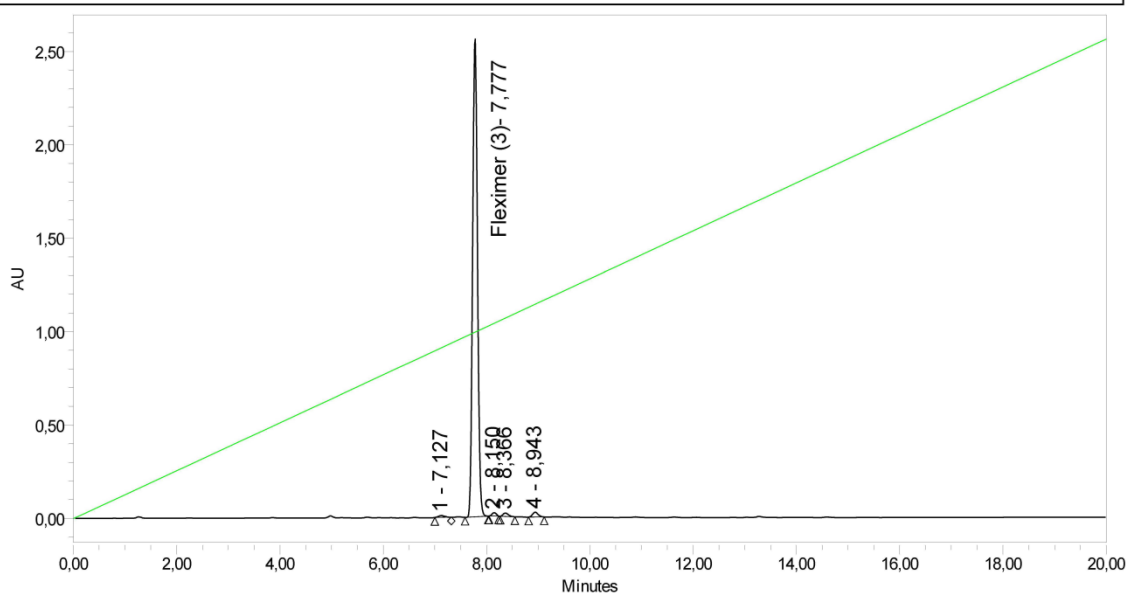


1-(β-D-2'-Deoxyribofuranosyl)-4-(4-benzoyloxypyrimidin-5-yl)pyrazole (2)

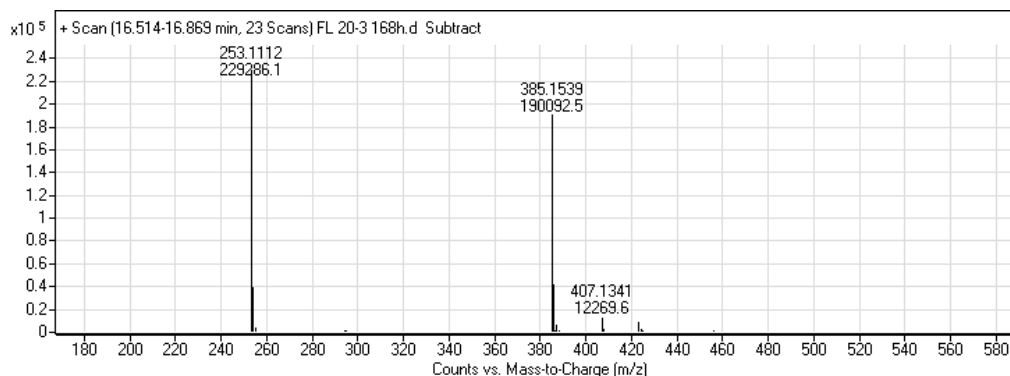
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Sample Name: Fleximer (3)  
 Sample Type: Unknown  
 Vial: 1  
 Injection #: 1  
 Injection Volume: 15,00 µl  
 Run Time: 20,00 Minutes  
 Column Type:

Acquired By: Breeze  
 Date Acquired: 02.03.2023 13:40:20 GMT-4  
 Acq. Method: 100B\_dual\_230nm\_05ml  
 Date Processed: 20.03.2023 18:59:13 GMT-4  
 Channel Name: W2489 ChB  
 Channel Desc.: W2489 ChB 254nm  
 Sample Set Name:



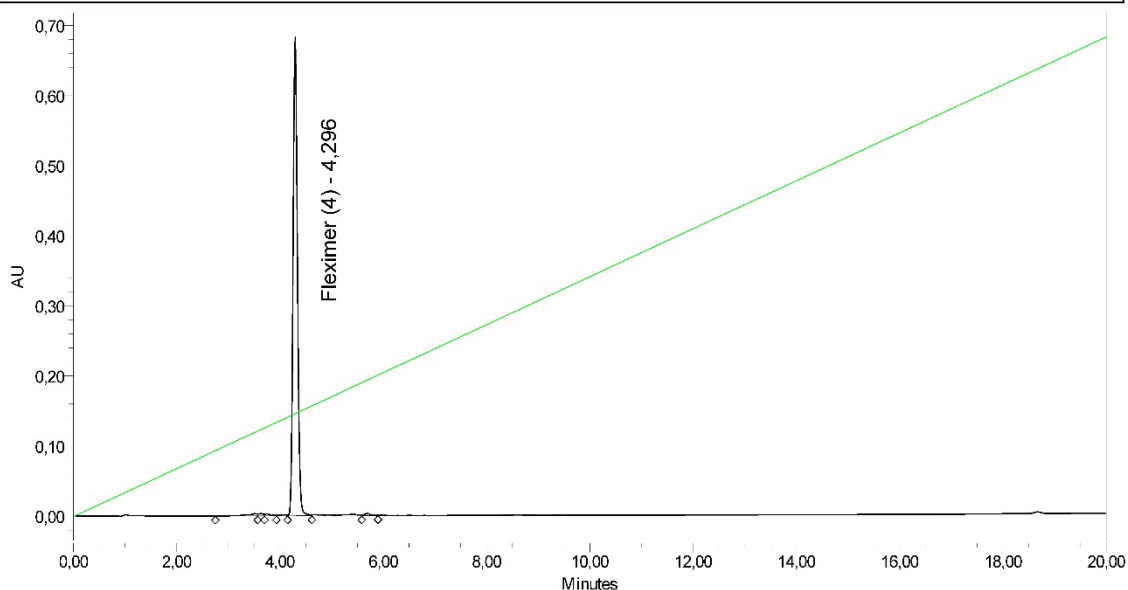
	Peak Name	RT (min)	Area (µV*sec)	% Area	Height (µV)	% Height
1	1	7,127	81342	0,48	9355	0,35
2	Fleximer (3)	7,777	16480090	97,03	2567521	97,29
3	2	8,150	100170	0,59	17952	0,68
4	3	8,366	129334	0,76	17959	0,68
5	4	8,943	194086	1,14	26299	1,00



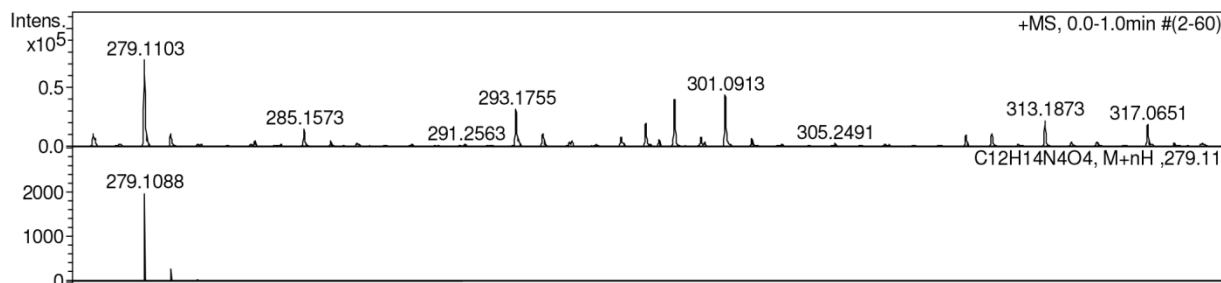
1-(β-D-Ribofuranosyl)-4-(4-benzoyloxypyrimidin-5-yl)pyrazole (3)

## SAMPLE INFORMATION

Sample Name:	Fleximer (4)	Acquired By:	Breeze
Sample Type:	Unknown	Date Acquired:	01.06.2023 16:22:01 GMT-4
Vial:	1	Acq. Method:	100B_dual_230nm_05ml
Injection #:	1	Date Processed:	01.06.2023 16:50:42 GMT-4
Injection Volume:	10,00 ul	Channel Name:	W2489 ChB
Run Time:	20,00 Minutes	Channel Desc.:	W2489 ChB 254nm
Column Type:		Sample Set Name:	



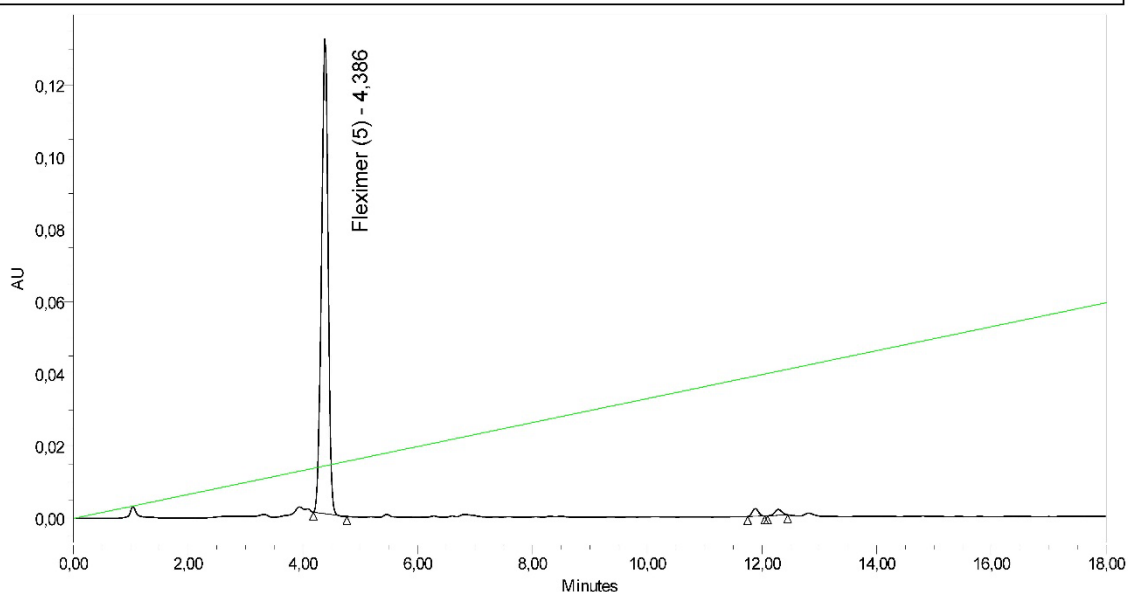
	Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	1	3,516	54322	1,31	3309	0,48
2	2	3,628	23993	0,58	3531	0,51
3	3	3,747	23156	0,56	2950	0,42
4	Fleximer (4)	4,296	4011516	96,84	682065	98,12
5	5	5,690	29295	0,71	3246	0,47



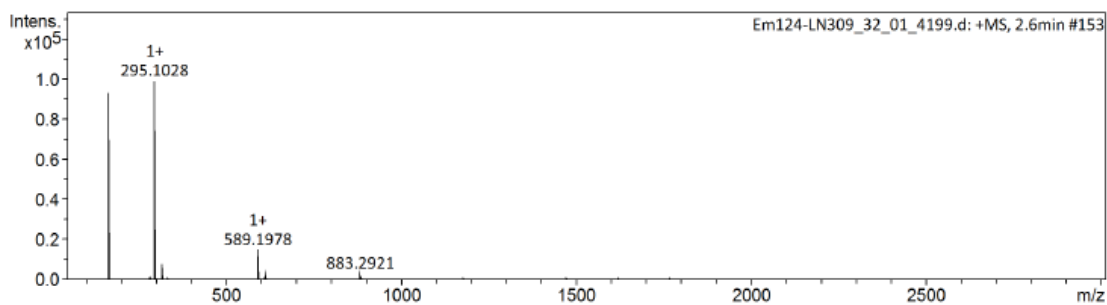
1-(β-D-2'-Deoxyribofuranosyl)-4-(pyrimidin-4(3*H*)-on-5-yl)pyrazole (4)

## SAMPLE INFORMATION

Sample Name:	Fleximer (5)	Acquired By:	Breeze
Sample Type:	Unknown	Date Acquired:	29.11.2022 17:06:42 GMT-4
Vial:	31	Acq. Method:	50B_dual_280_05ml
Injection #:	1	Date Processed:	14.06.2023 13:29:44 GMT-4
Injection Volume:	10,00 ul	Channel Name:	W2489 ChB
Run Time:	18,00 Minutes	Channel Desc.:	W2489 ChB 280nm
Column Type:		Sample Set Name:	Fleximers



	Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	Fleximer (5)	4,386	1049920	97,16	131302	97,18
2	3	11,884	16271	1,51	2141	1,59
3	4	12,286	14453	1,34	1664	1,23

1-(β-D-Ribofuranosyl)-4-(pyrimidin-4(3*H*)-on-5-yl)pyrazole (5)

# HPLC of side products from transglycosylation reaction mixture (fleximer riboside synthesis)

IBCH RAS

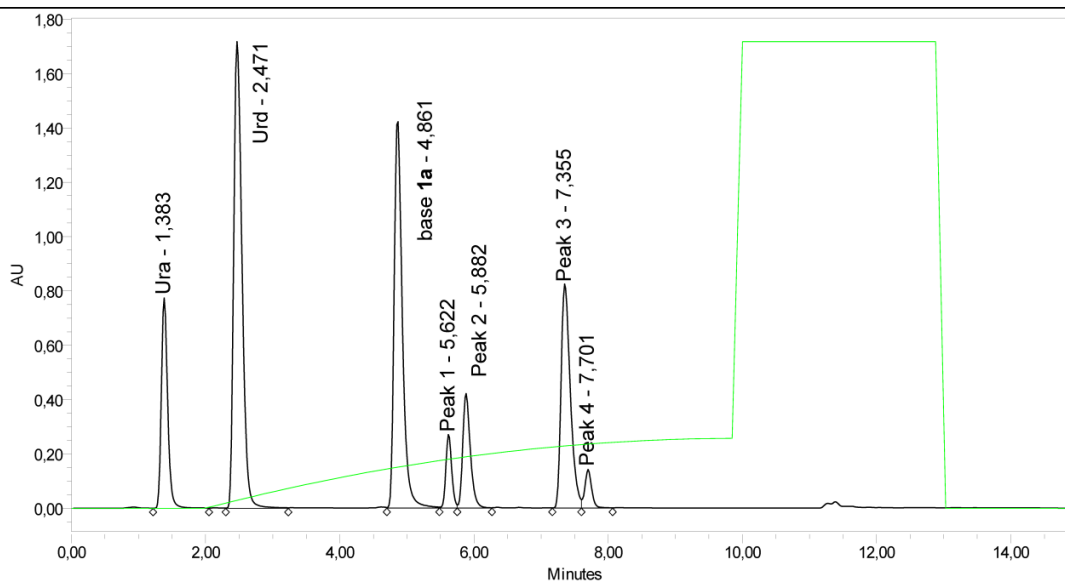
Project Name Defaults

Reported by User: Breeze user (Breeze)



## SAMPLE INFORMATION

Sample Name:	FL-11/1 1h	Acquired By:	Breeze
Sample Type:	Unknown	Date Acquired:	24.05.2021 15:58:16 GMT-4
Vial:	7	Acq. Method:	Fleximers_0_15B_10 min
Injection #:	1	Date Processed:	02.08.2023 13:42:16 GMT-4
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Run Time:	15,00 Minutes	Channel Desc.:	W2489 ChB 280nm
Column Type:		Sample Set Name:	Fleximers



	Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	Ura	1,383	5043469	11,01	769387	13,80
2	Urd	2,471	14716294	32,14	1720877	30,86
3	base 1a	4,861	12149922	26,53	1426226	25,58
4	Peak 1	5,622	1632296	3,56	270525	4,85
5	Peak 2	5,882	3334549	7,28	420576	7,54
6	Peak 3	7,355	7906597	17,27	826918	14,83
7	Peak 4	7,701	1008487	2,20	141244	2,53

Report Method: Gradient Overlay Report ASC

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Printed: 02.08.2023

13:45:09 Etc/GMT-4

# HPLC of side products from transglycosylation reaction mixture (fleximer 2'-deoxyriboside synthesis)

IBCH RAS

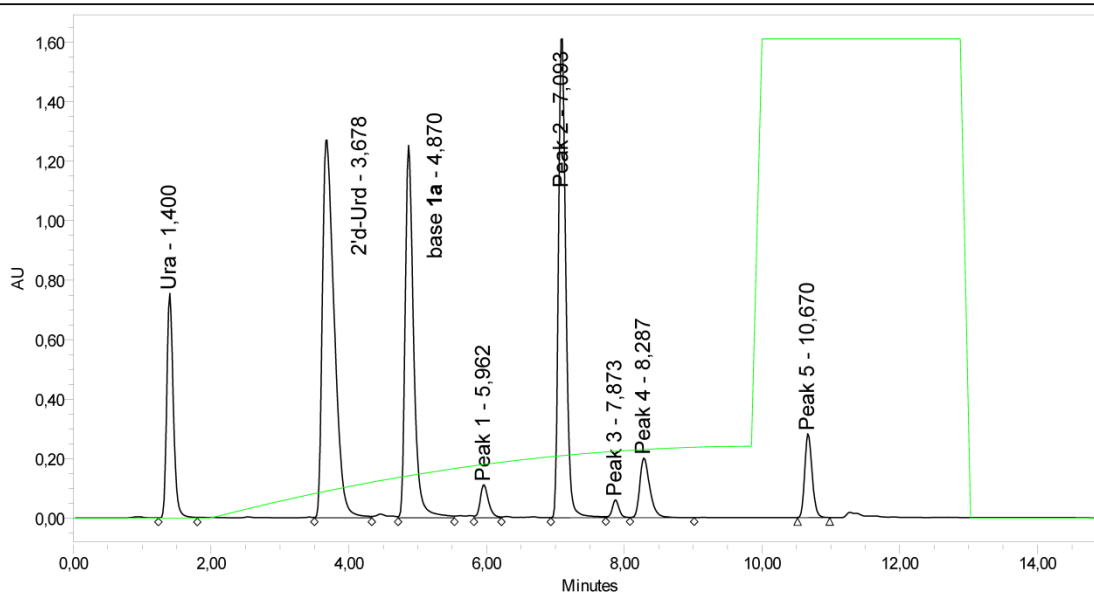
Project Name Defaults

Reported by User: Breeze user (Breeze)



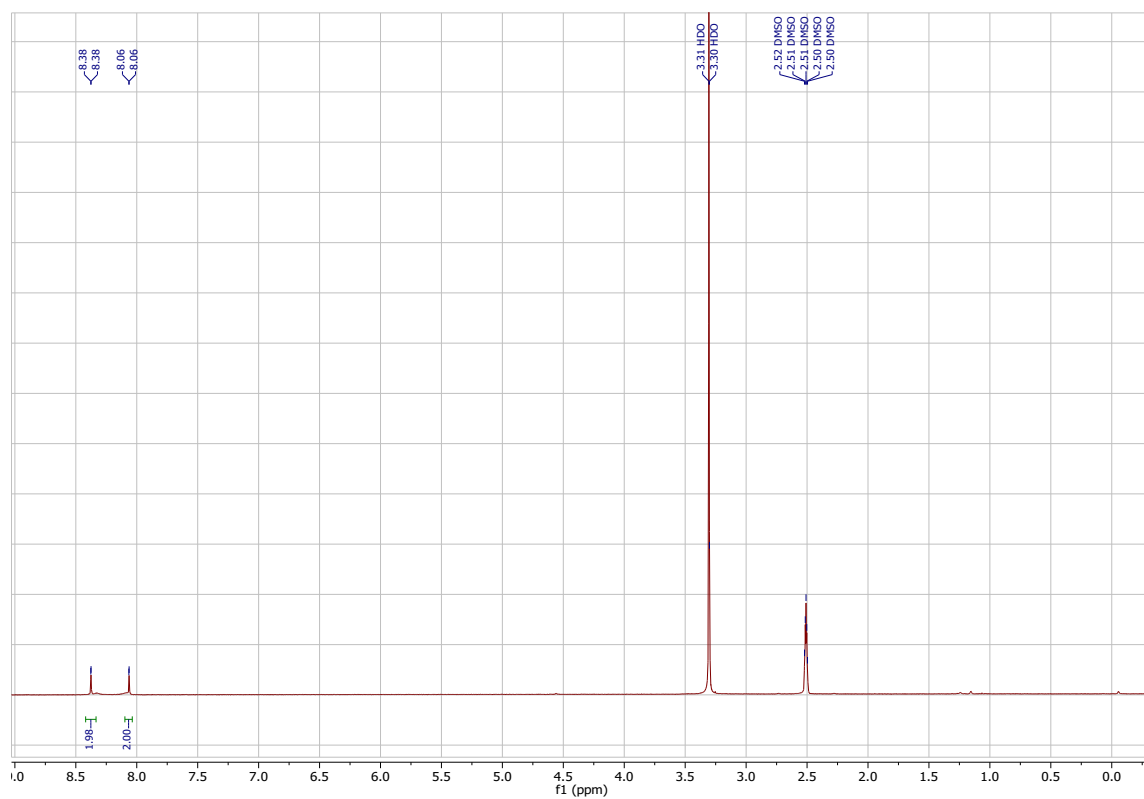
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Injection #:	1	Date Processed:	02.08.2023 13:51:27 GMT-4
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Column Type:		Sample Set Name:	Fleximers

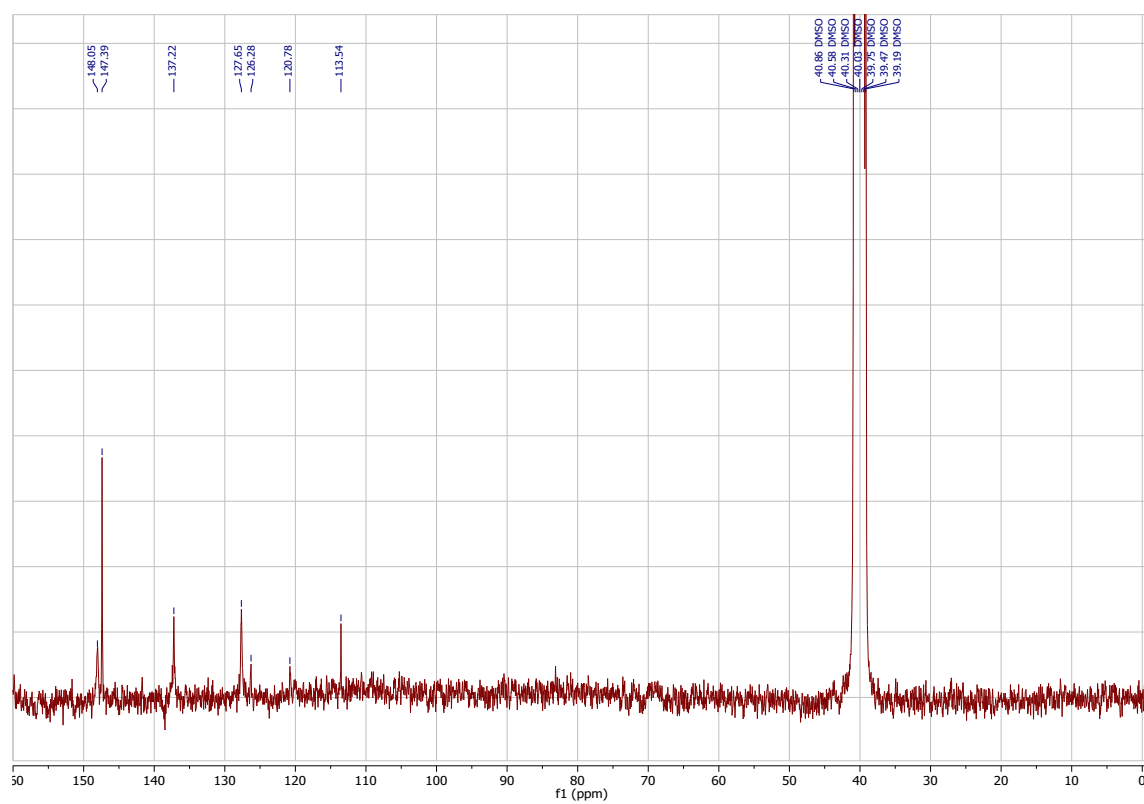


	Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	Ura	1,400	4974523	10,30	751107	13,54
2	2'd-Urd	3,678	15205213	31,47	1272912	22,94
3	base 1a	4,870	10682803	22,11	1251423	22,55
4	Peak 1	5,962	938773	1,94	110914	2,00
5	Peak 2	7,093	11945274	24,72	1619756	29,19
6	Peak 3	7,873	417468	0,86	60052	1,08
7	Peak 4	8,287	2045992	4,23	200852	3,62
8	Peak 5	10,670	2102629	4,35	282025	5,08

## NMR spectra of compounds

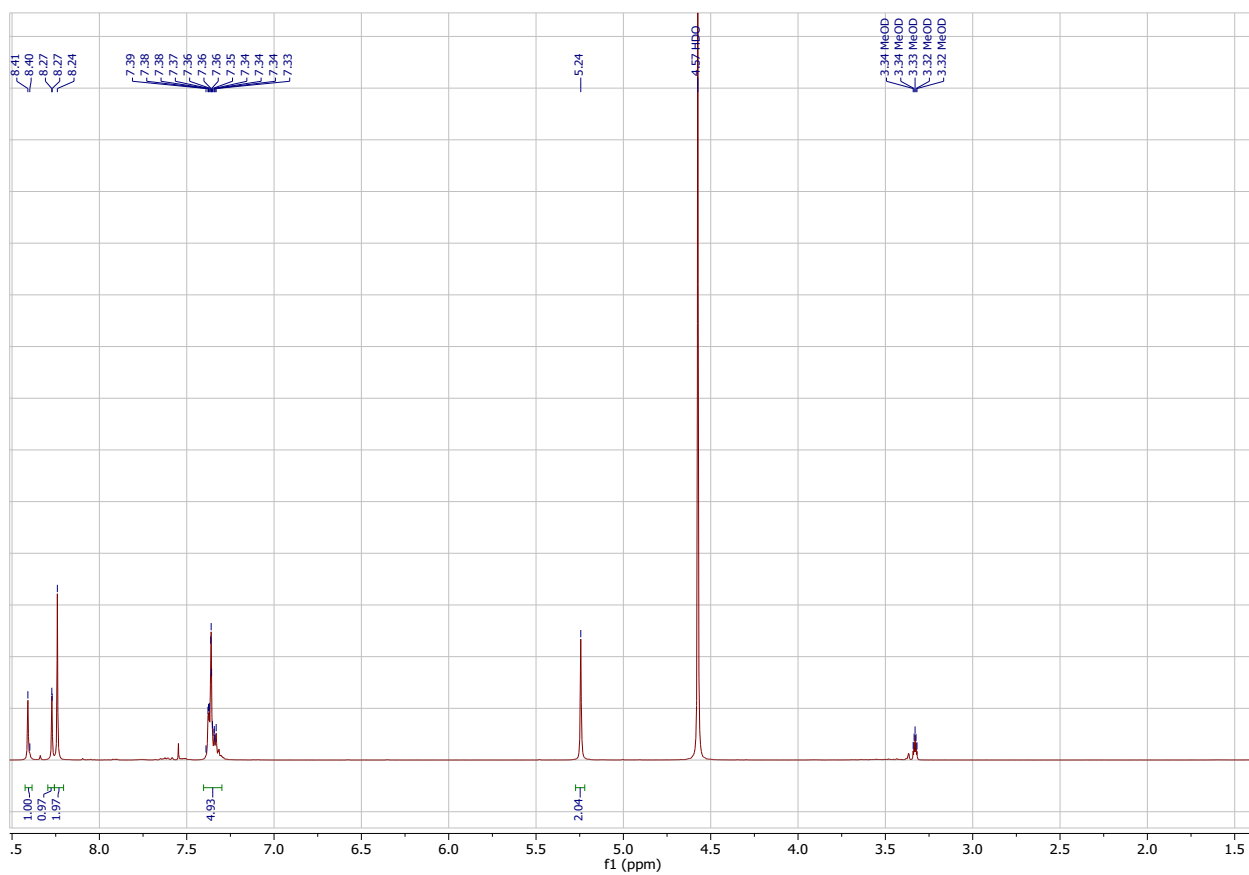


$^1\text{H}$  NMR spectrum of **1a** in  $\text{CD}_3\text{OD}$

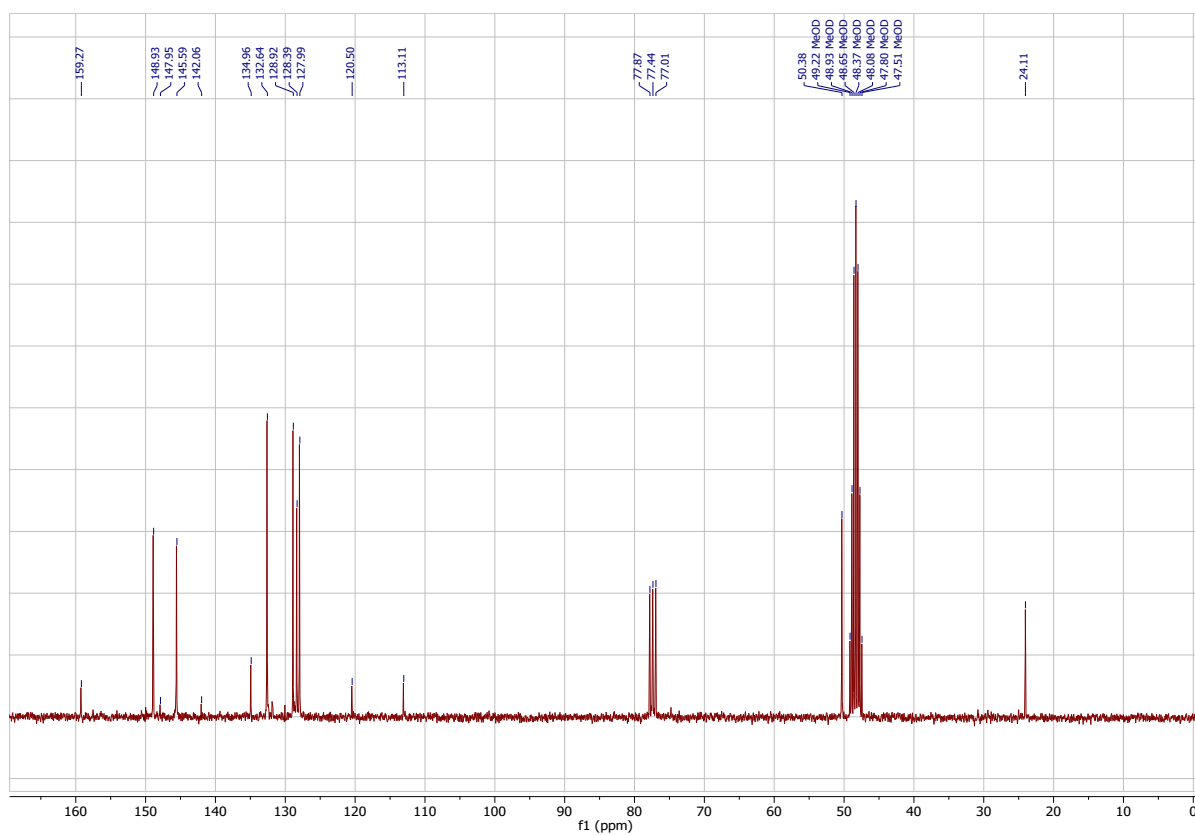


$^{13}\text{C}$  NMR spectrum of **1a** in  $\text{CD}_3\text{OD}$

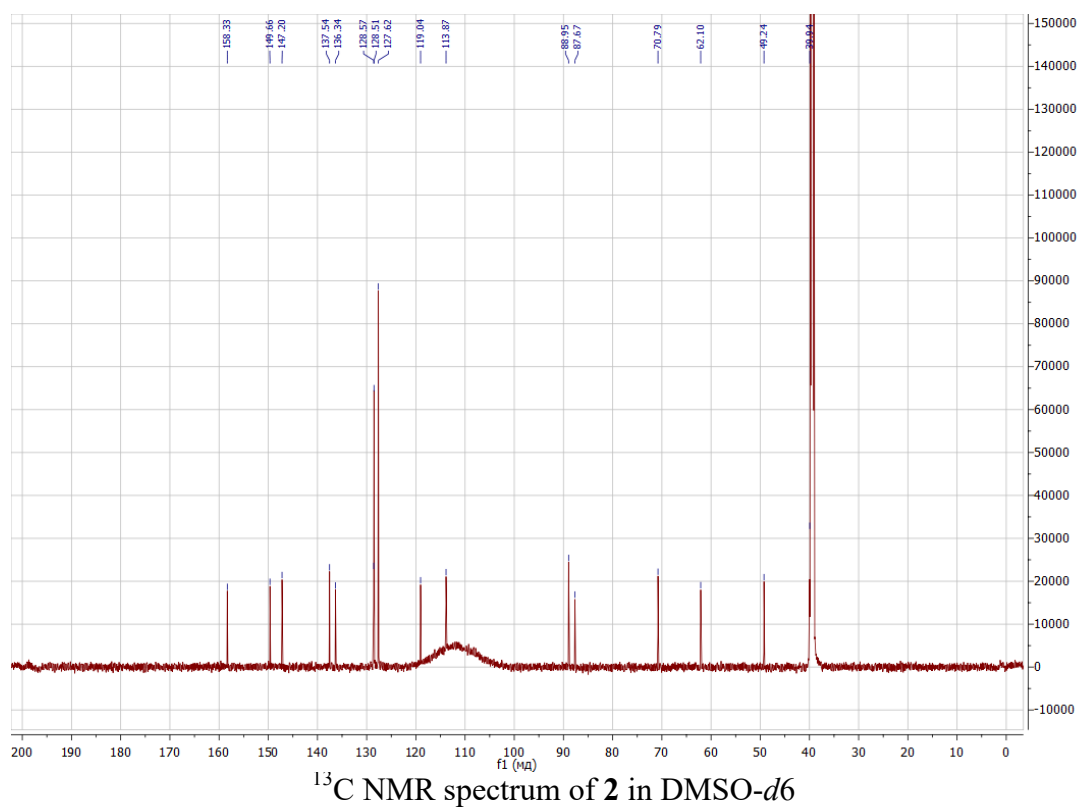
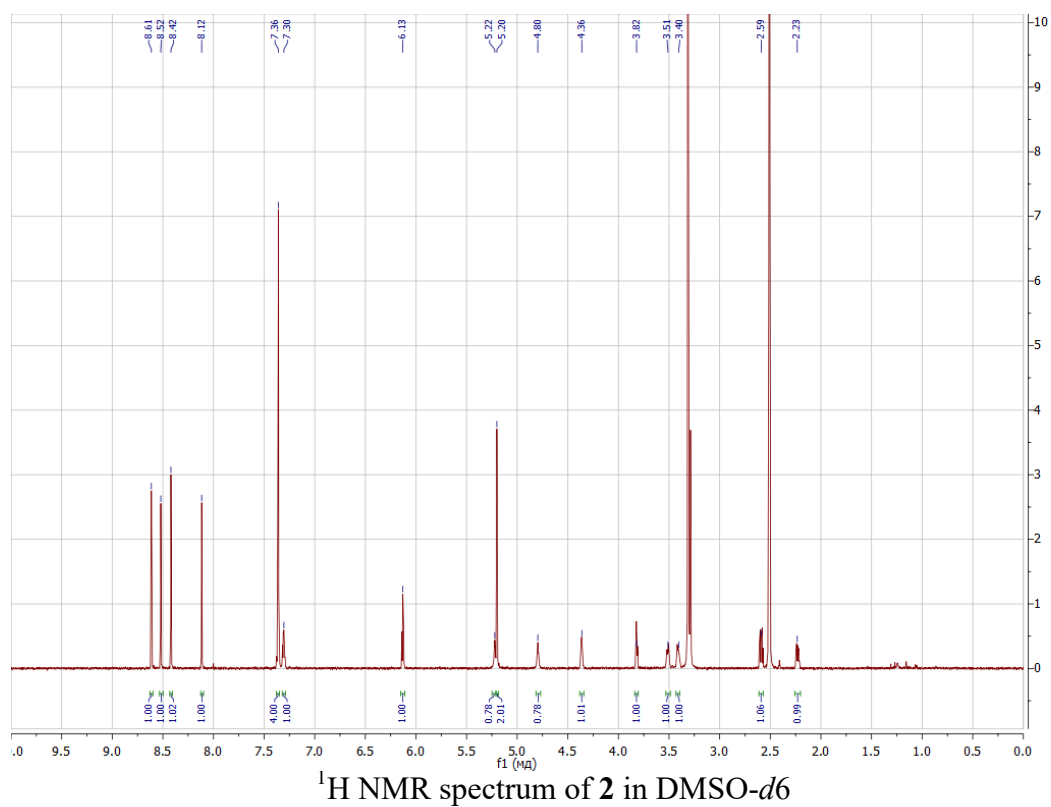


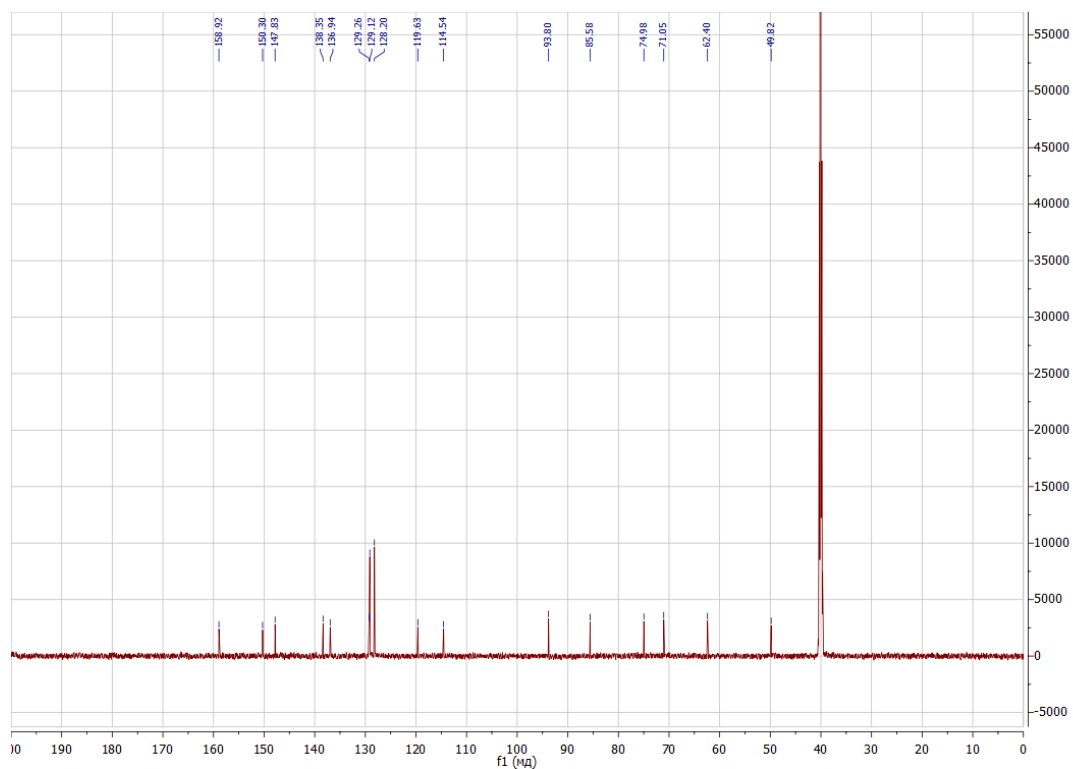
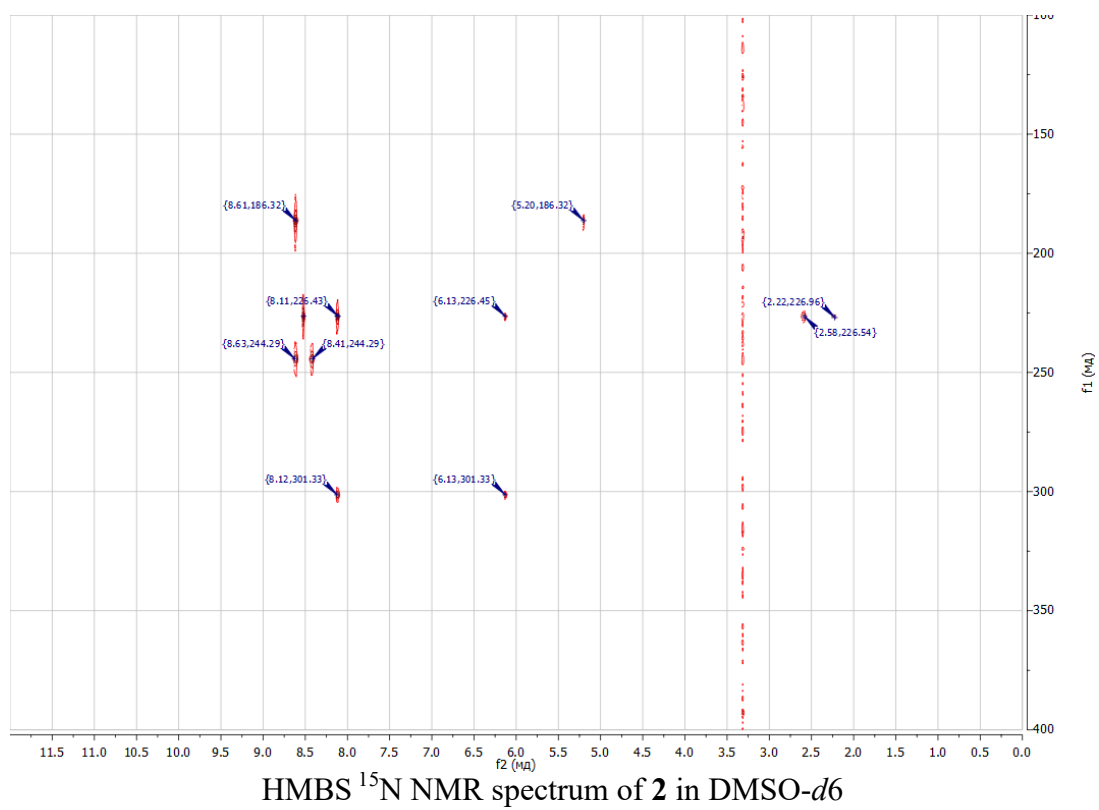


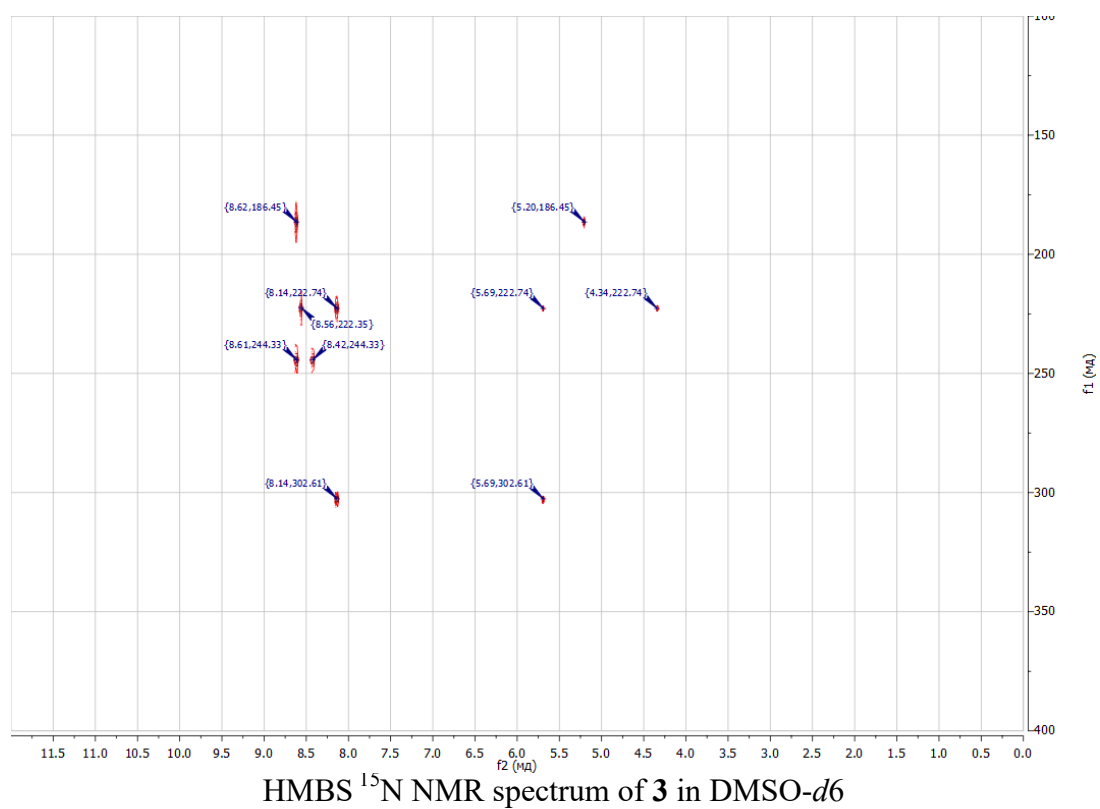
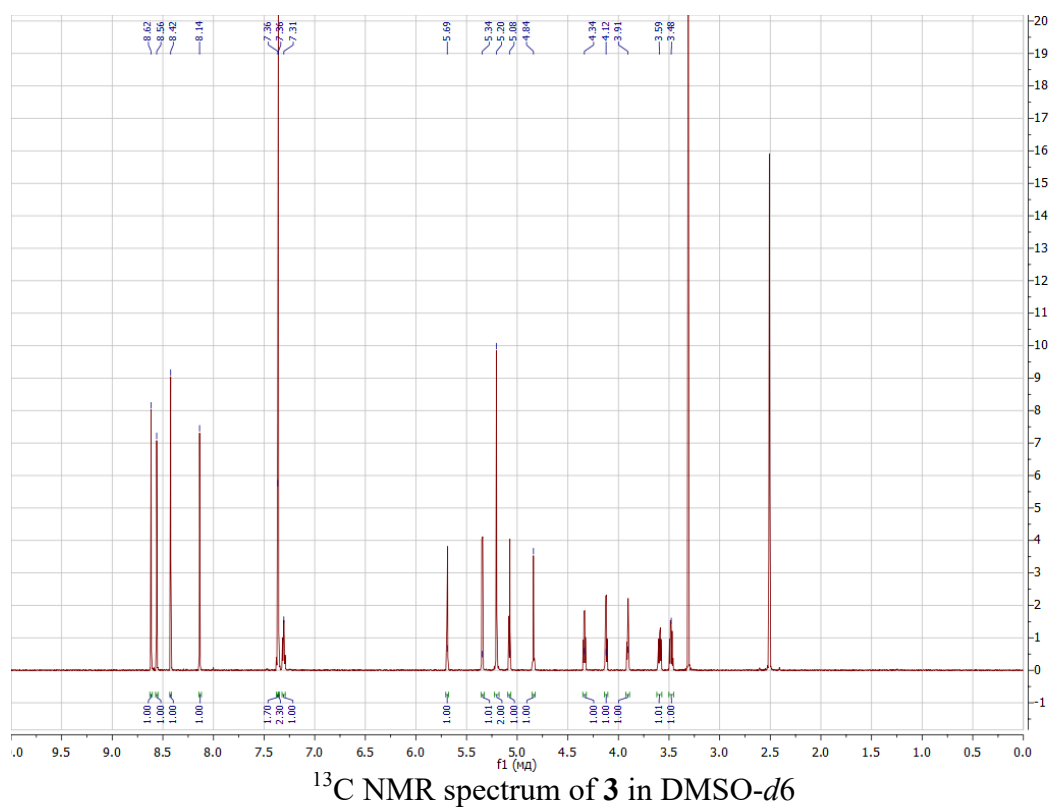
<sup>1</sup>H NMR spectrum of **1b** in CD<sub>3</sub>OD

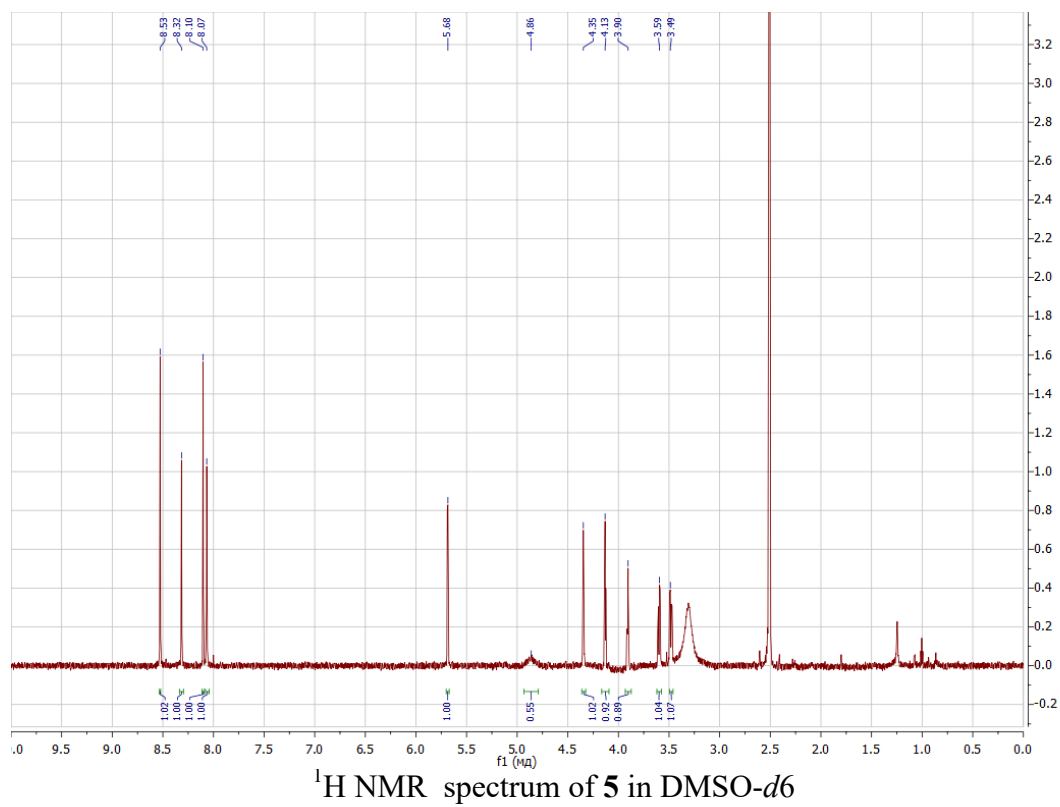
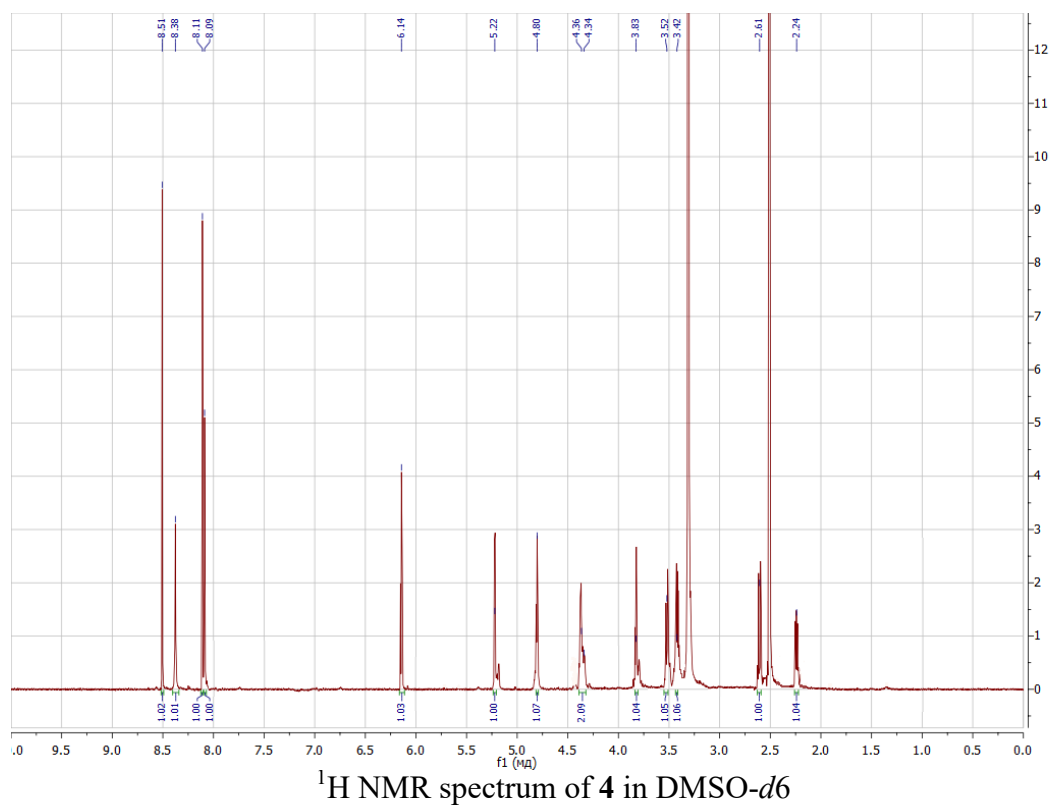


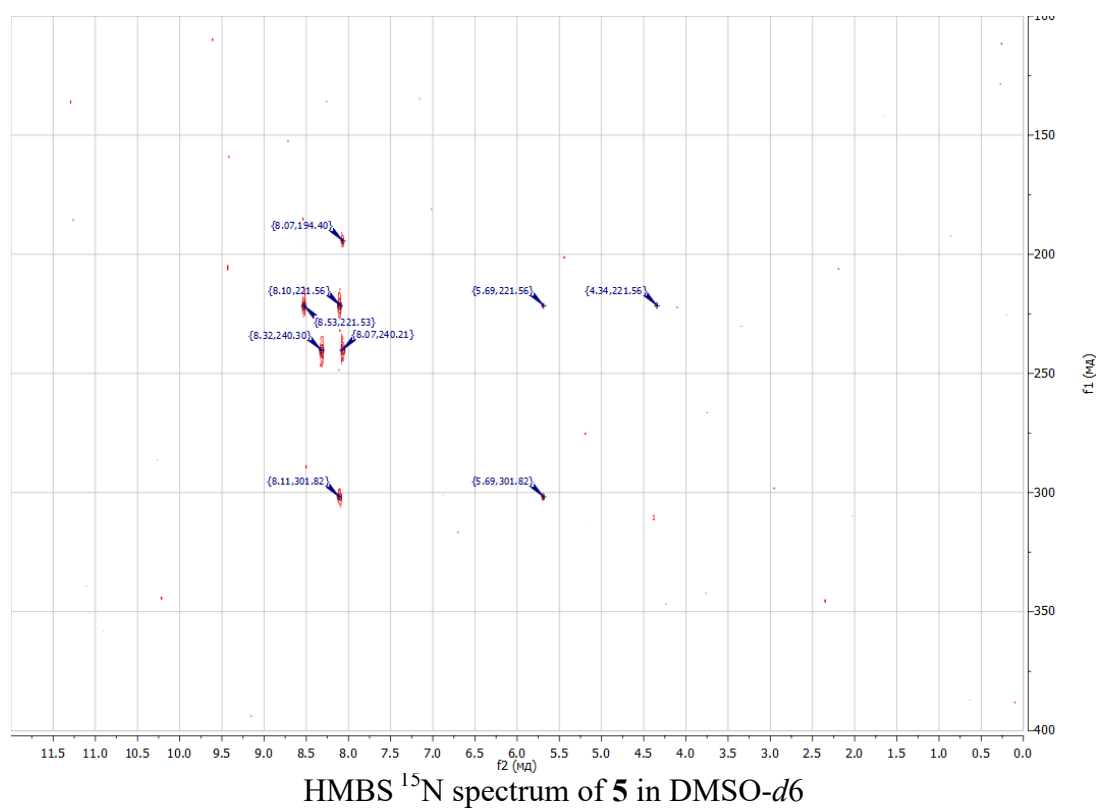
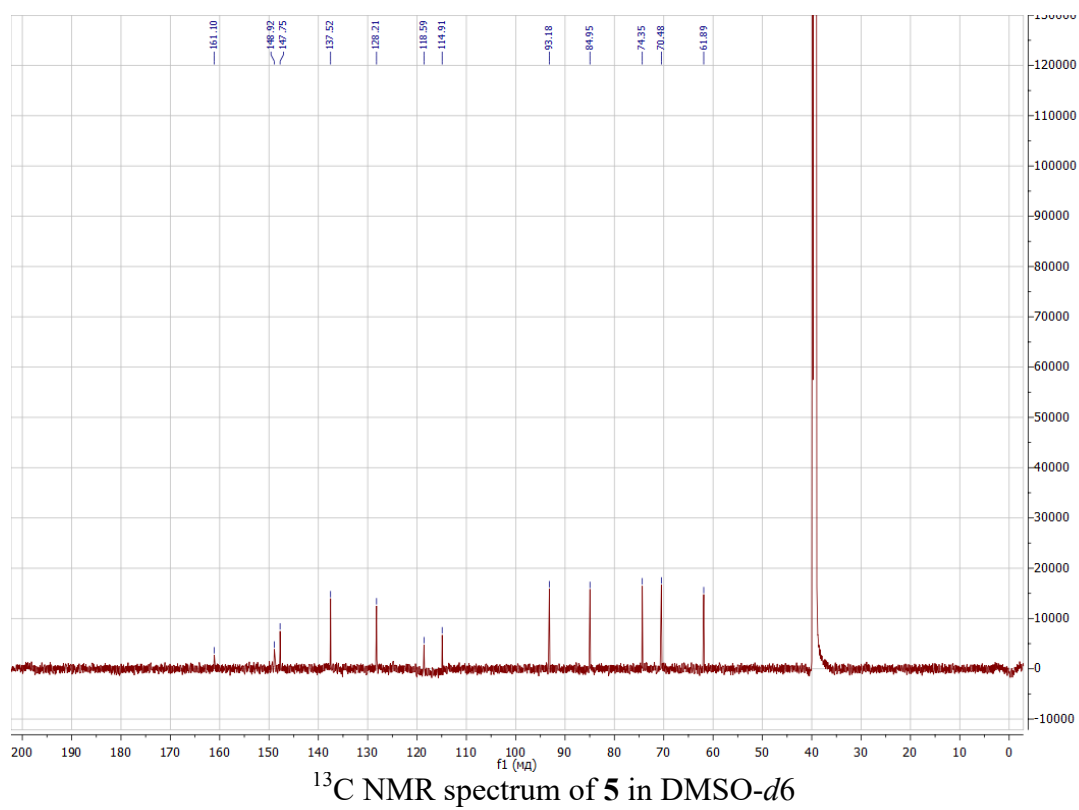
<sup>13</sup>C NMR spectrum of **1b** in CD<sub>3</sub>OD

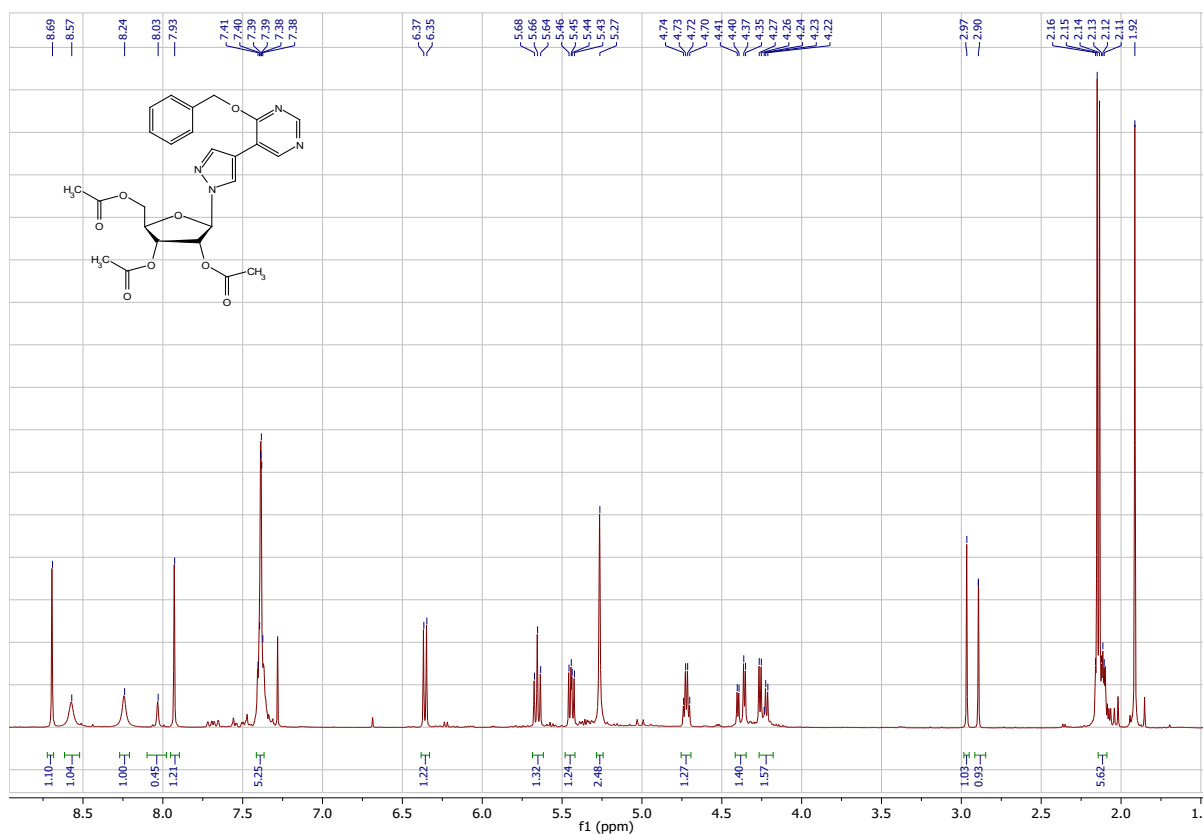




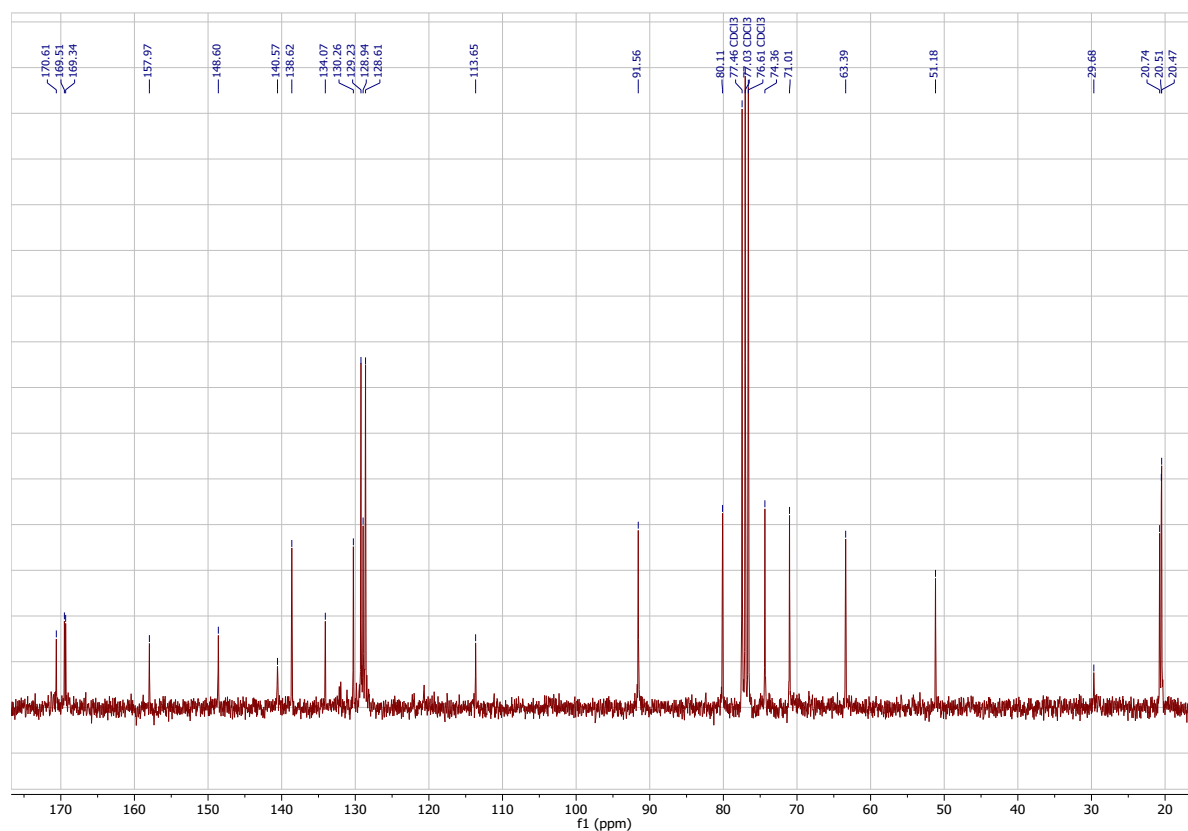




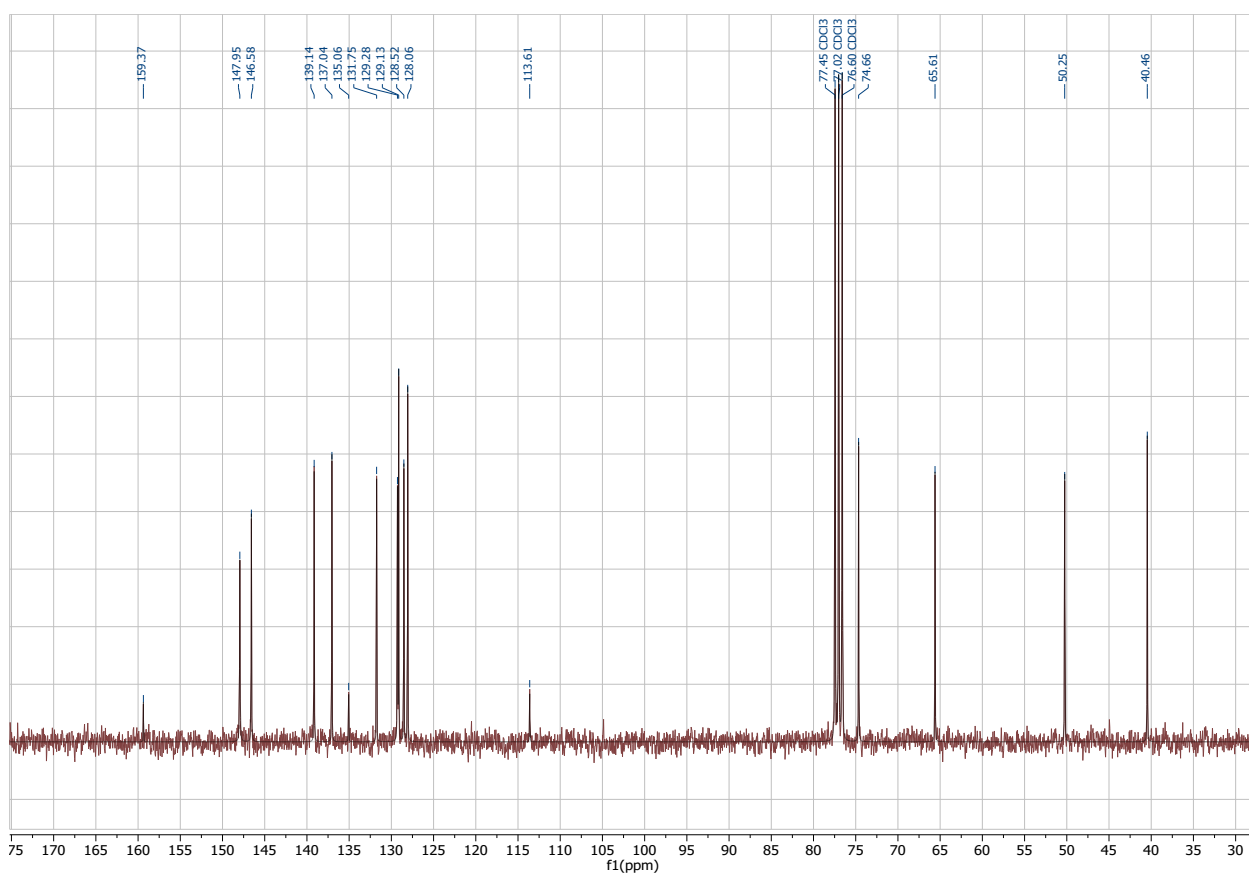
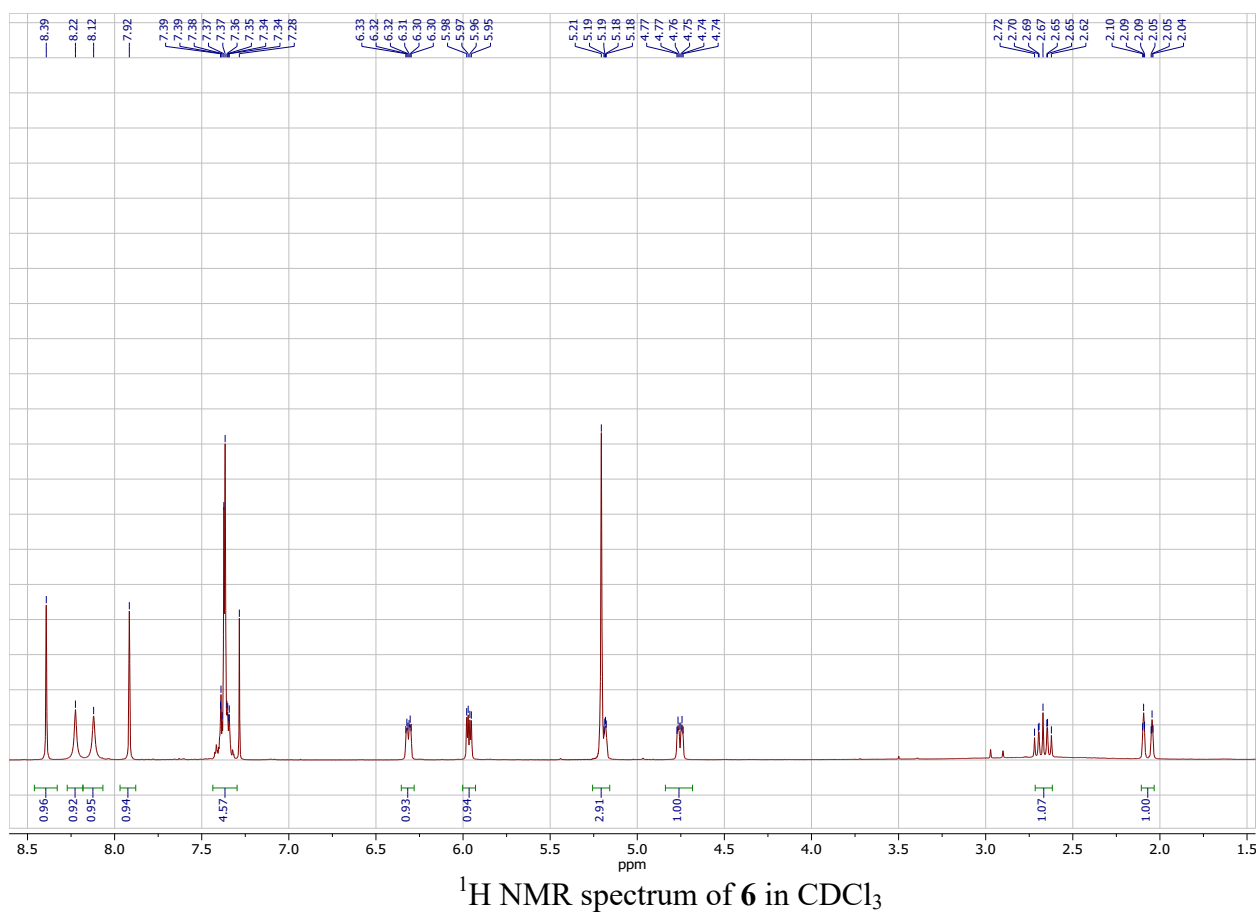




<sup>1</sup>H NMR spectrum of 1-(β-D-(2',3',5'-triacetylribofuranosyl))-4-(4-benzoyloxypyrimidin-5-yl)pyrazole in CDCl<sub>3</sub>

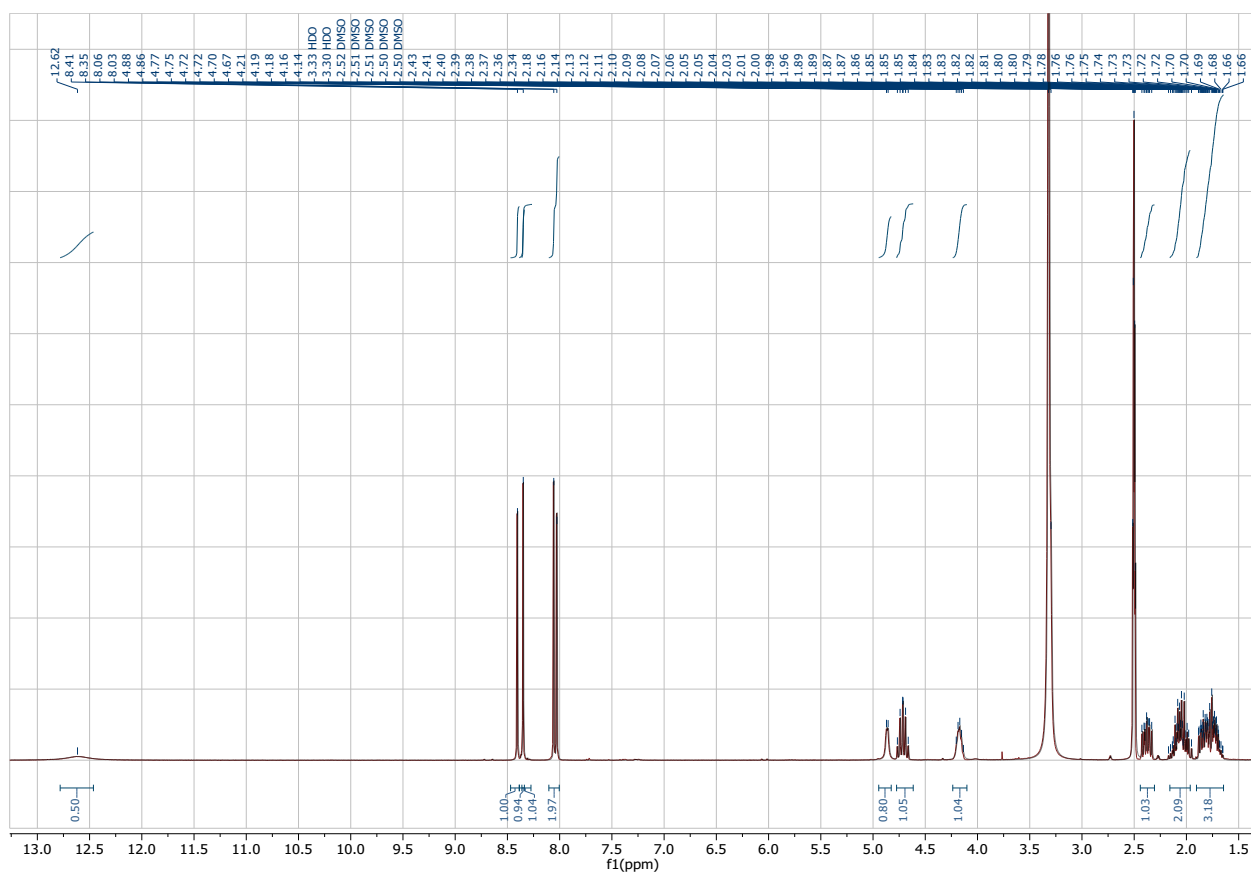


<sup>13</sup>C NMR spectrum of 1-(β-D-(2',3',5'-triacetylribofuranosyl))-4-(4-benzoyloxypyrimidin-5-yl)pyrazole in CDCl<sub>3</sub>

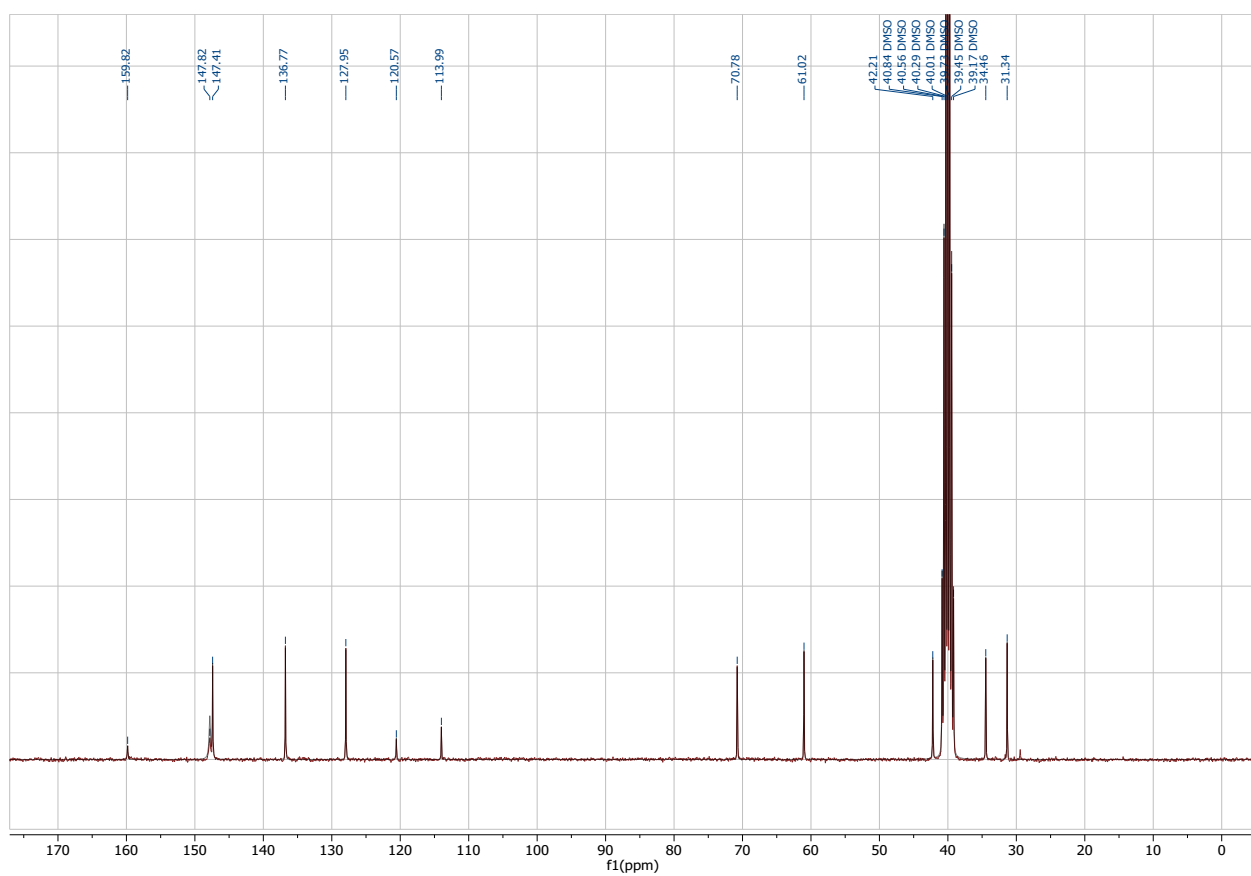


$^{13}\text{C}$  NMR spectrum of **6** in  $\text{CDCl}_3$

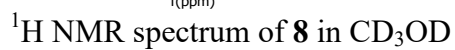
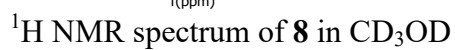


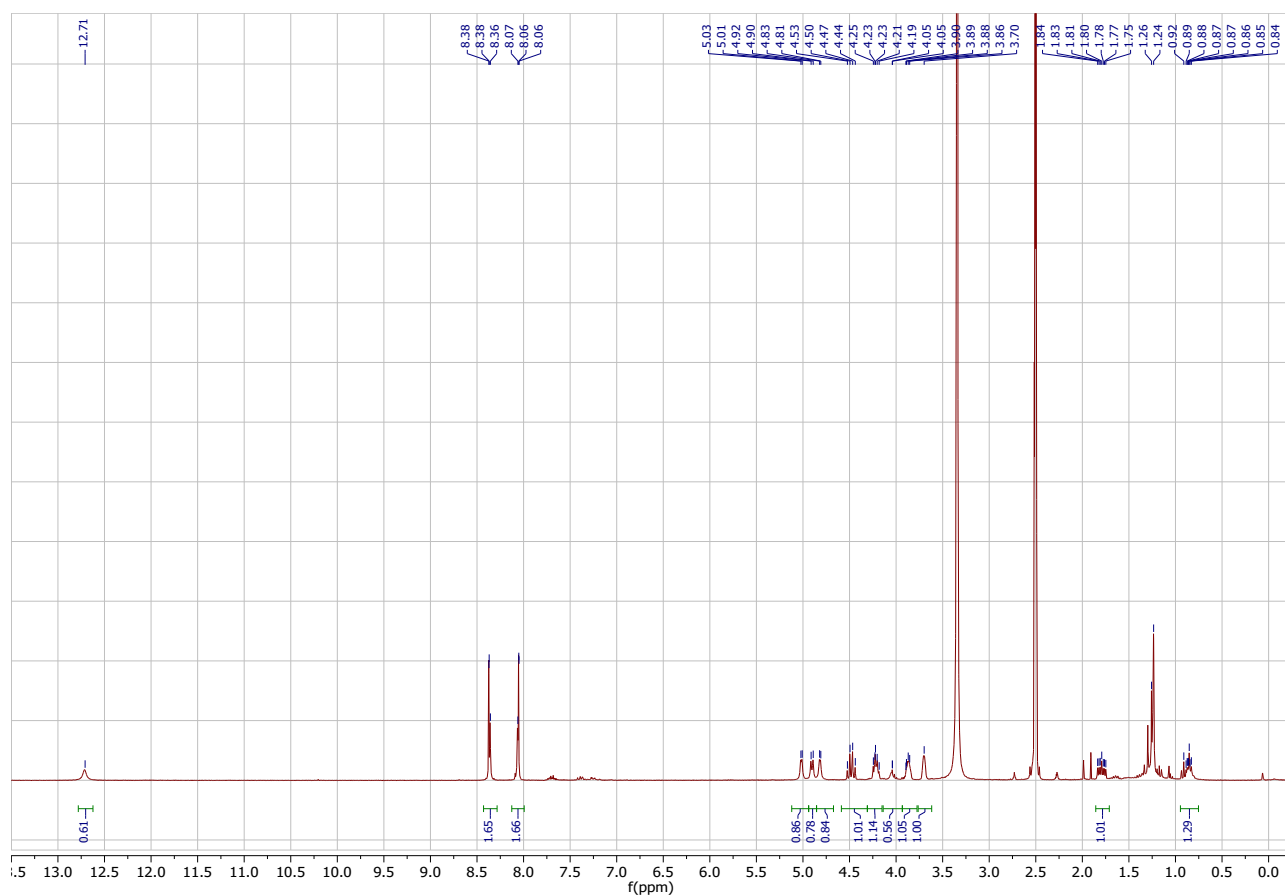


<sup>1</sup>H NMR spectrum of 7 in DMSO-*d*<sub>6</sub>

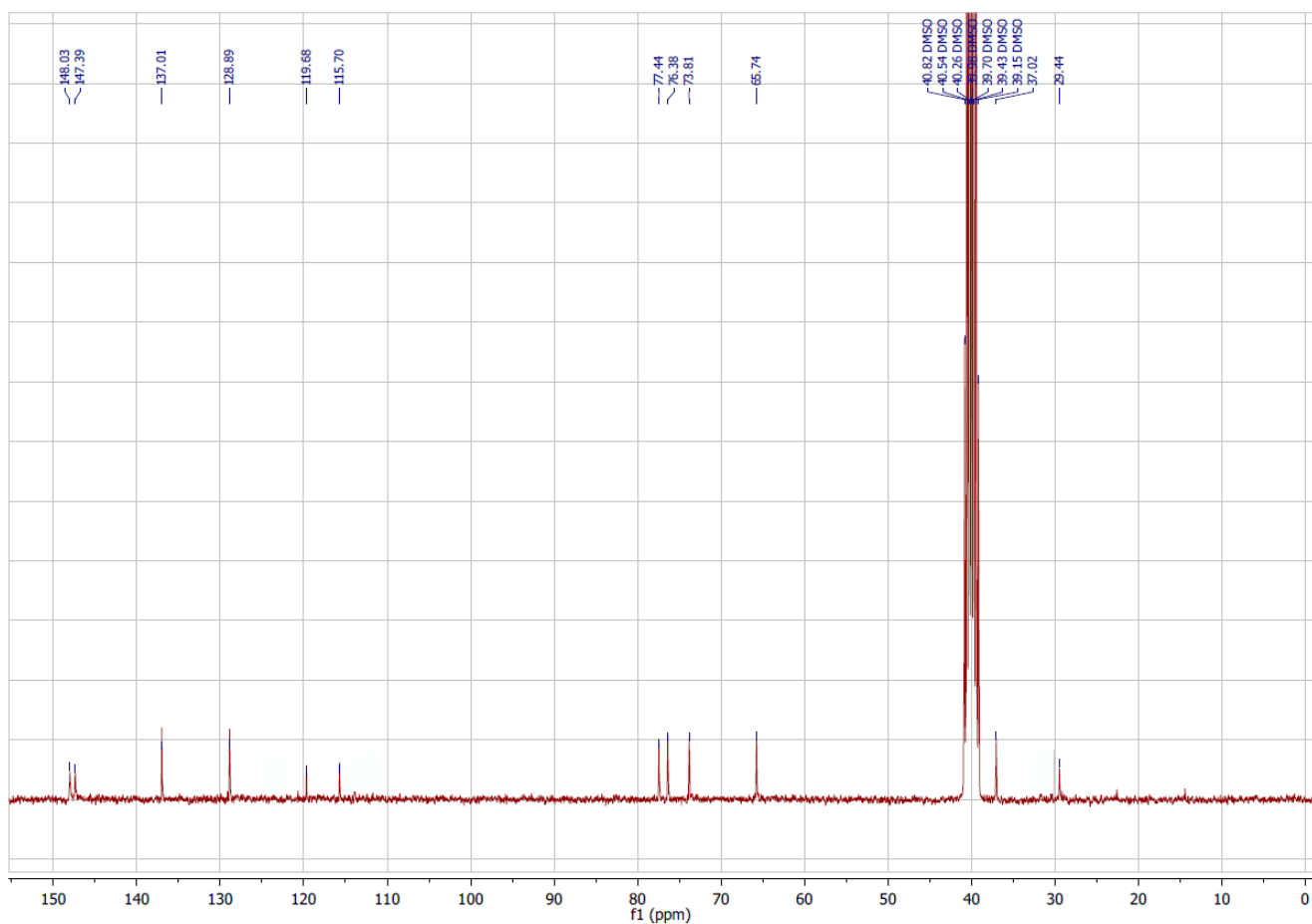


<sup>13</sup>C NMR spectrum of 7 in DMSO-*d*<sub>6</sub>





$^1\text{H}$  NMR spectrum of **9** in  $\text{DMSO}-d_6$



$^{13}\text{C}$  NMR spectrum of **9** in  $\text{DMSO}-d_6$

# HRMS spectrum of 1a

## Display Report

### Analysis Info

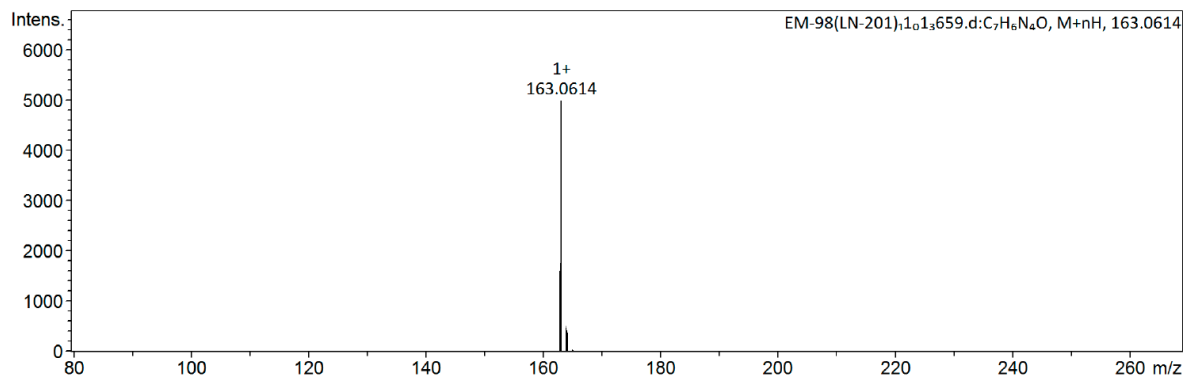
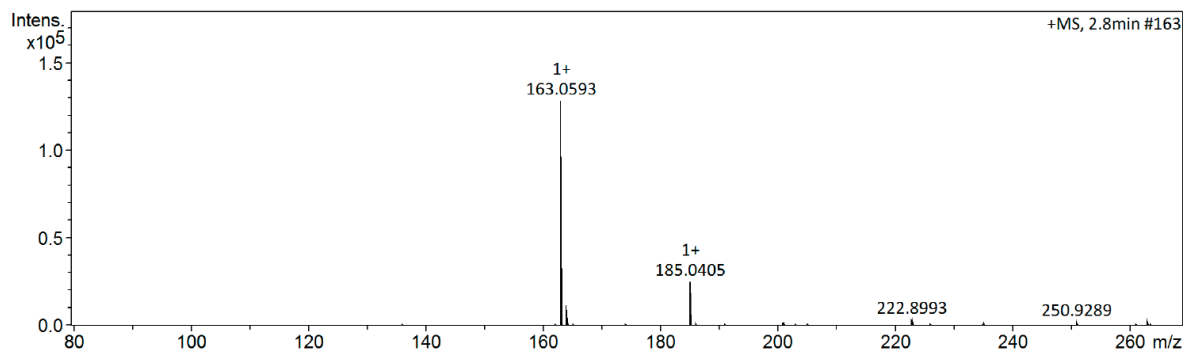
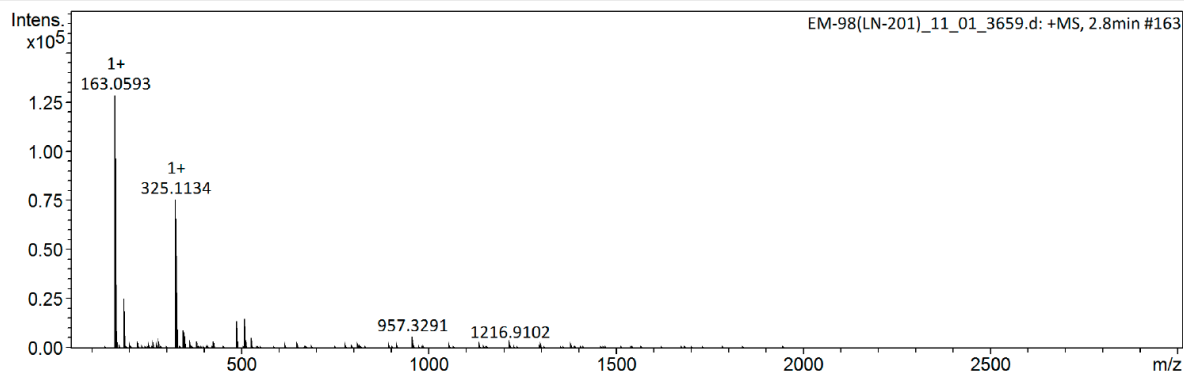
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 Sample Name 1a  
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Operator BDAL@DE  
 Instrument compact 8255754.20088

### Acquisition Parameter

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# HRMS spectrum of **1b**

## Display Report

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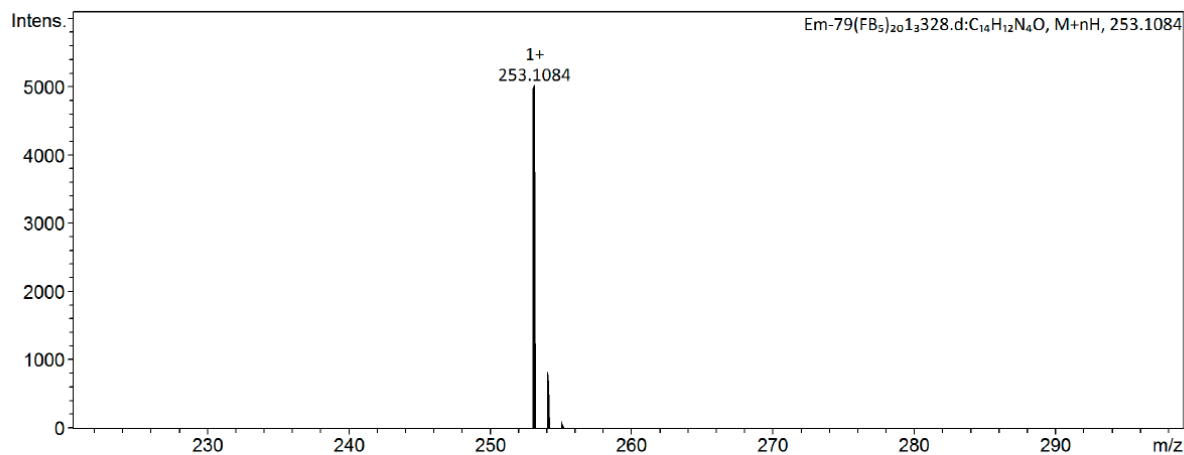
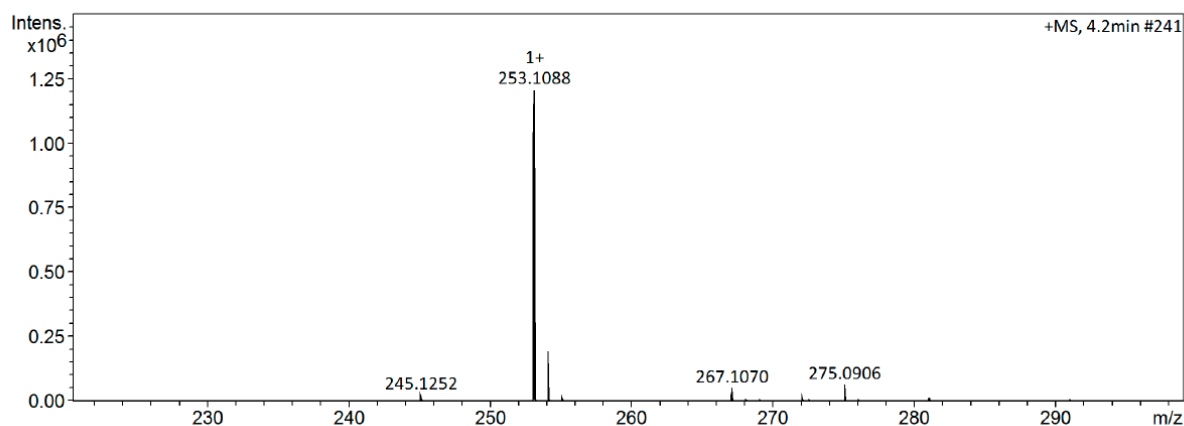
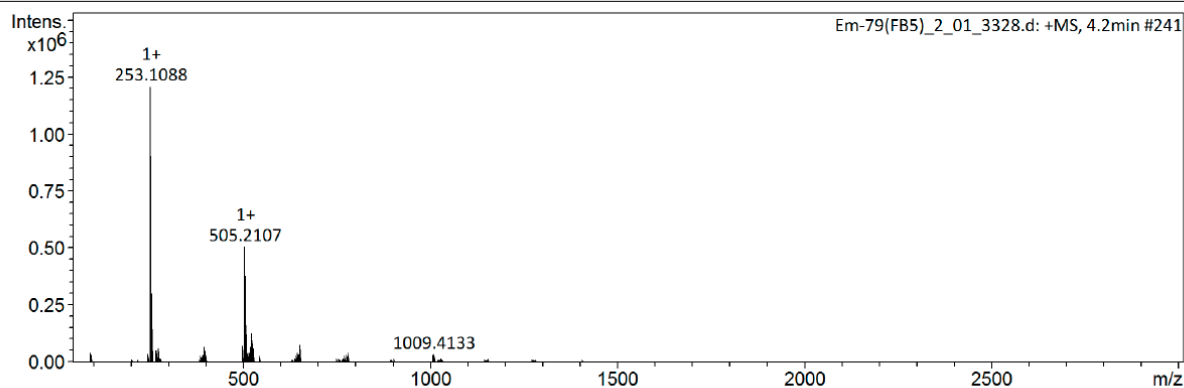
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 Sample Name 1b  
 Comment

Acquisition Date 3/27/2020 2:41:34 PM

Operator BDAL@DE  
 Instrument compact 8255754.20088

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
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# HRMS spectrum of 6

## Display Report

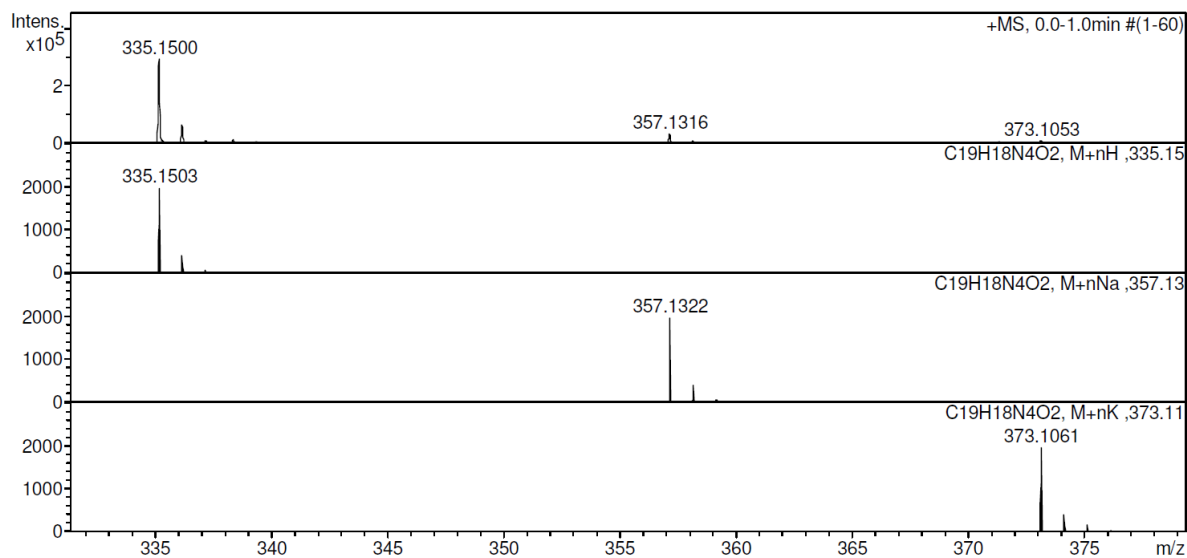
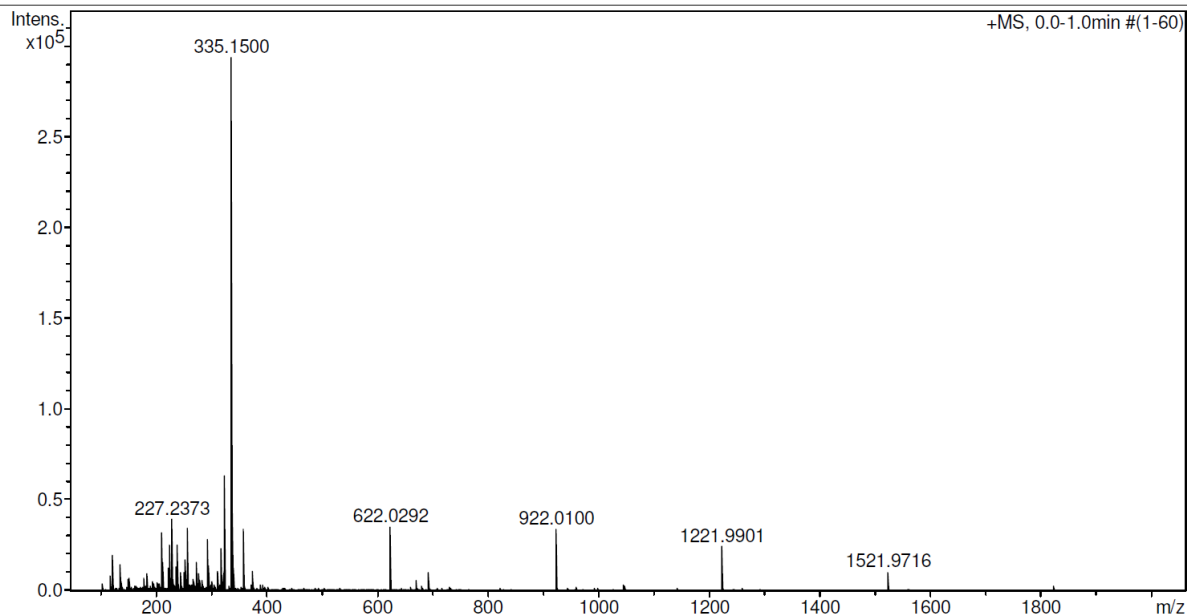
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 Sample Name 6  
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Acquisition Date 07.08.2023 14:51:03  
 Operator BDAL@DE  
 Instrument / Ser# microTOF CH3CN : 10248

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Focus	Not active			Set Dry Heater	180 °C
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# HRMS spectrum of 7

## Display Report

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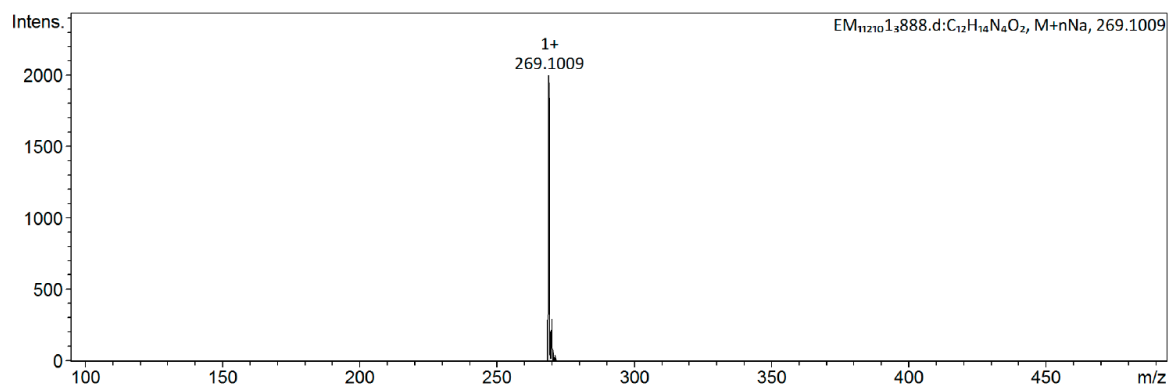
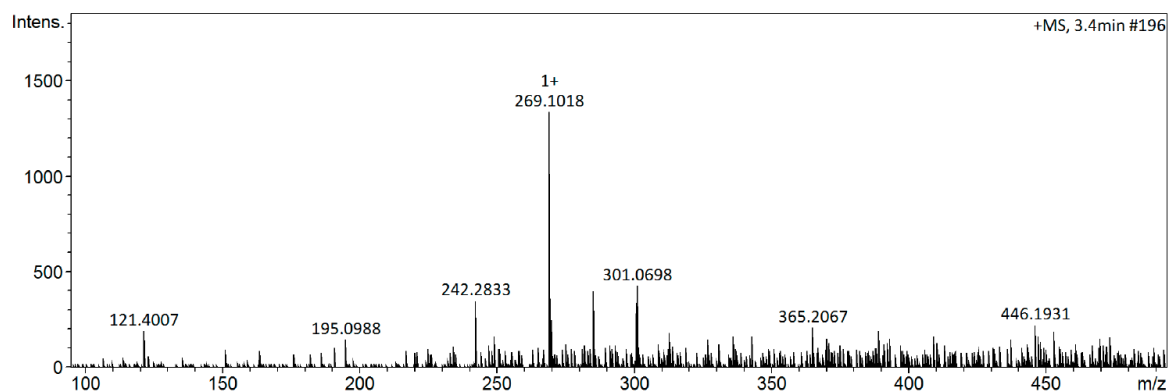
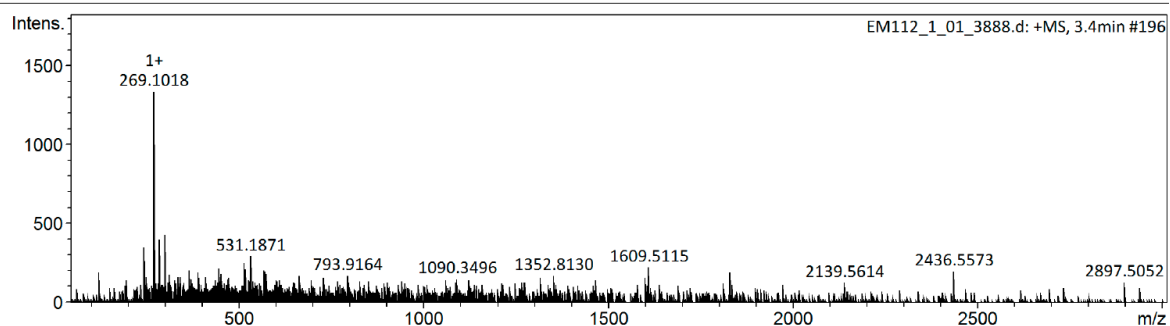
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Comment

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Operator BDAL@DE  
Instrument compact 8255754.20088

### Acquisition Parameter

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Bruker Compass DataAnalysis 4.3

printed: 9/27/2021 3:49:59 PM

by: BDAL@DE

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# HRMS spectrum of 8

## Display Report

### Analysis Info

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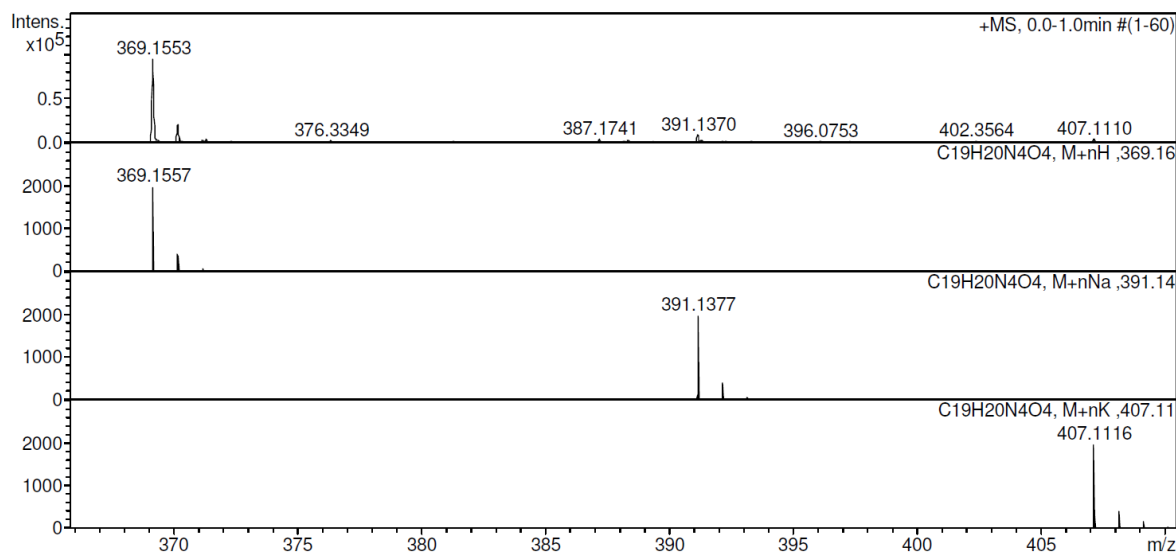
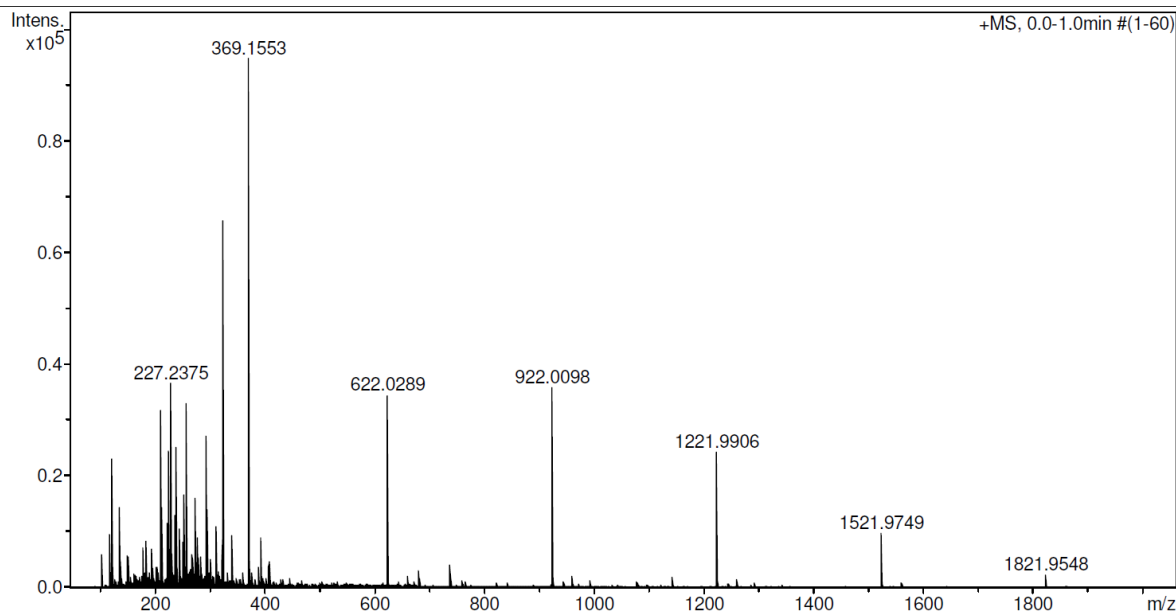
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Operator BDAL@DE

Instrument / Ser# micrOTOF CH3CN : 10248

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





# HRMS spectrum of 9

## Display Report

### Analysis Info

Analysis Name D:\Data\Em123-LN261\_31\_01\_4198.d

Method la\_2.2\_small2.m

Sample Name 9

Comment

Acquisition Date 6/23/2023 3:53:39 PM

Operator BDAL@DE

Instrument compact 8255754.20088

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

