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AF-153.1.{1H}.1.fid
/TERN vil1940

9.63

9.17

7.76

7.74

7.56

7.54

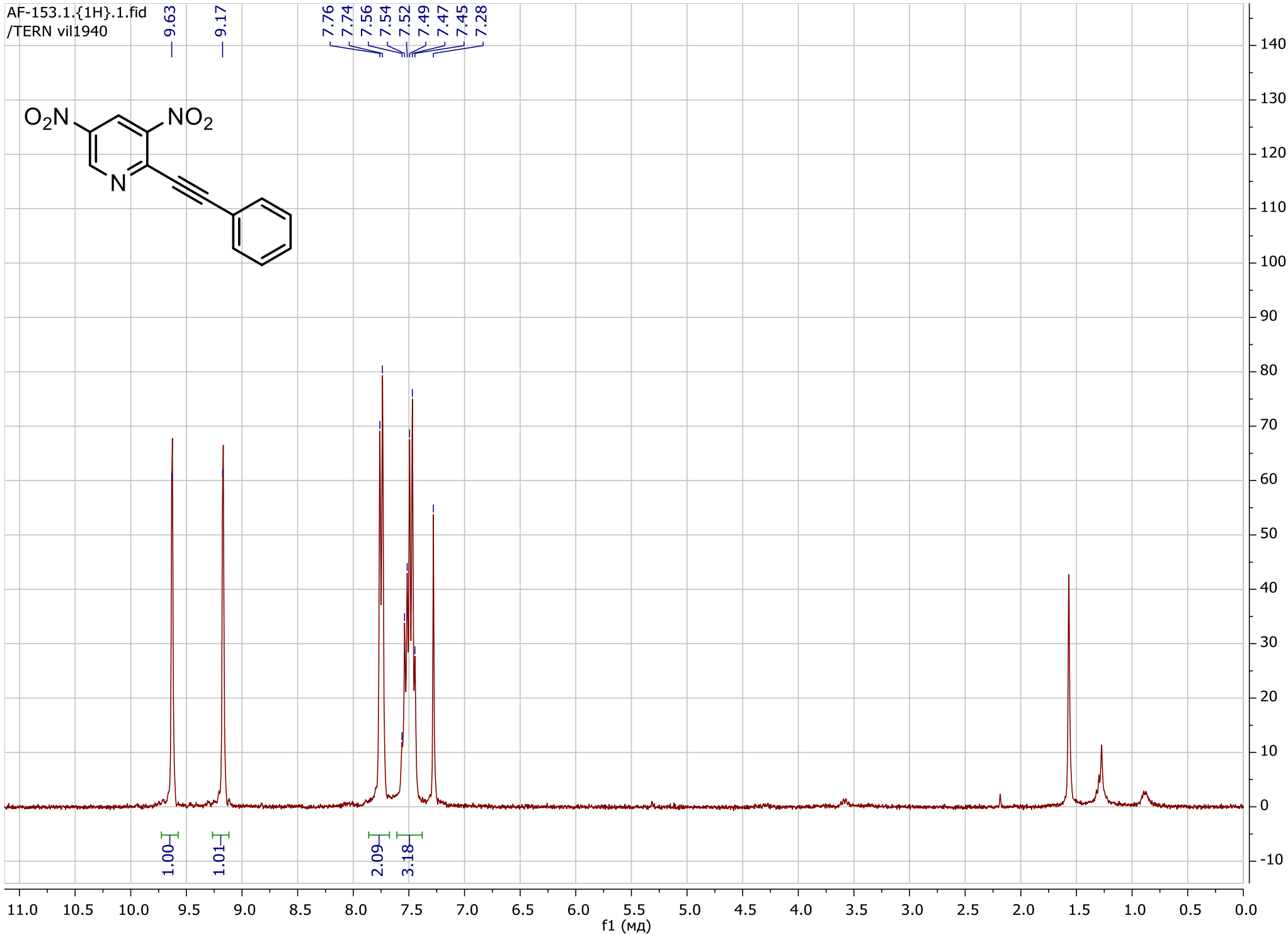
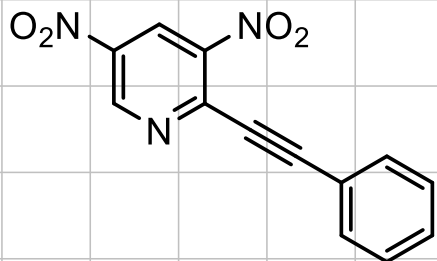
7.52

7.49

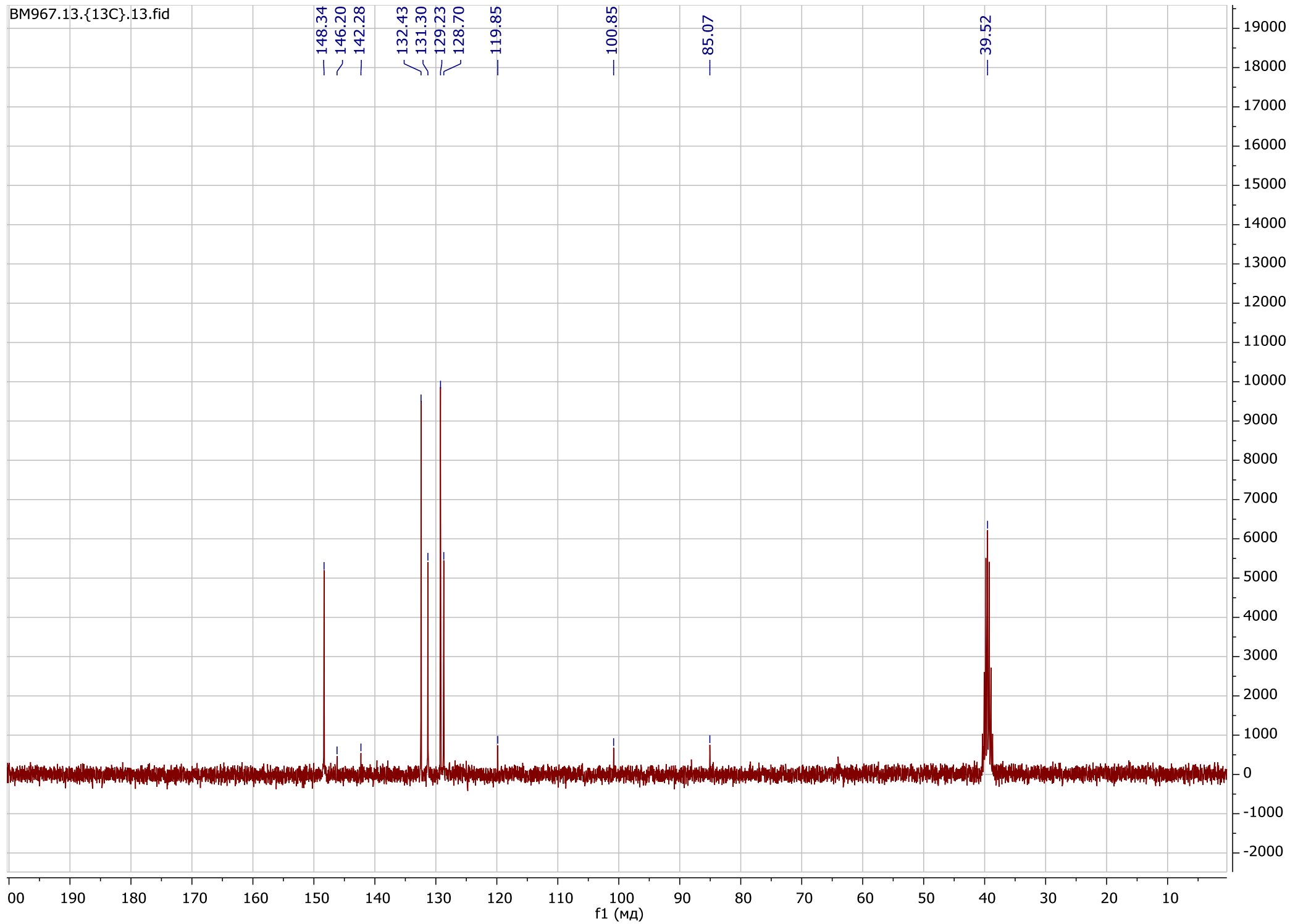
7.47

7.45

7.28



BM967.13.{13C}.13.fid



Display Report

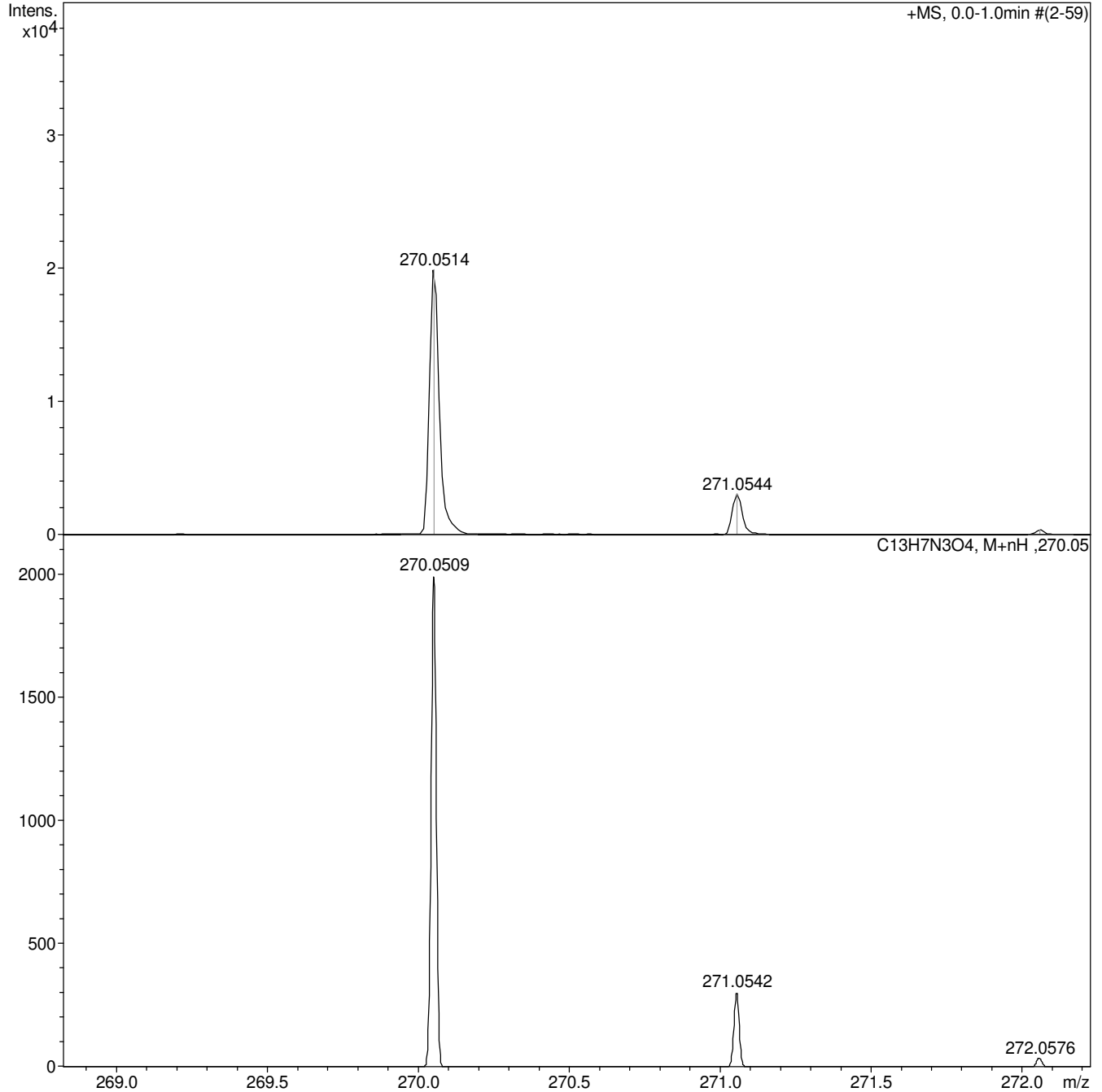
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Method tune_low.m
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Comment C13H7N3O4 mw 269 calibrant added

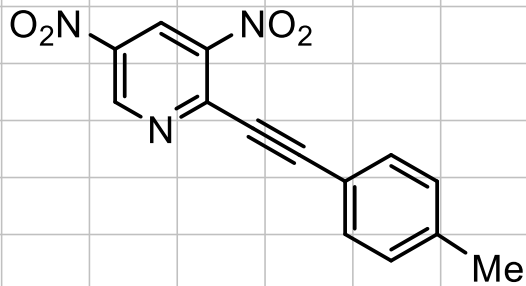
Acquisition Date 05.03.2014 14:47:17
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-160.{1H}.1.fid
/LB58 IYT2495



9.64
9.63

9.19
9.18

7.68
7.65

7.31
7.29

7.28

2.46

1.00

0.98

2.06

3.32

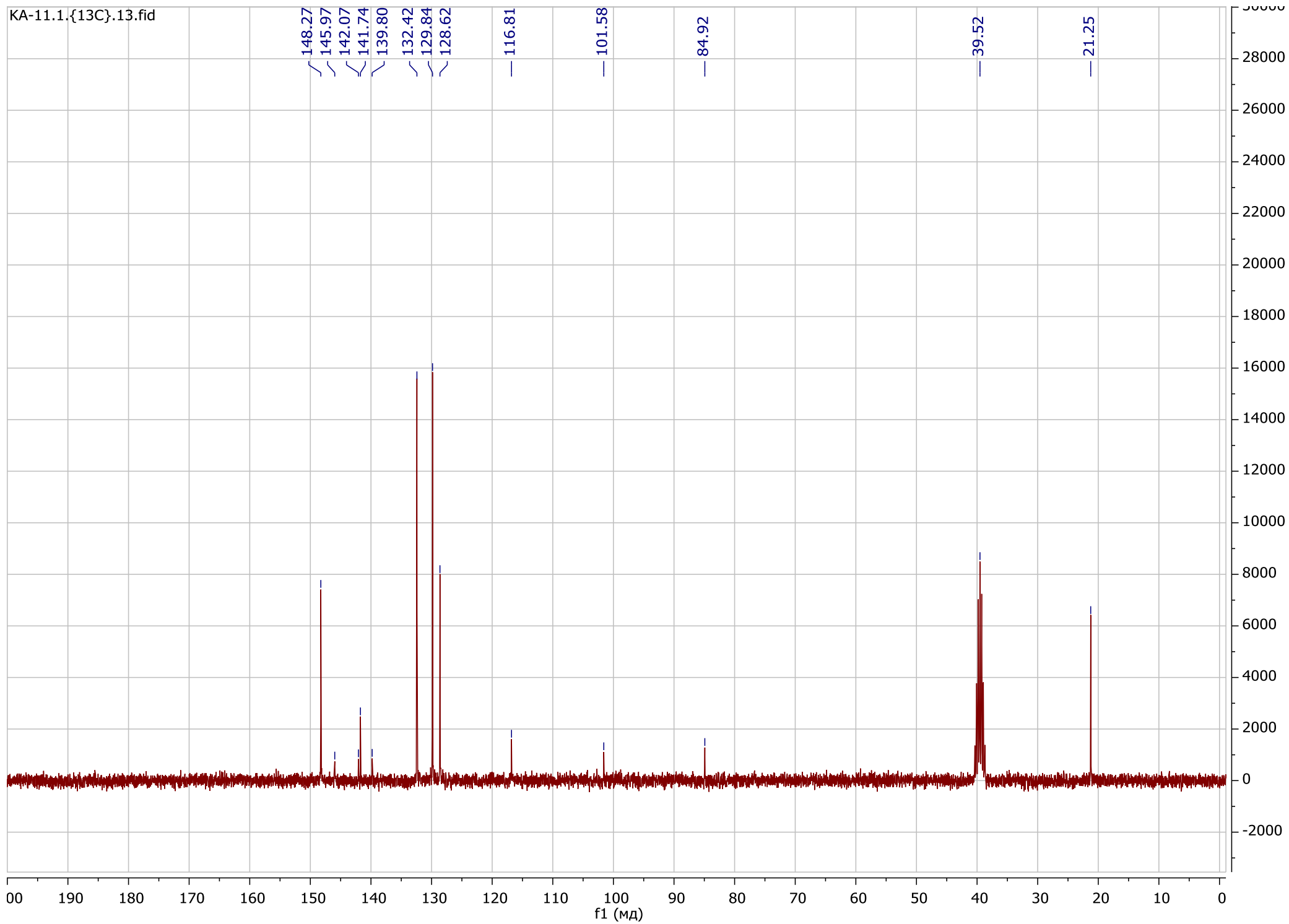
3.13

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f1 (M δ)

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20

KA-11.1.{13C}.13.fid



Display Report

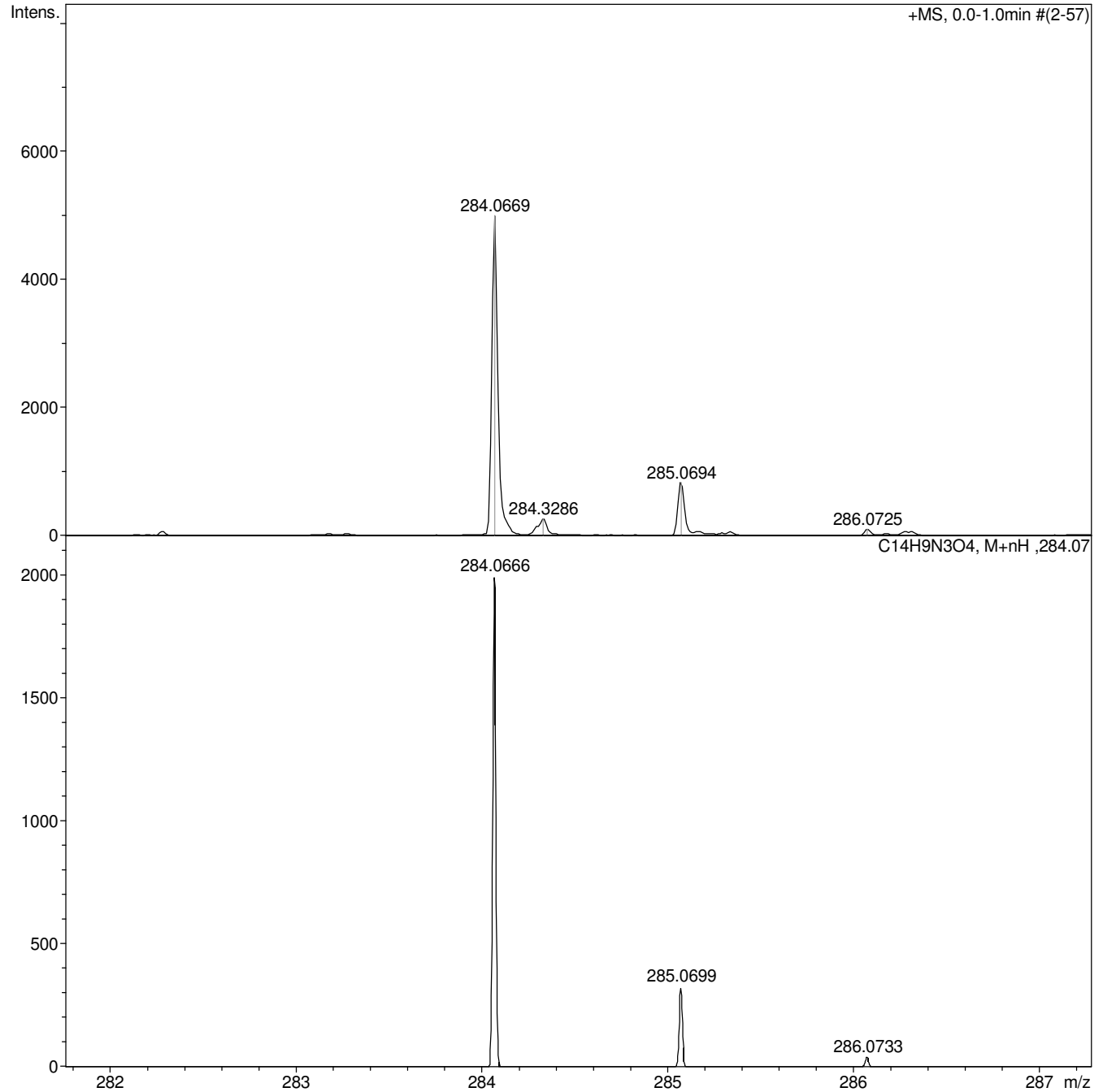
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Comment C14H9N3O4 mw 283 calibrant added

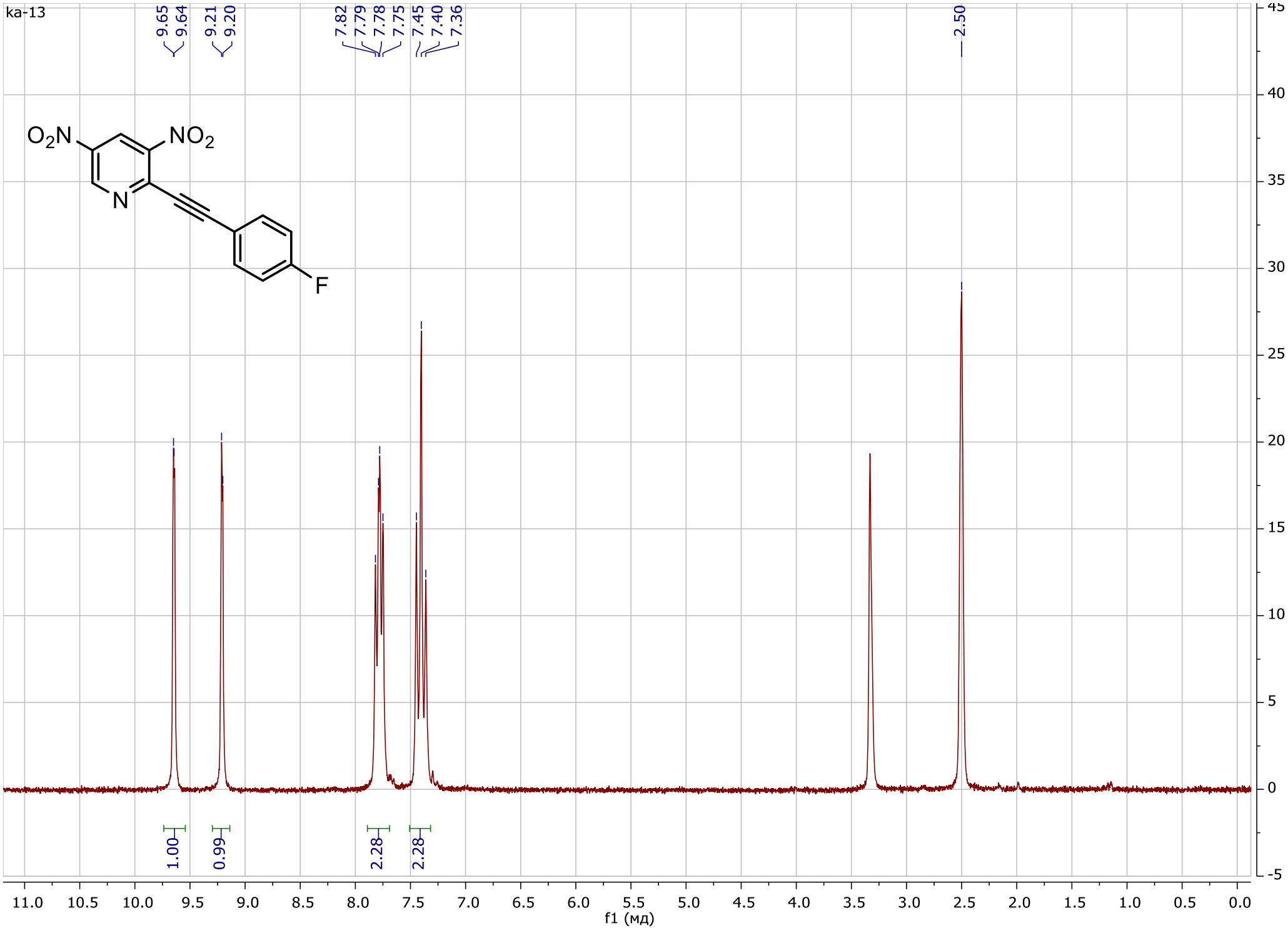
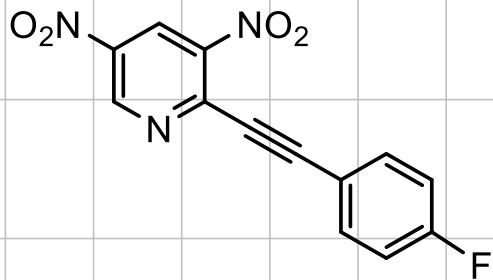
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Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

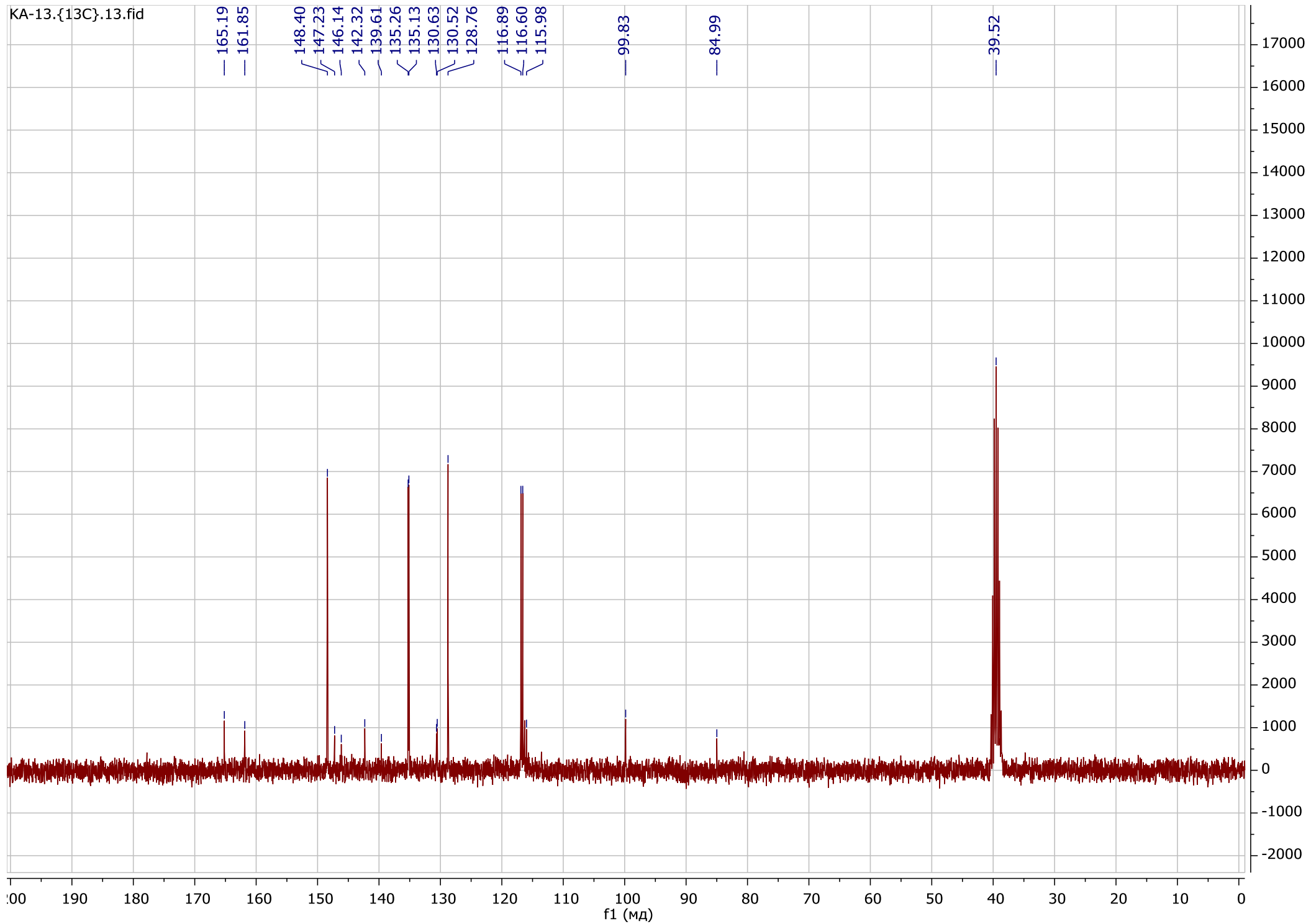
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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



ka-13



KA-13.{13C}.13.fid



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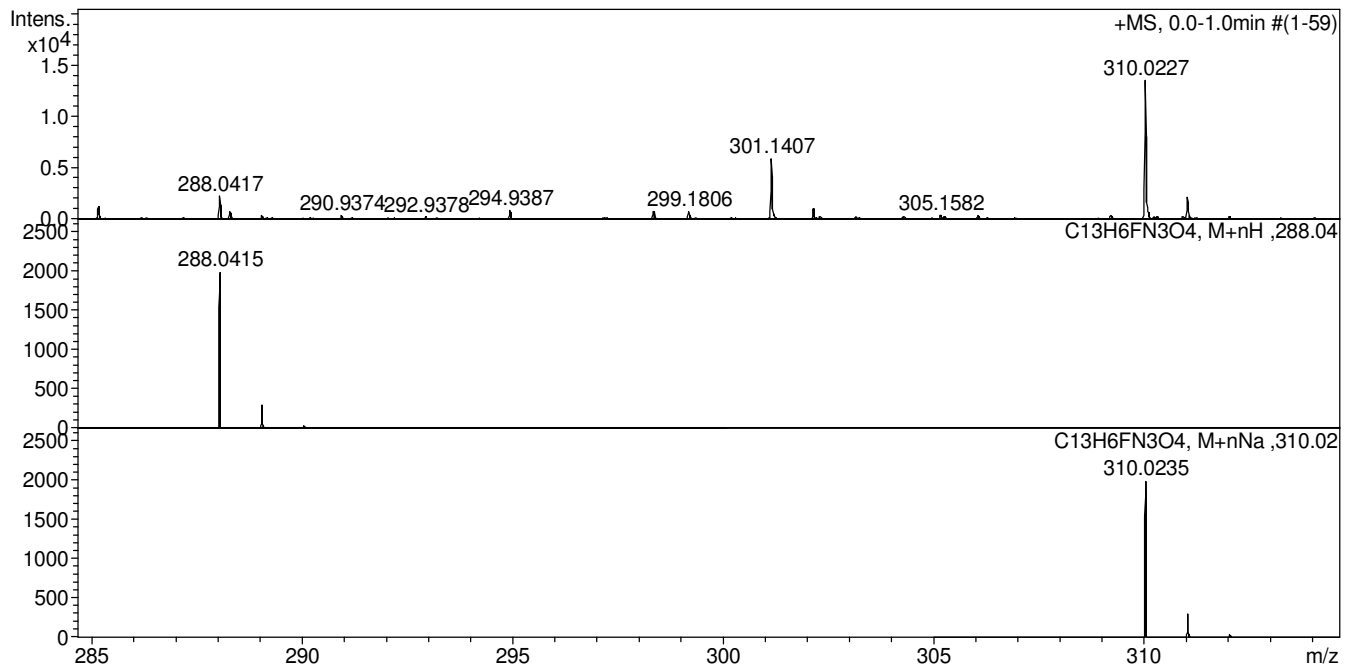
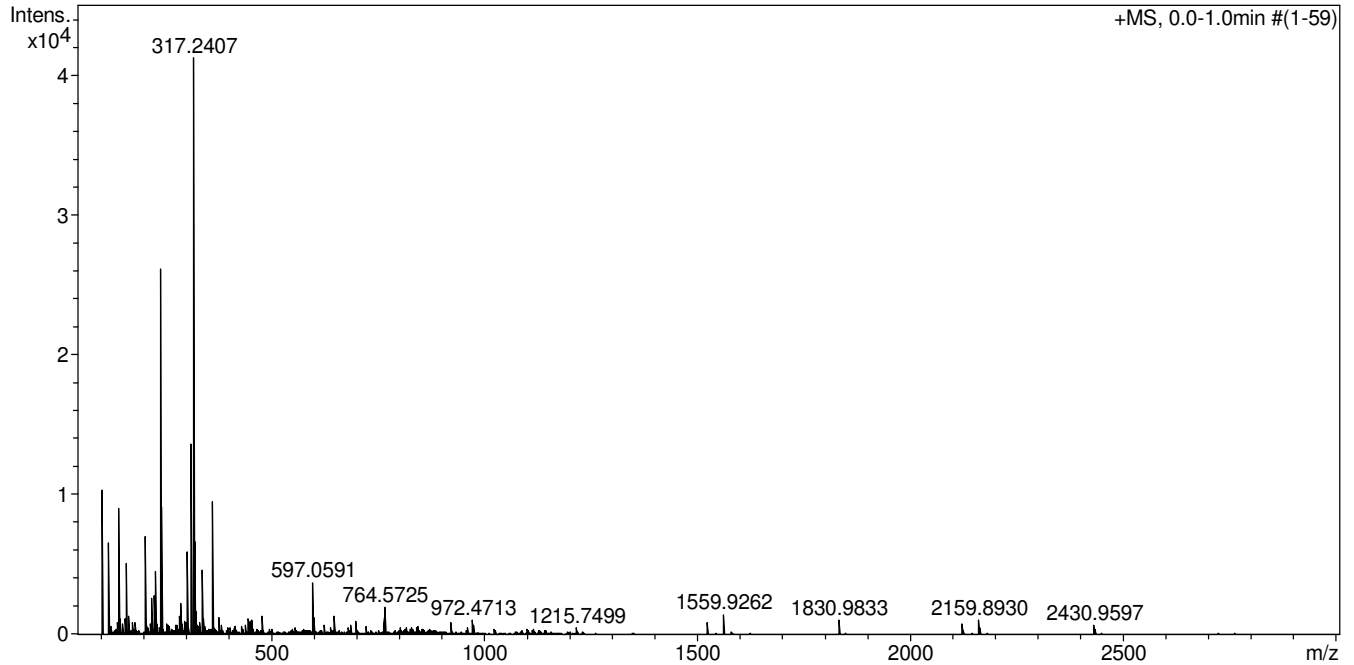
Analysis Info

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Method tune_low.m
Sample Name /LPIK KA-13
Comment CH3CN 100 %, dil. 2, calibrant added

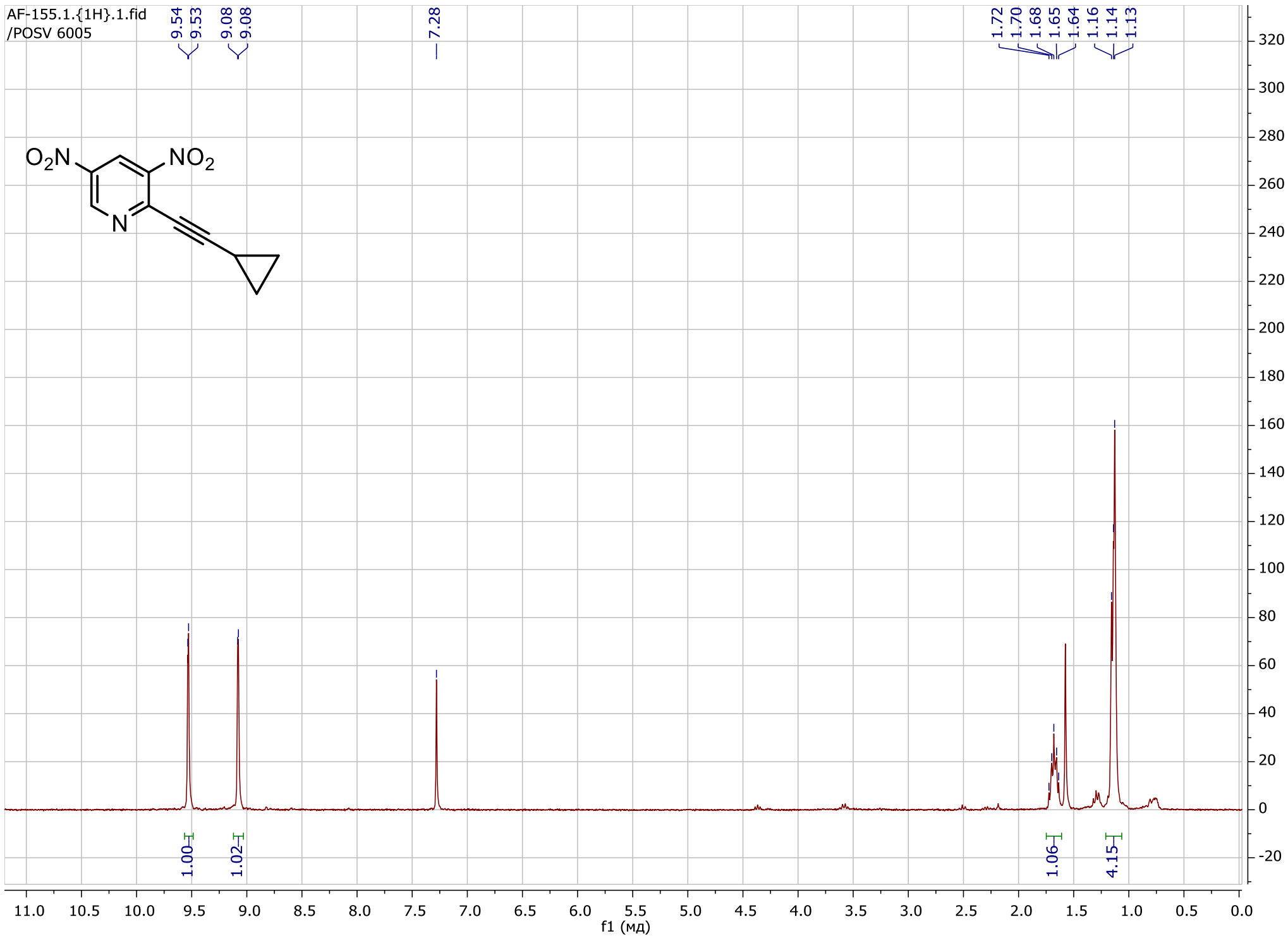
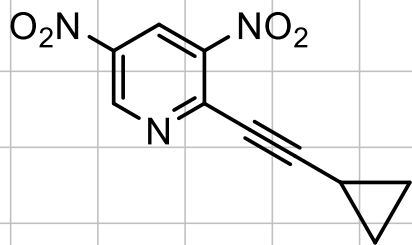
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Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

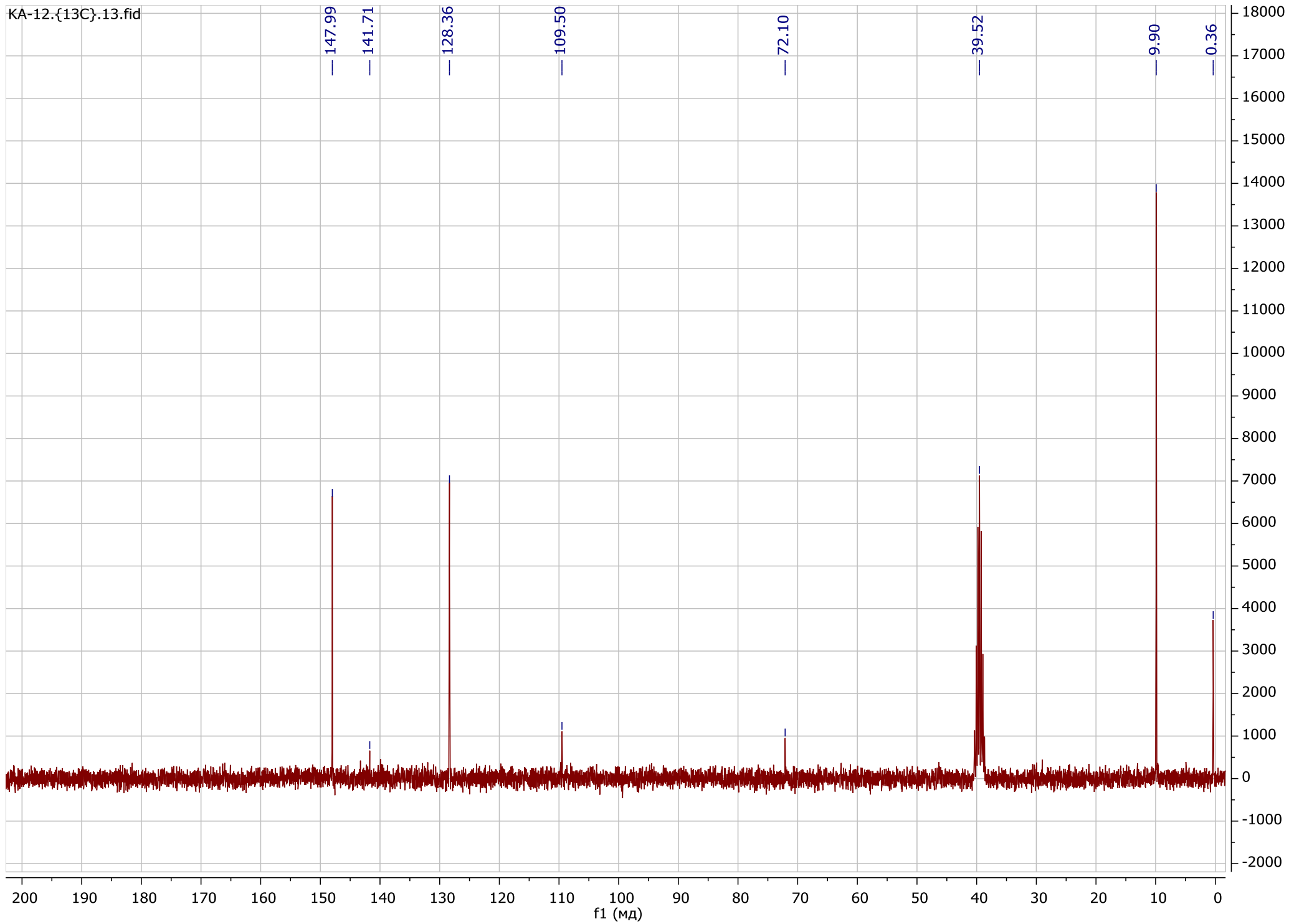
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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-155.1.1.1.fid
/POSV 6005



KA-12-¹³C}.13.fid



Display Report

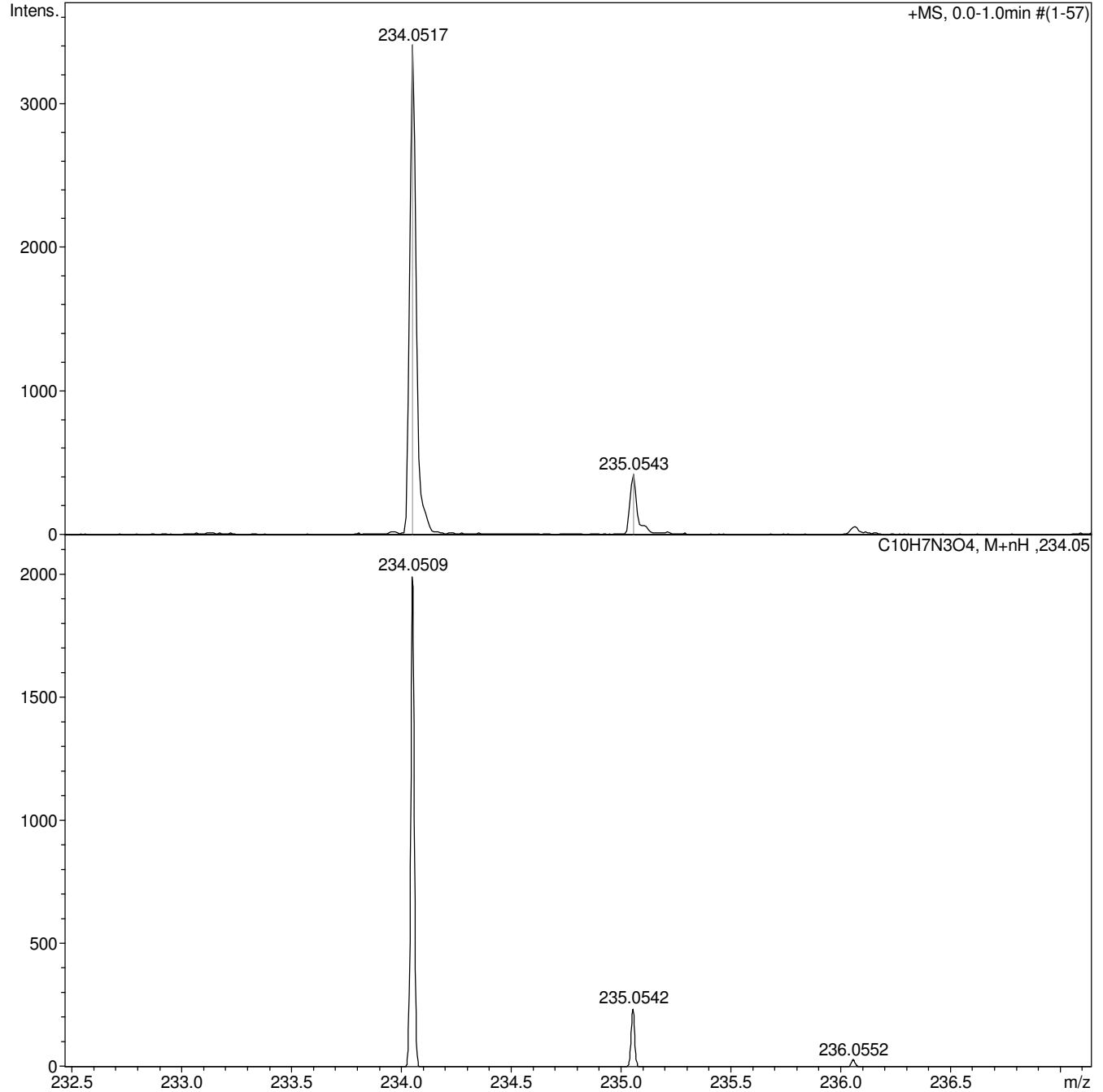
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Method tune_low.m
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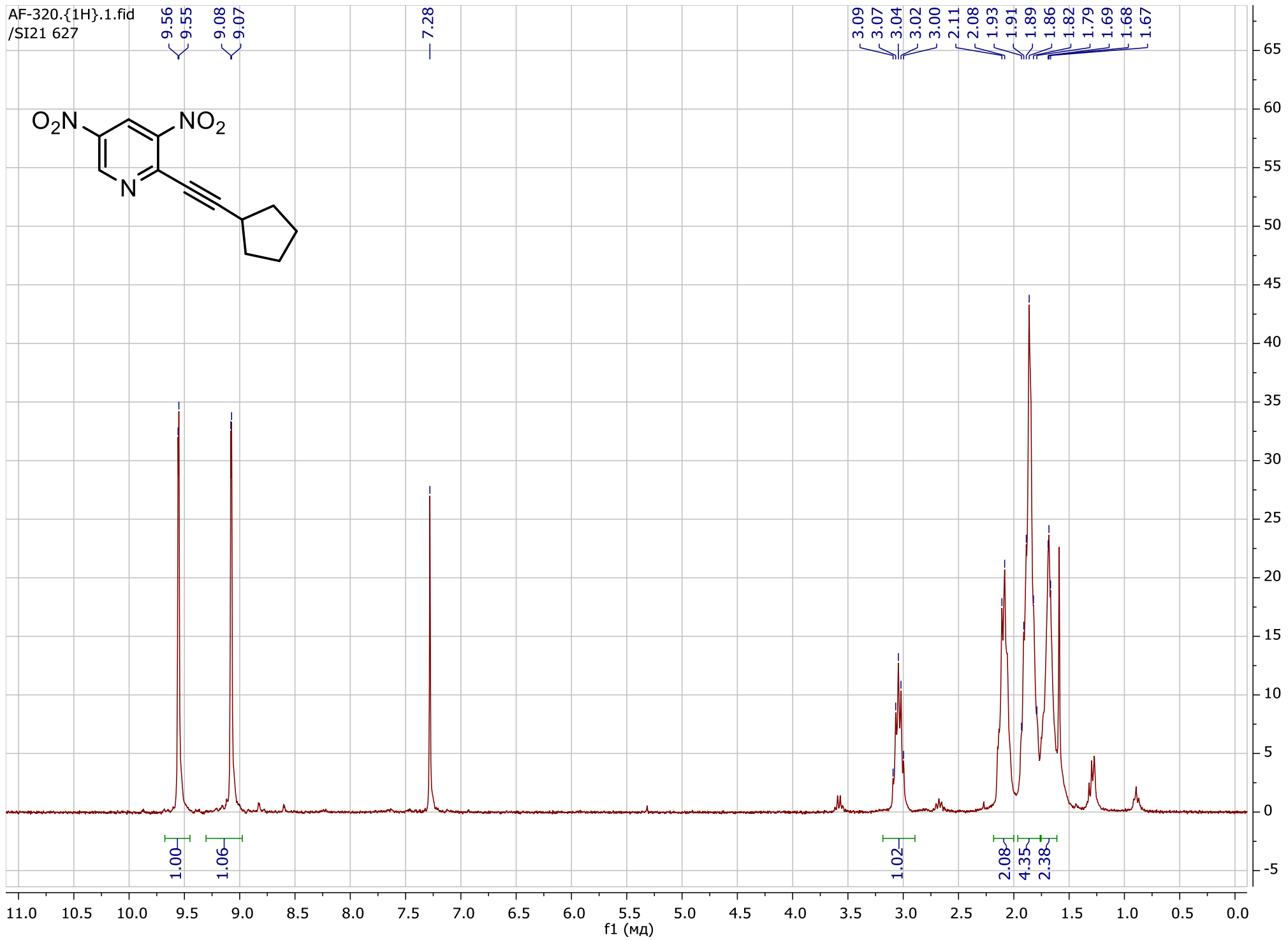
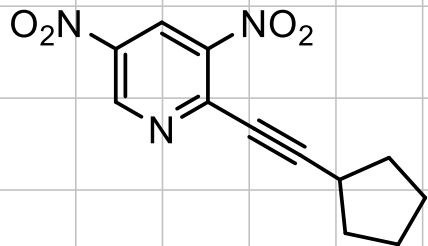
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Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

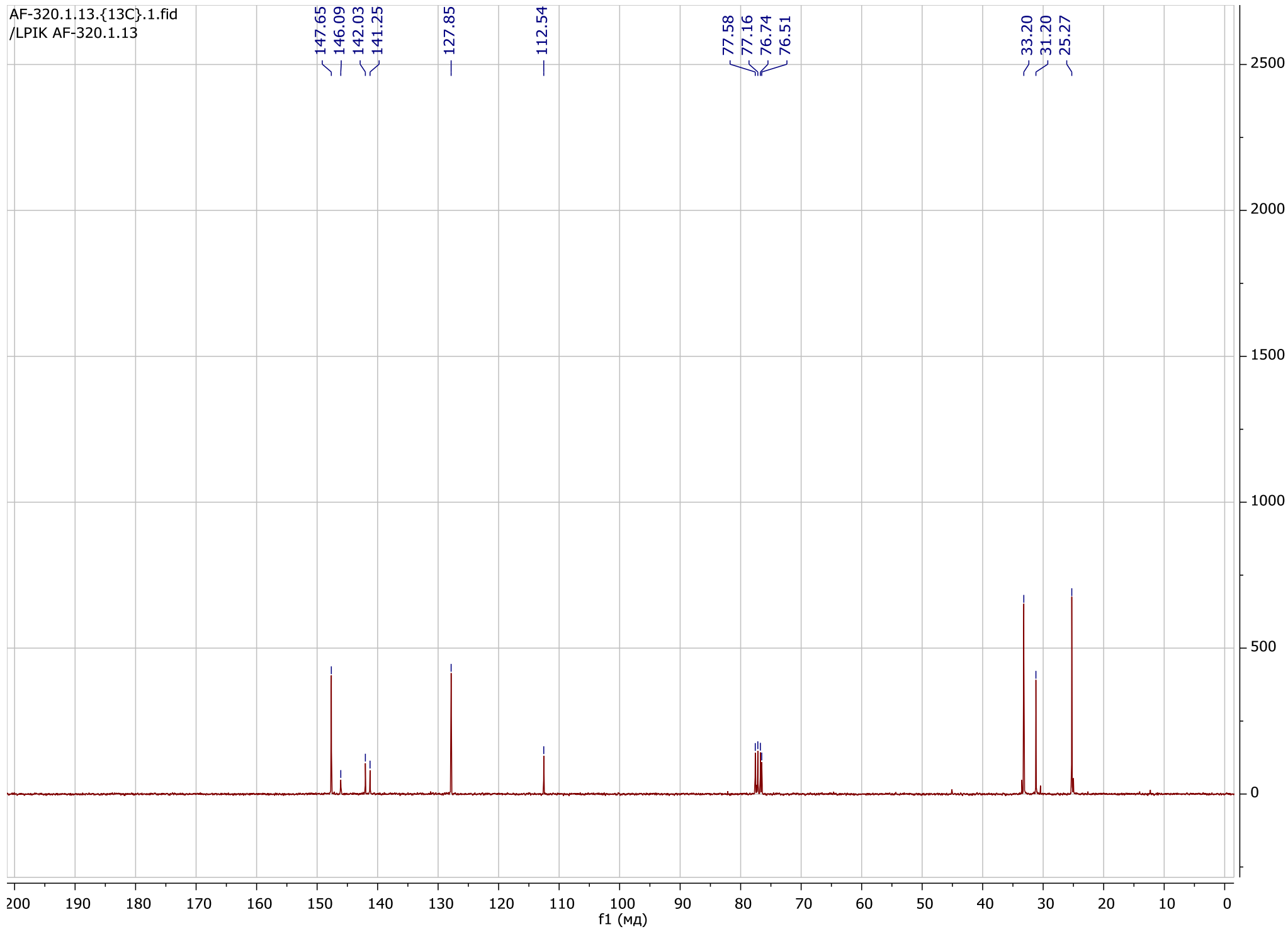
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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-320.{1H}.1.fid
/SI21 627



AF-320.1.13.{13C}.1.fid
/LPIK AF-320.1.13



Display Report

Analysis Info

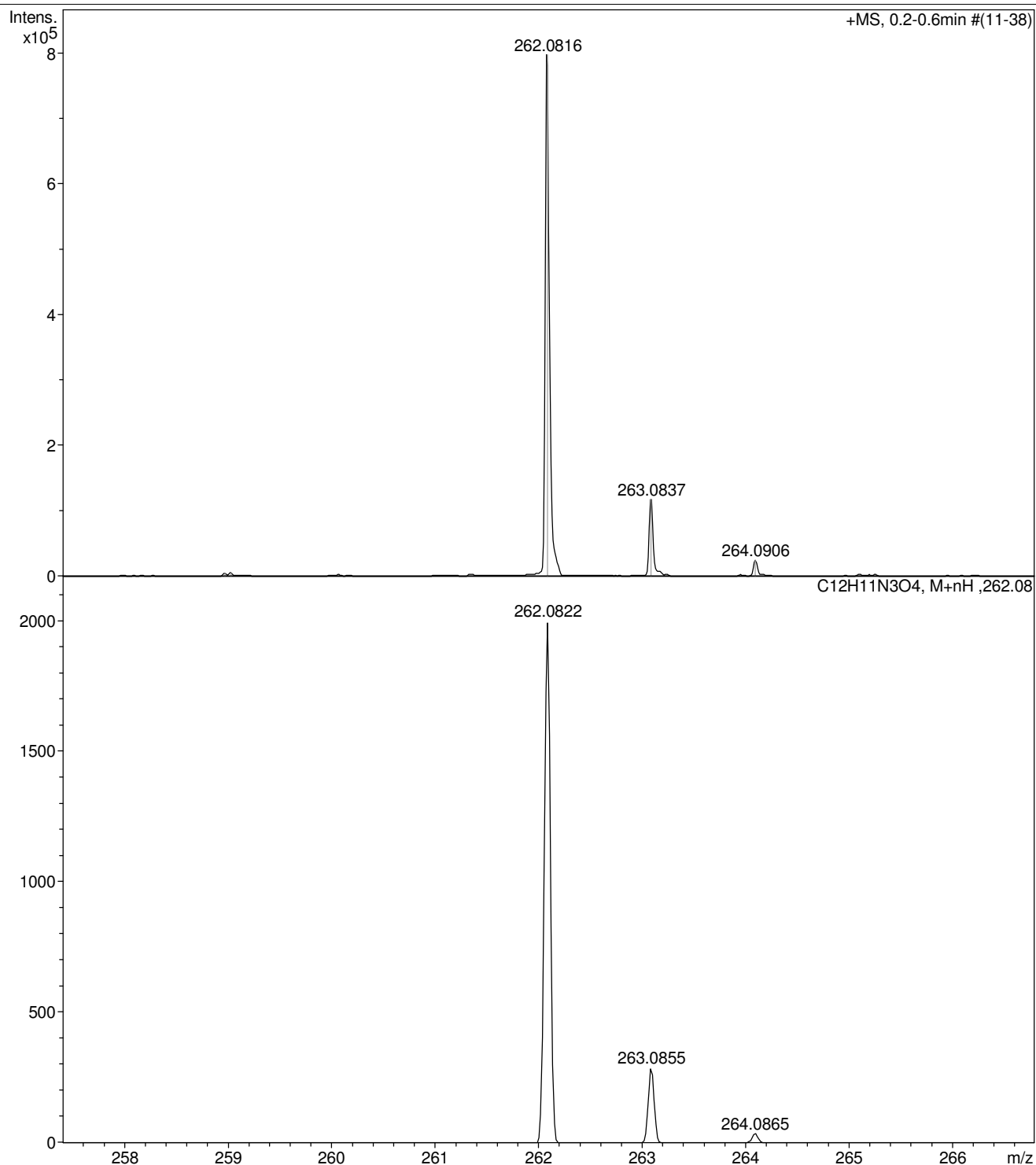
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Comment C12H11N3O4 mH 262.0822 calibrant added

Acquisition Date 25.09.2019 13:14:51

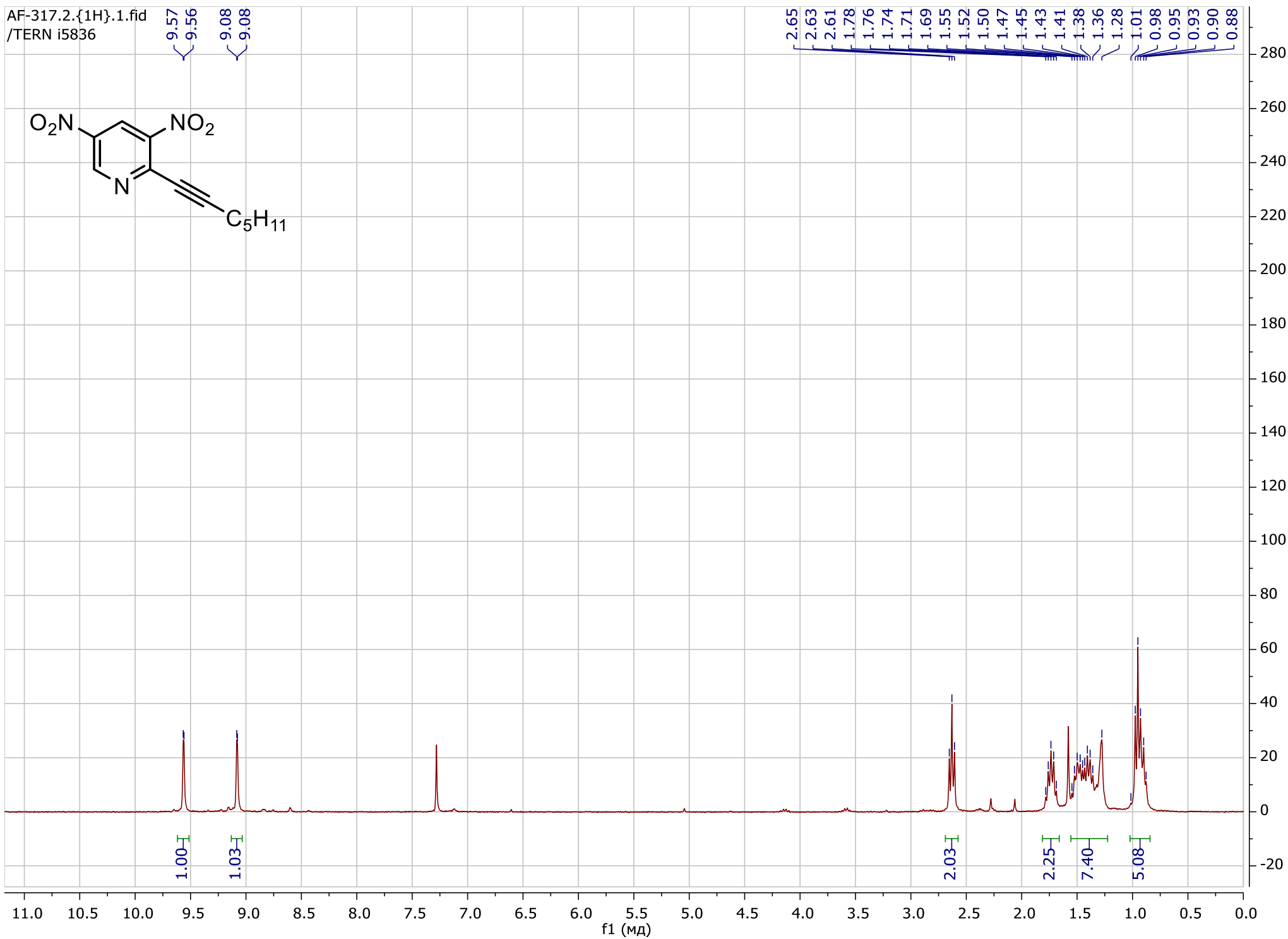
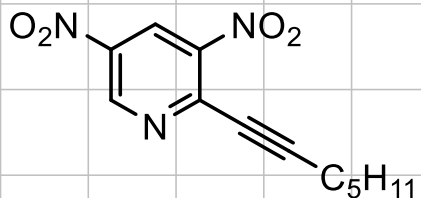
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

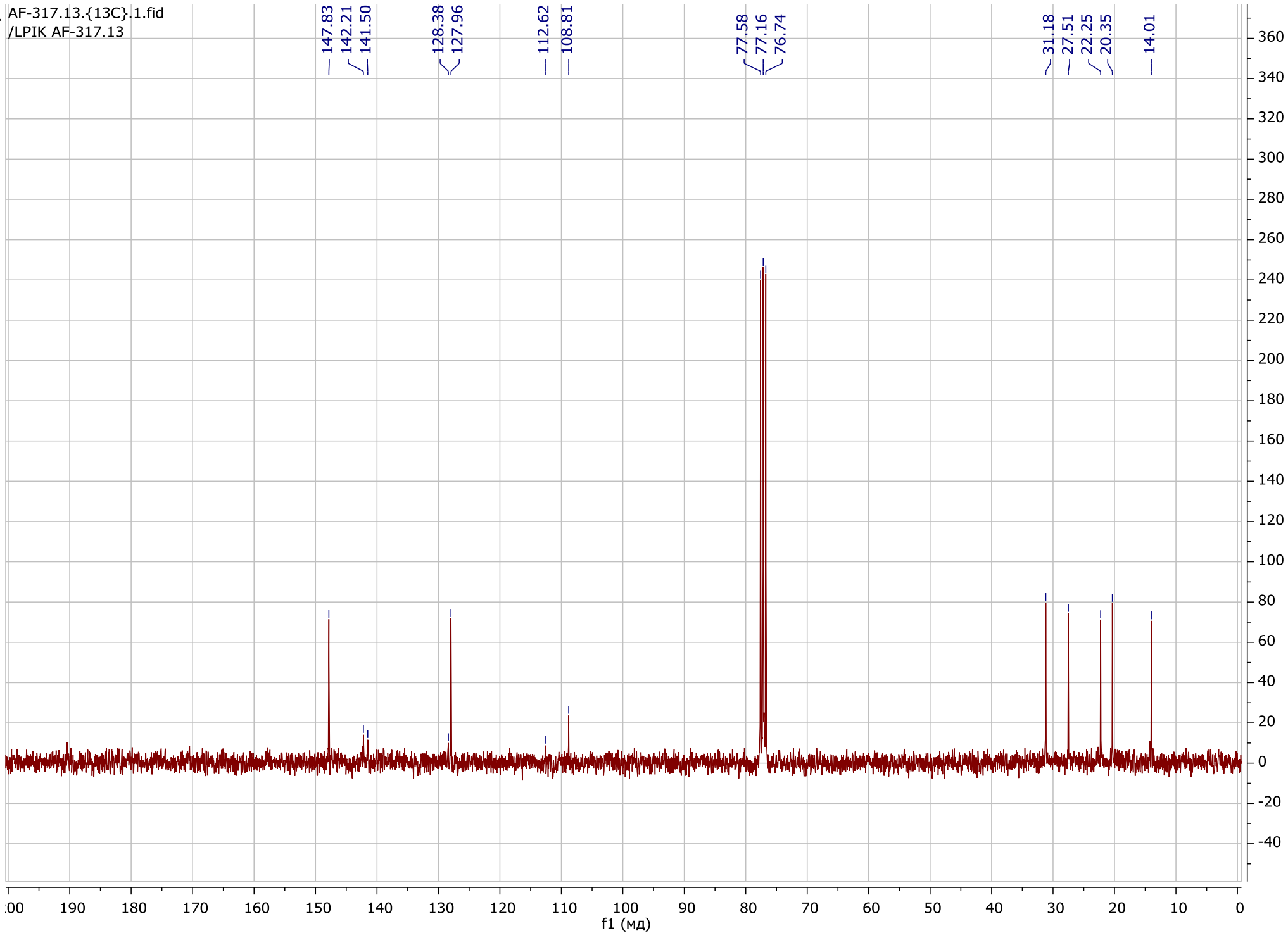
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Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-317.2.{1H}.1.fid
/TERN i5836



AF-317.13.¹³C}.1.fid
/LPIK AF-317.13



Display Report

Analysis Info

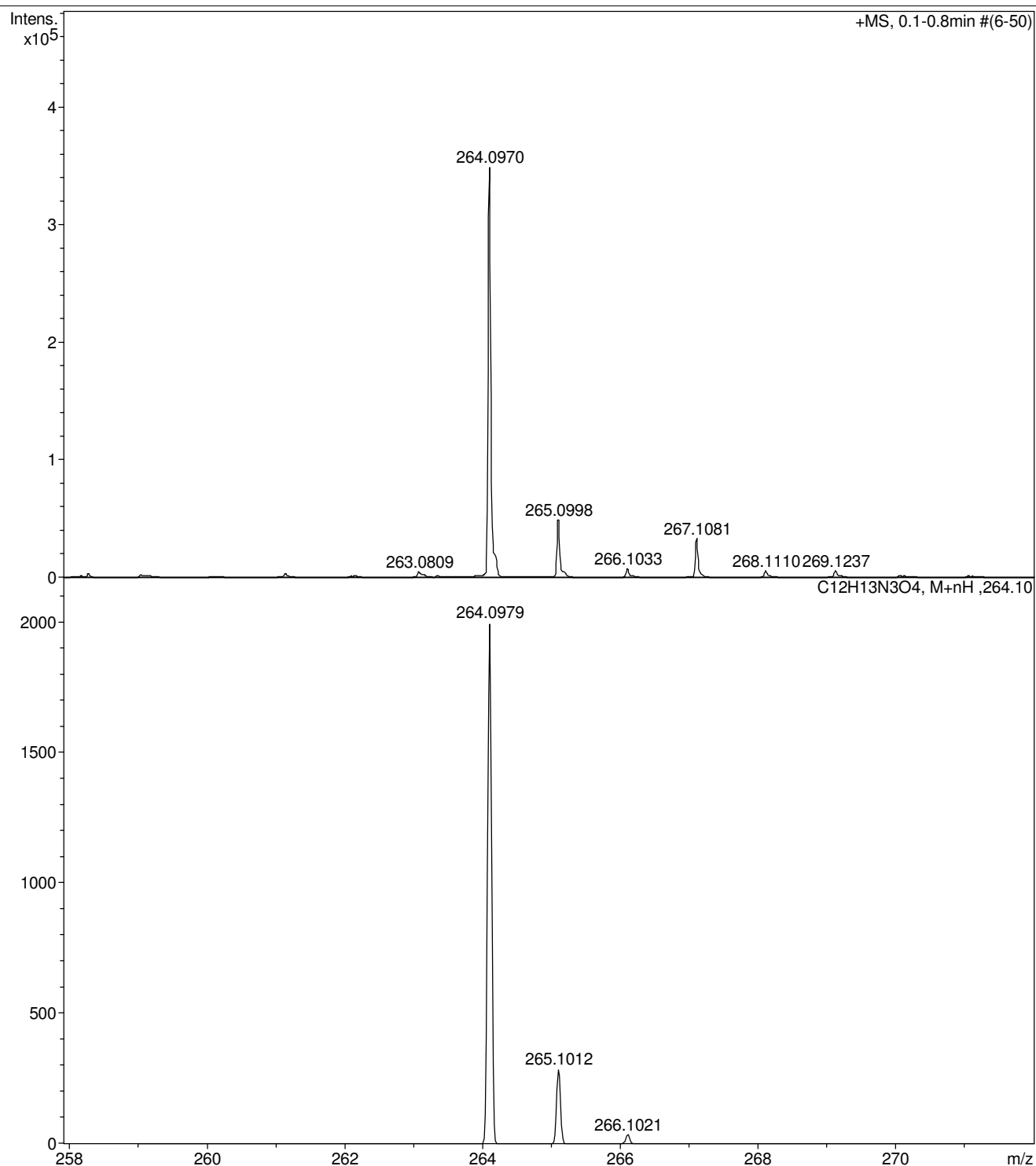
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Sample Name /LPIK AF-317
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Acquisition Date 25.09.2019 12:13:31

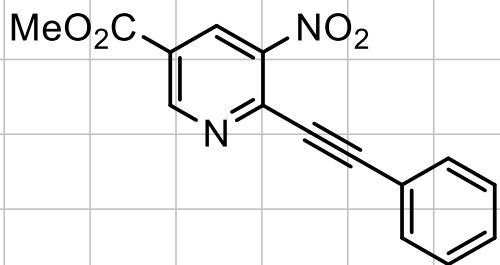
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

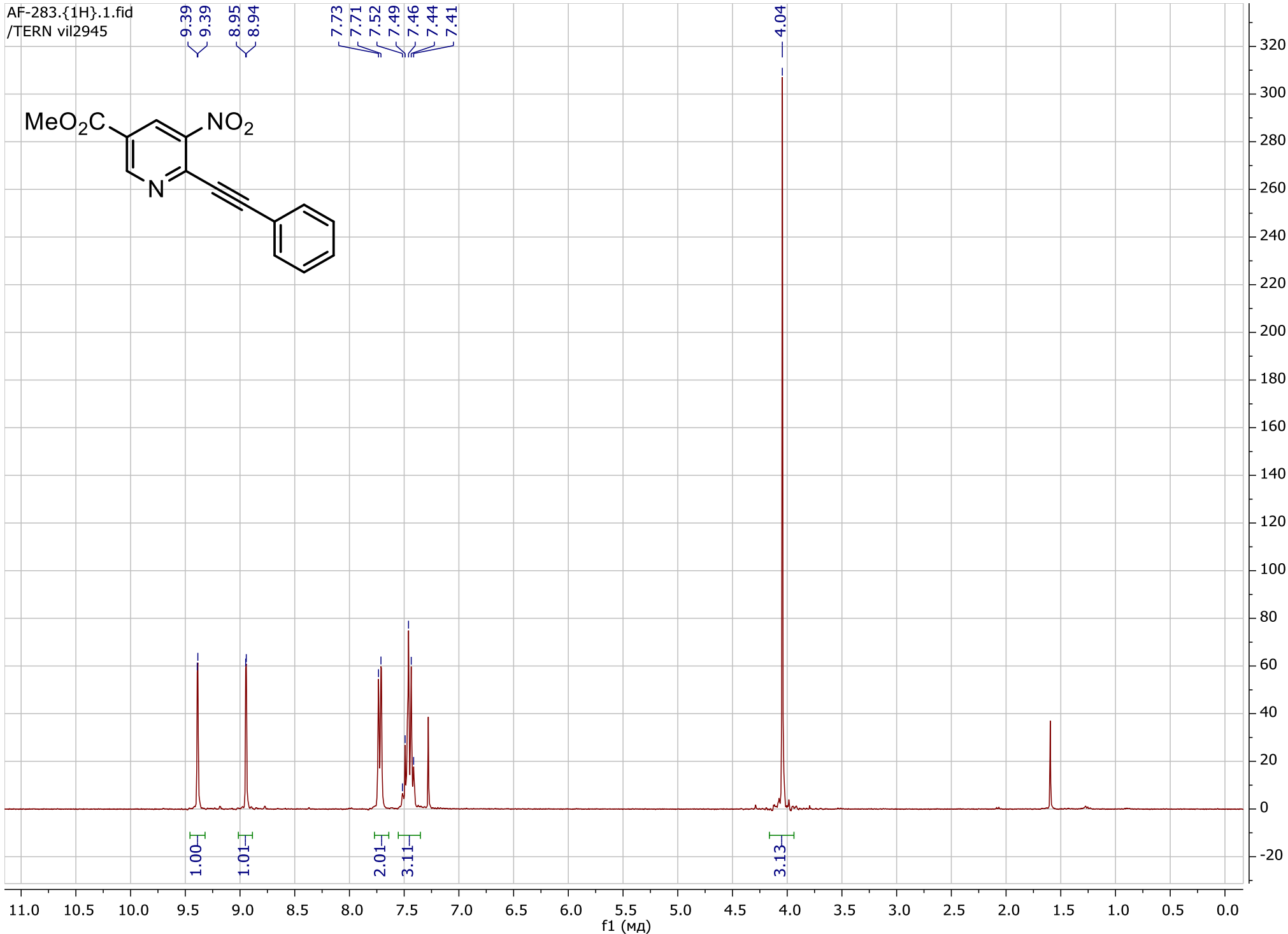


AF-283.{1H}.1.fid
/TERN vil2945



9.39
9.39
8.95
8.94
7.73
7.71
7.52
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7.46
7.44
7.41

4.04



1.00

1.01

2.01

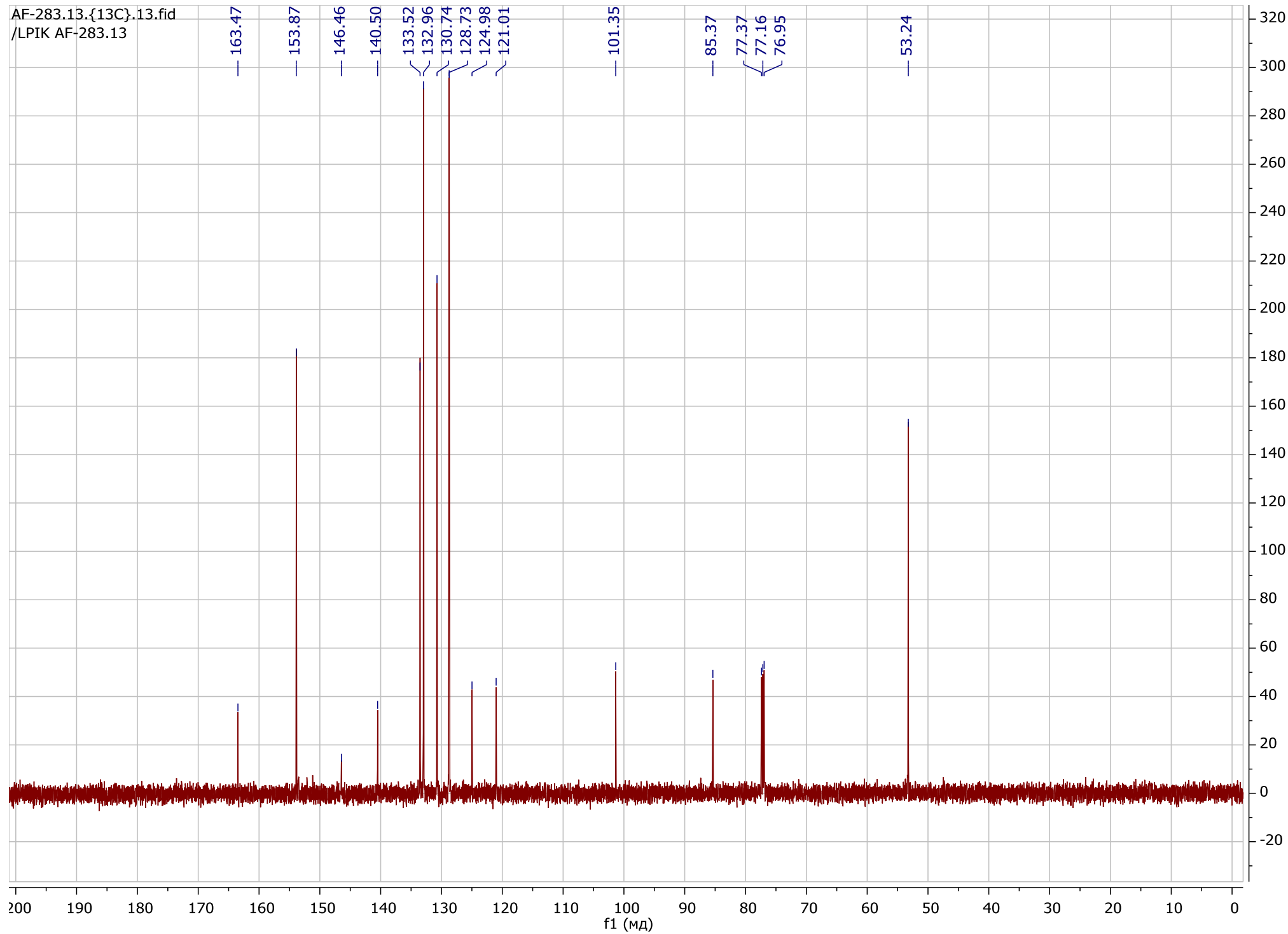
3.11

3.13

11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (Mn)

AF-283.13.{13C}.13.fid
/LPIK AF-283.13



Display Report

Analysis Info

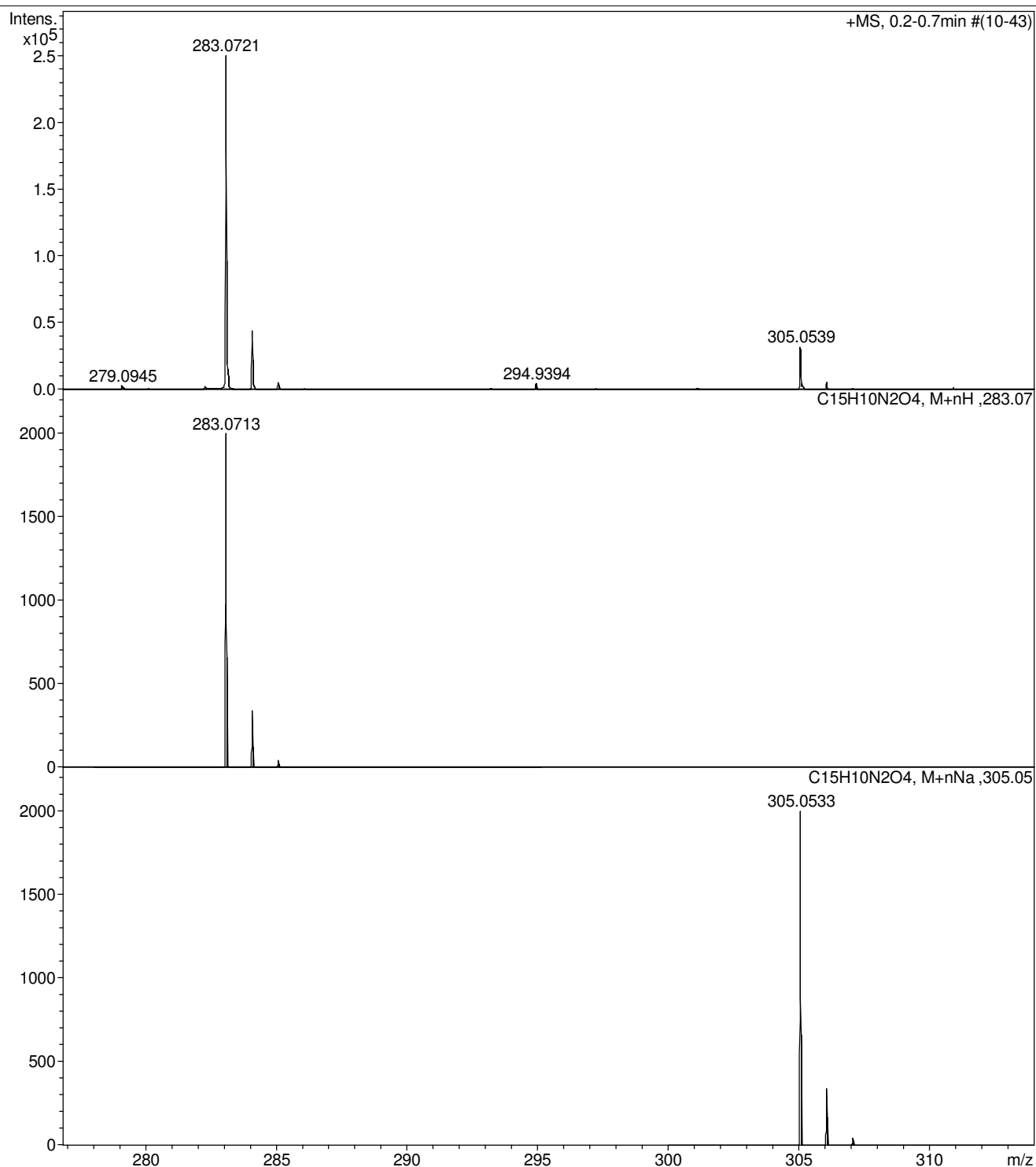
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Acquisition Date 23.04.2019 12:33:25

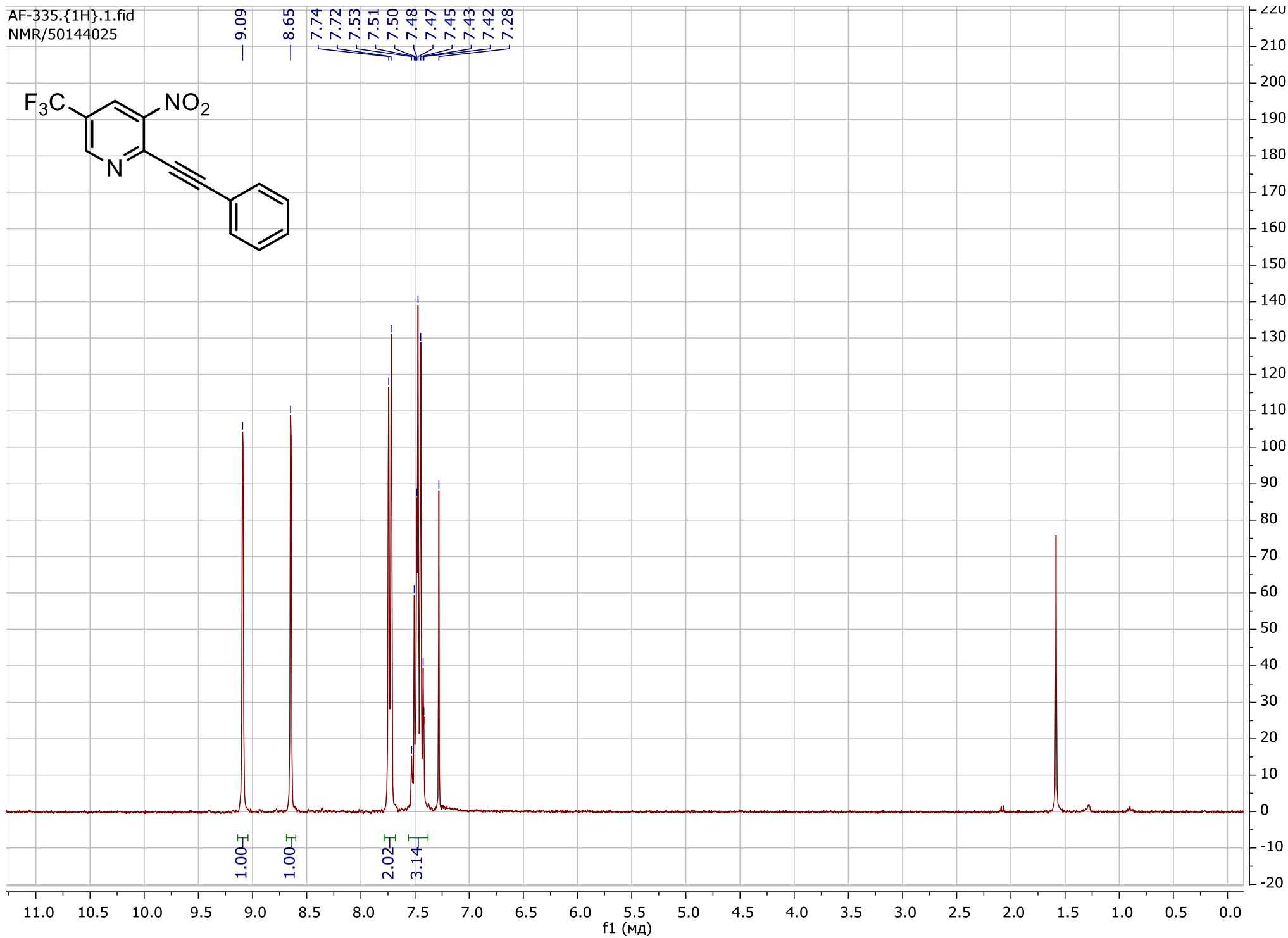
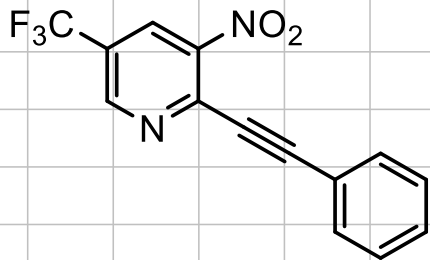
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

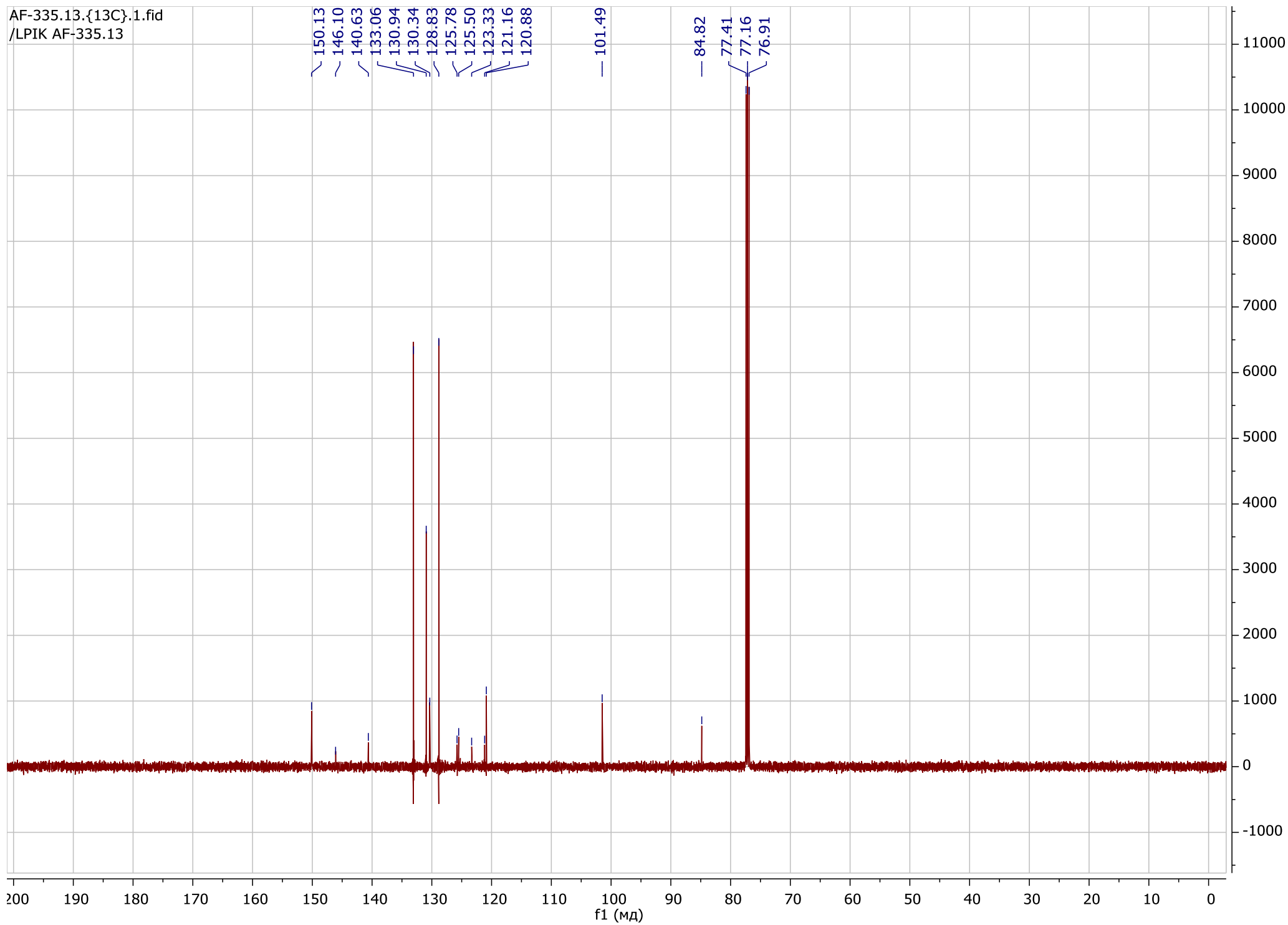
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Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-335.{1H}.1.fid
NMR/50144025



AF-335.13.{13C}.1.fid
/LPIK AF-335.13



Display Report

Analysis Info

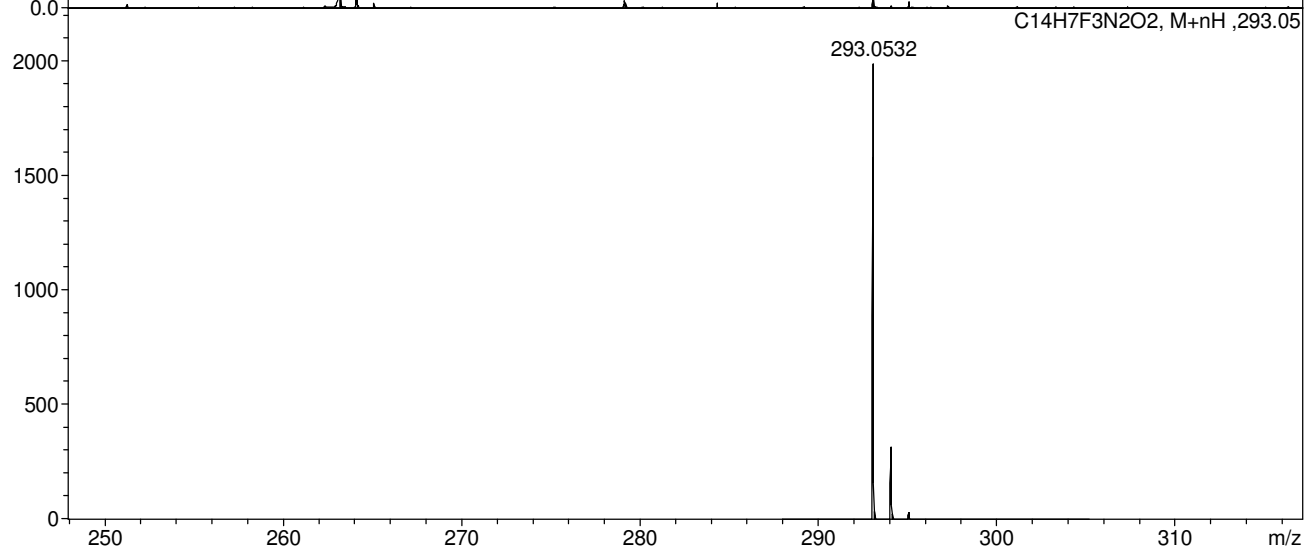
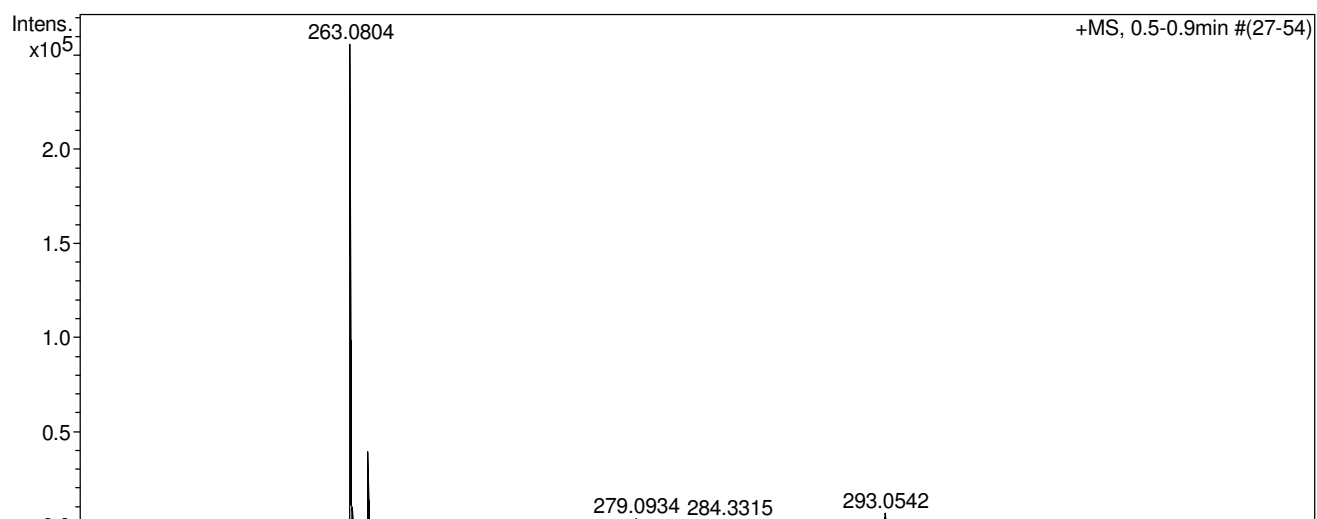
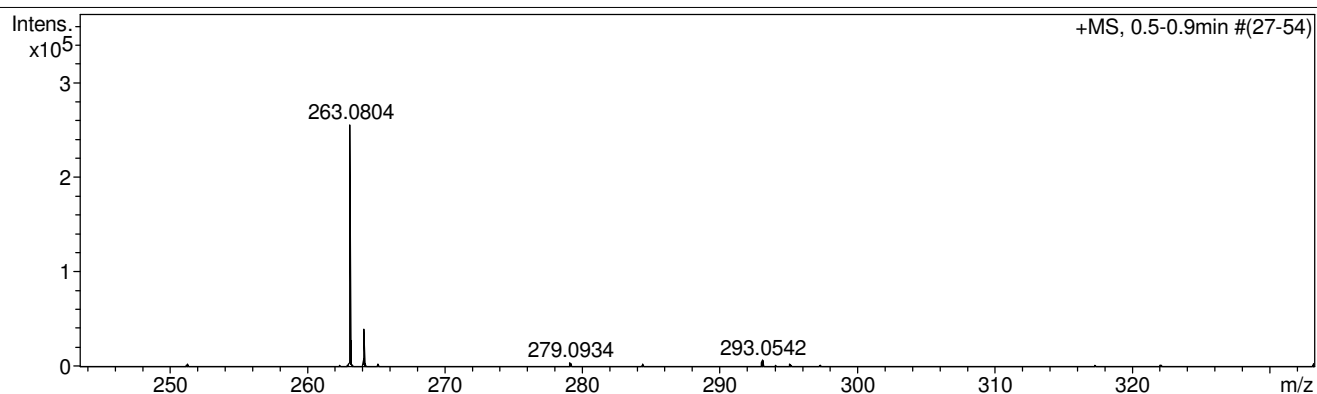
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Sample Name /LPIK AF-335
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Acquisition Date 21.01.2020 15:17:23

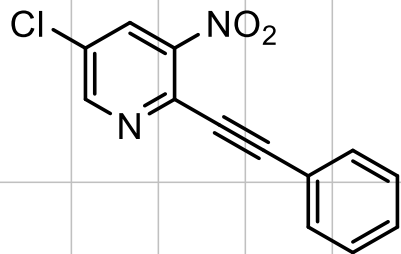
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-308.{1H}.1.fid
/VMIG P358



8.82
8.81
8.41
8.41
7.71
7.69
7.50
7.47
7.45
7.42
7.41

11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (Mд)

1.00
0.98
2.07
3.21

250

200

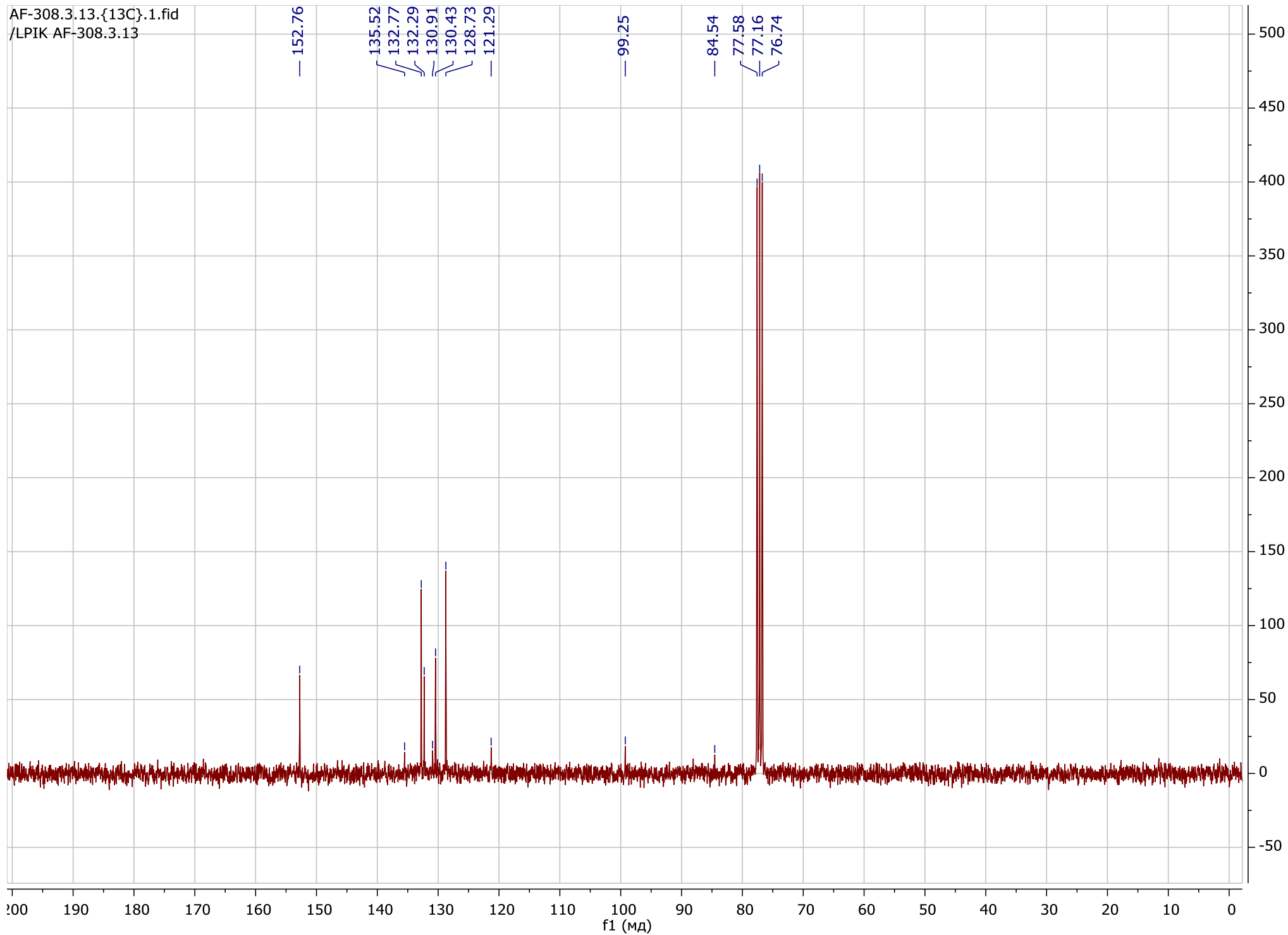
150

100

50

0

AF-308.3.13.{13C}.1.fid
/LPIK AF-308.3.13



Display Report

Analysis Info

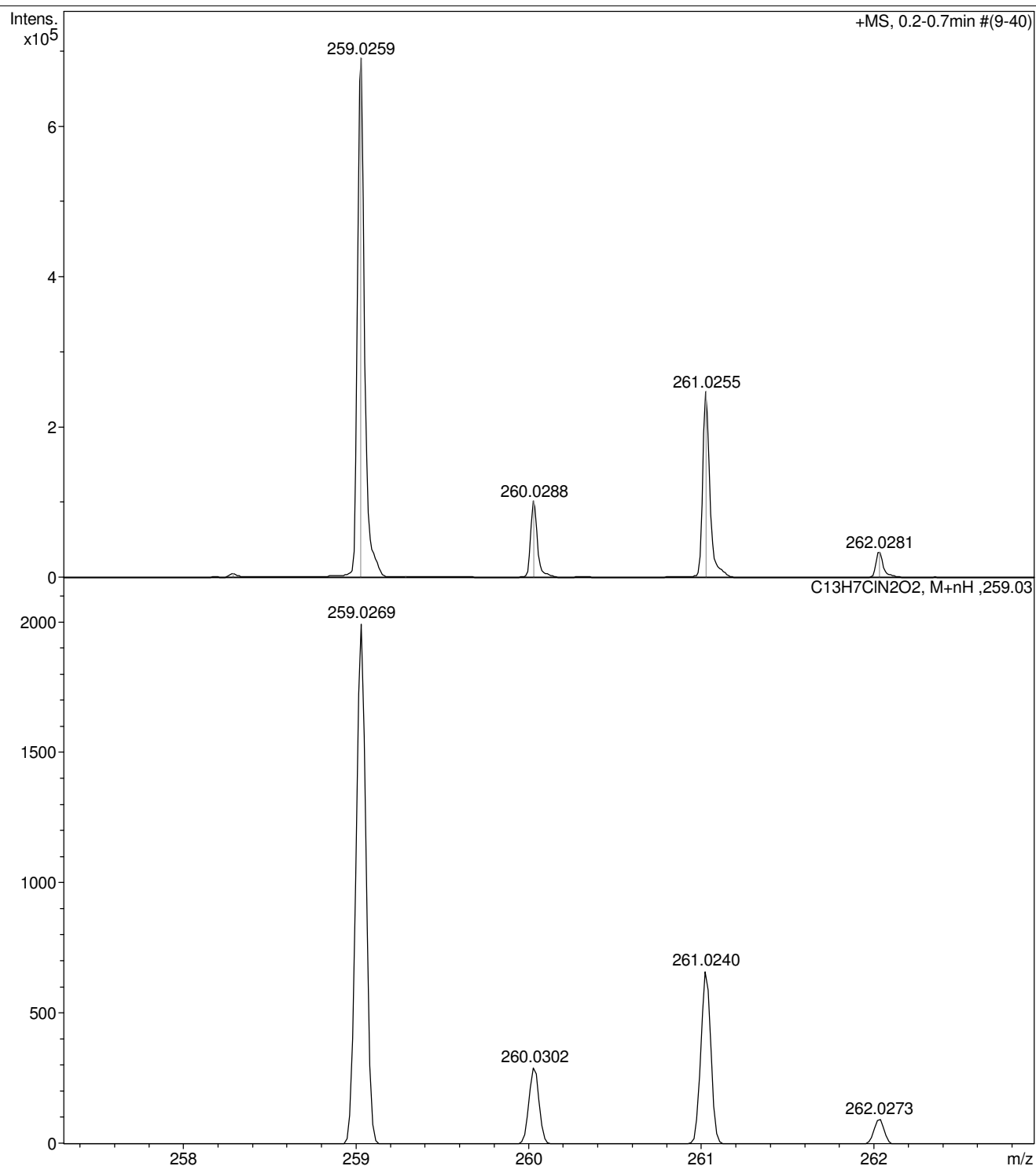
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Sample Name /LPIK AF-308
Comment C13H7CIN2O2 mH 259.0268 calibrant added

Acquisition Date 25.09.2019 12:36:54

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

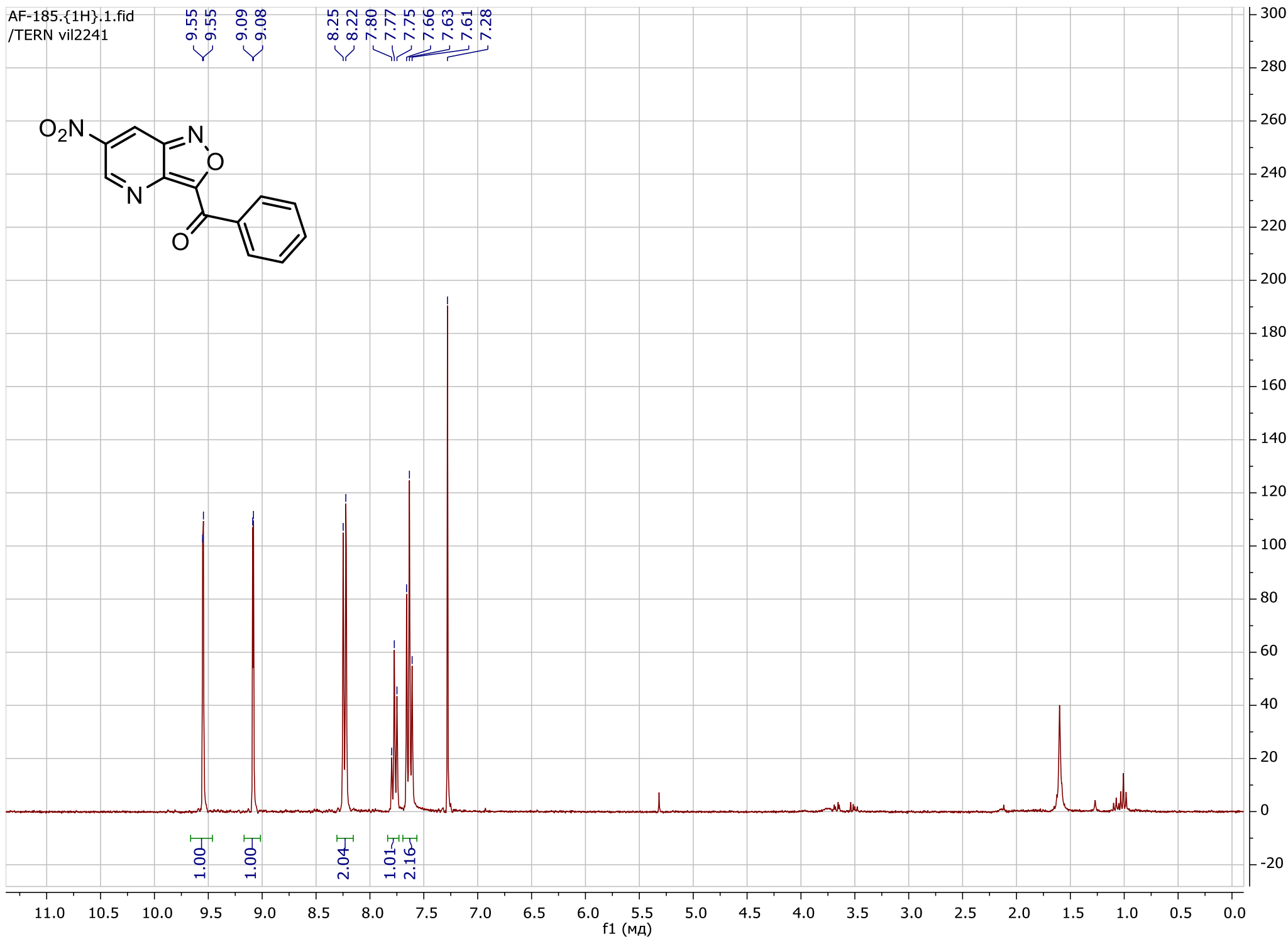
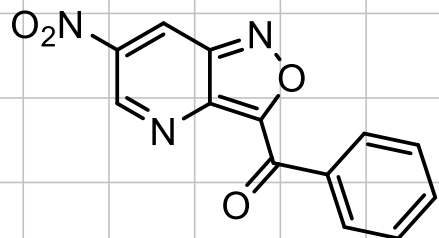
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Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

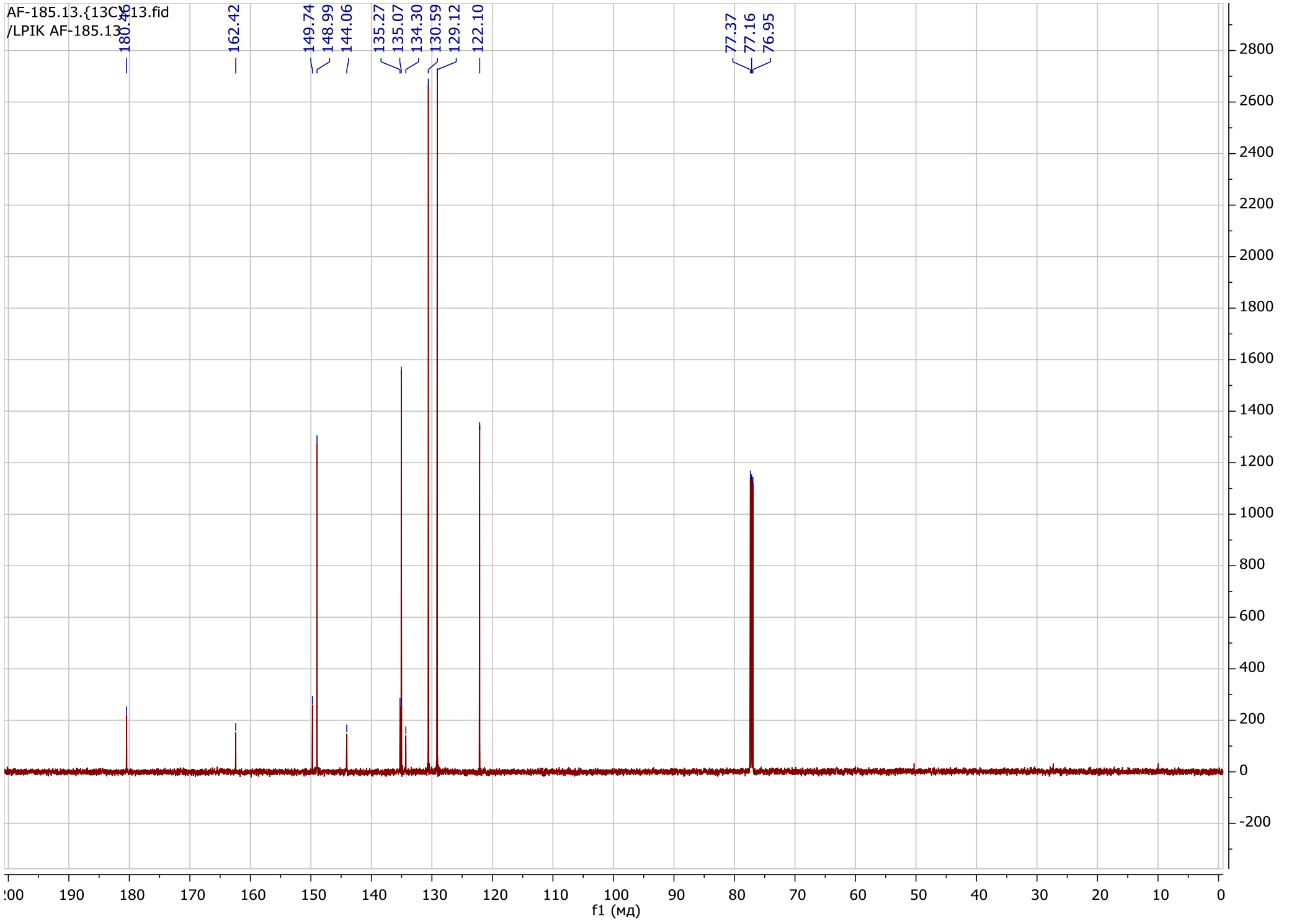


AF-185-¹H}.1.fid
/TERN vil2241

9.55
9.55
9.09
9.08
8.25
8.22
7.80
7.77
7.75
7.75
7.66
7.63
7.61
7.28



AF-185.13.{13C}.13.fid
/LPIK AF-185.13



Display Report

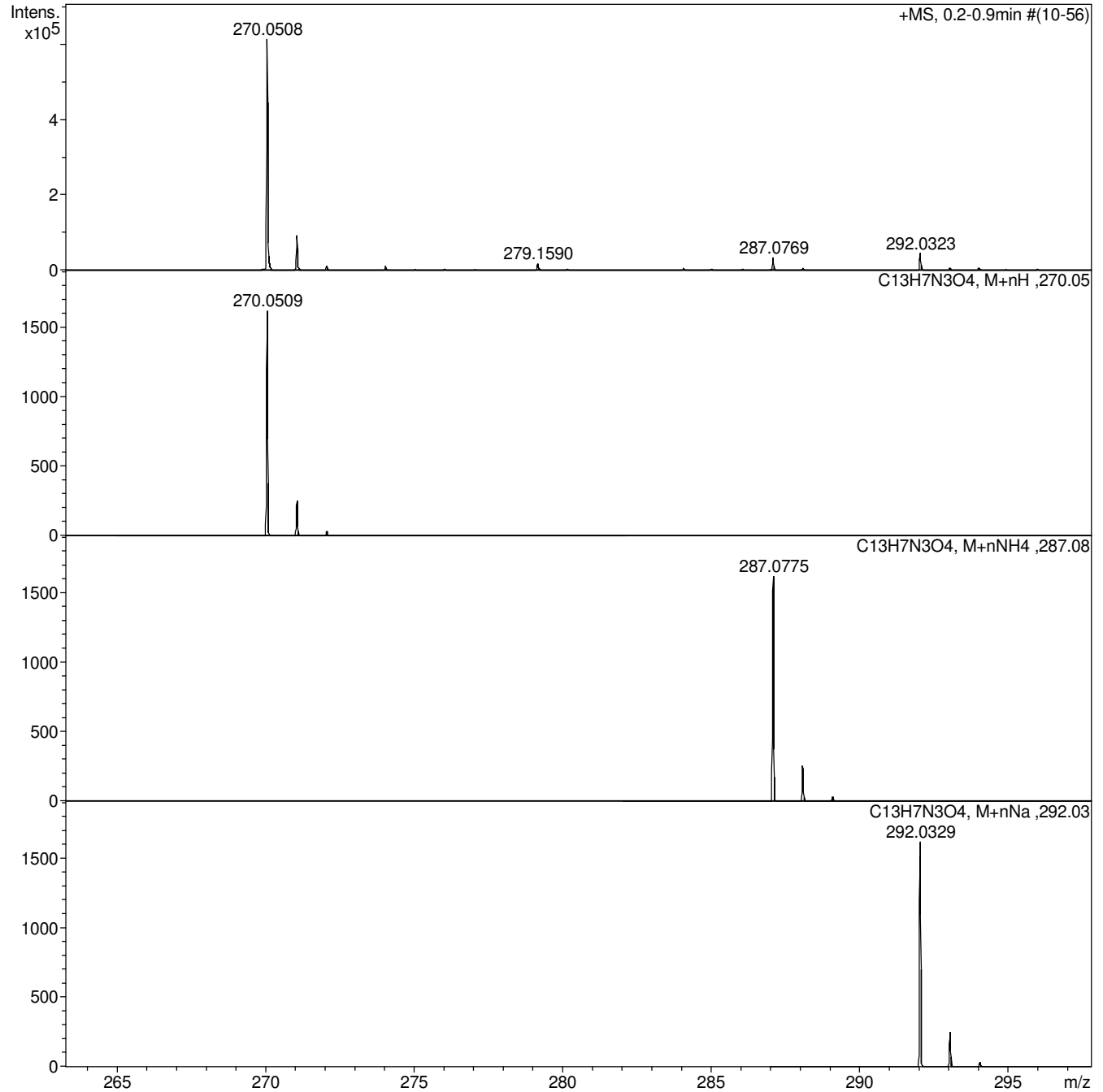
Analysis Info

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Sample Name /LPIK AF-185
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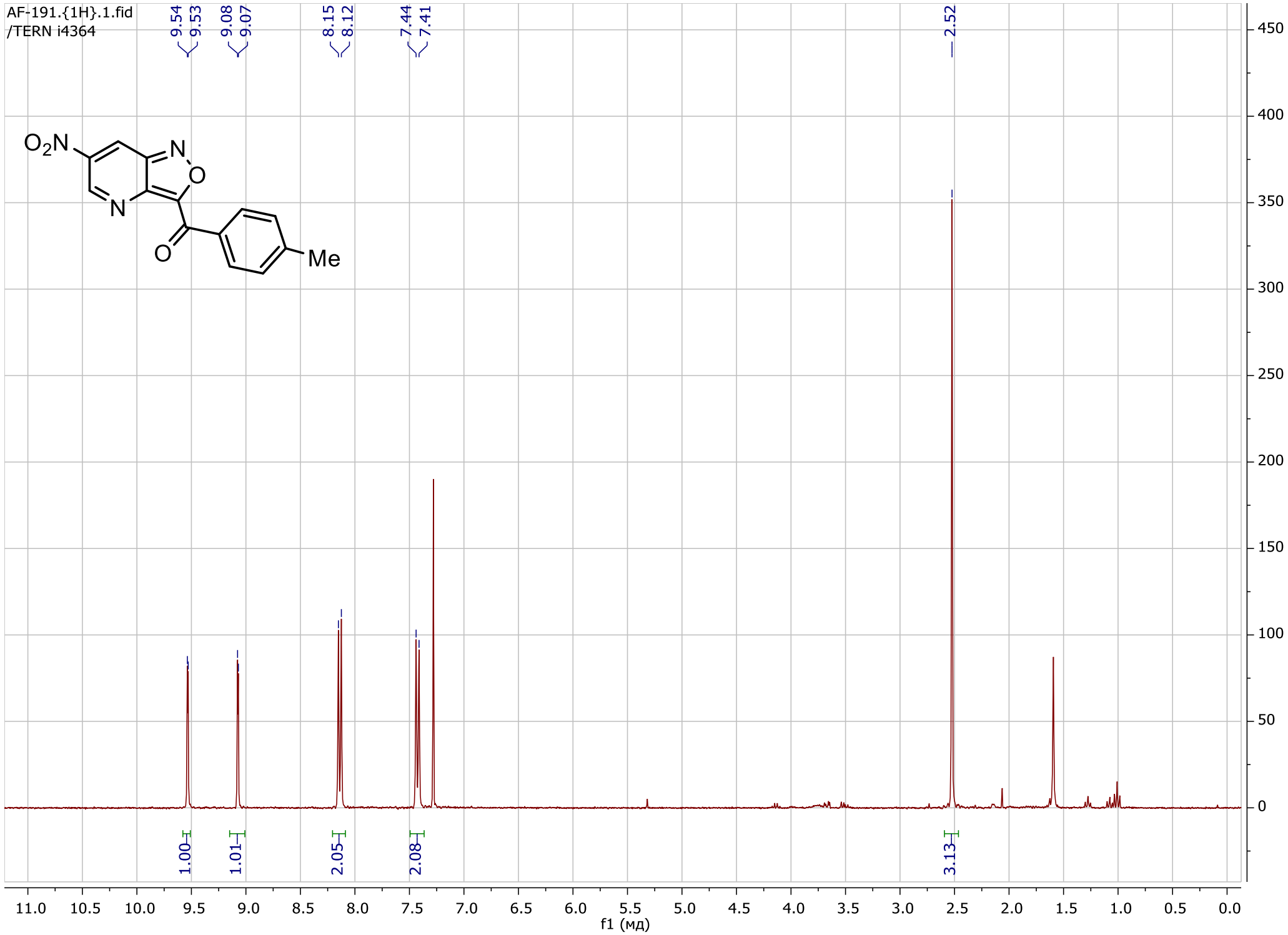
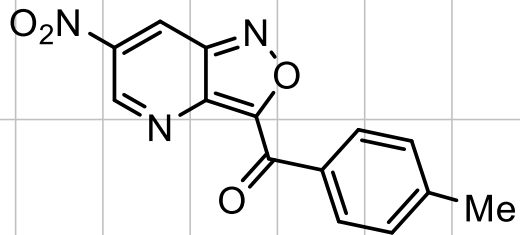
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Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

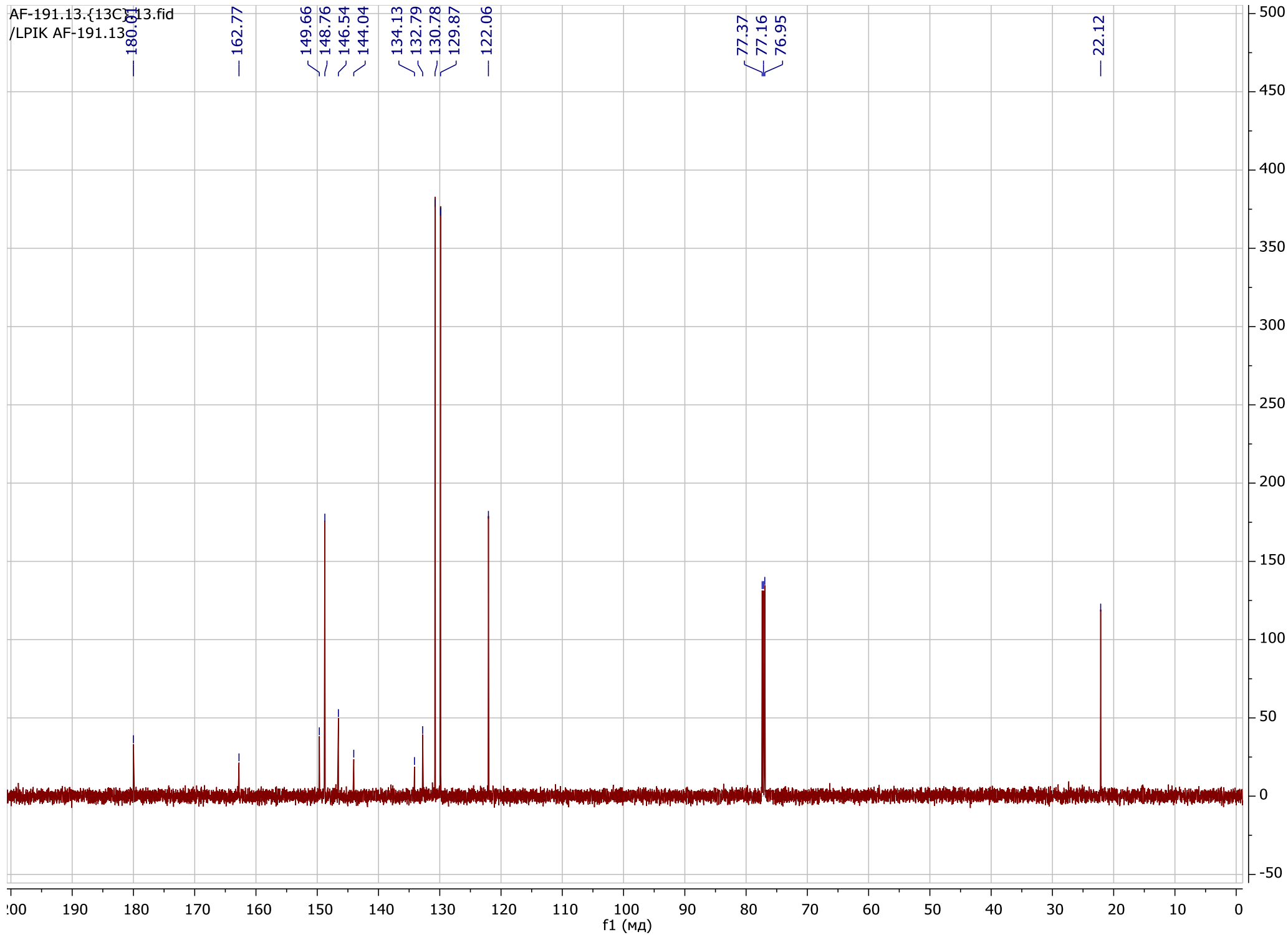
Acquisition Parameter

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Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
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AF-191.{1H}.1.fid
/TERN i4364





Display Report

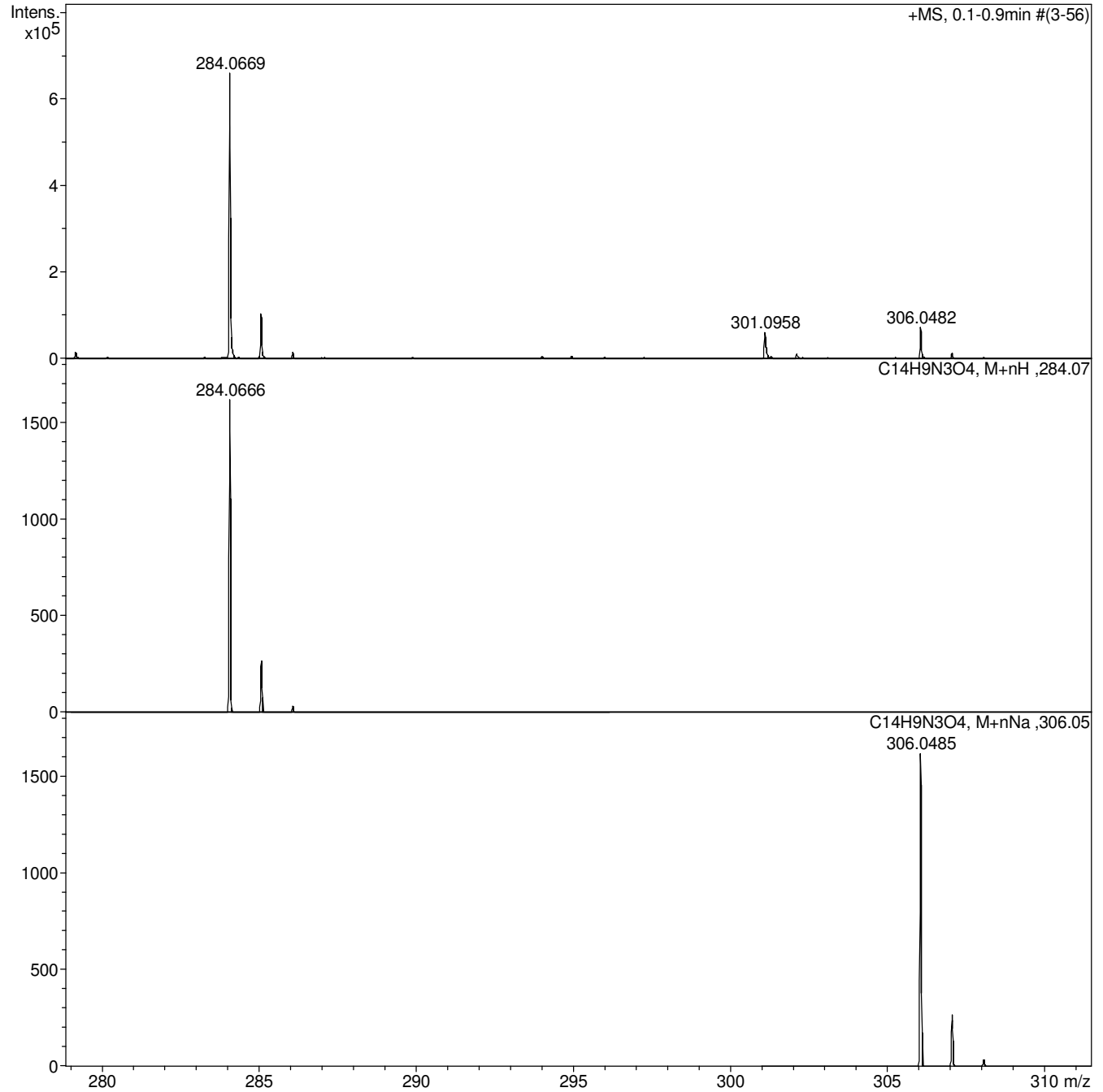
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2018\Bastrakov\1113028.d
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Sample Name /LPIK AF-191
Comment C14H9N3O4 mH 284.0665 calibrant added

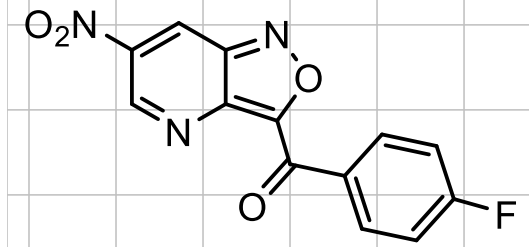
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Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

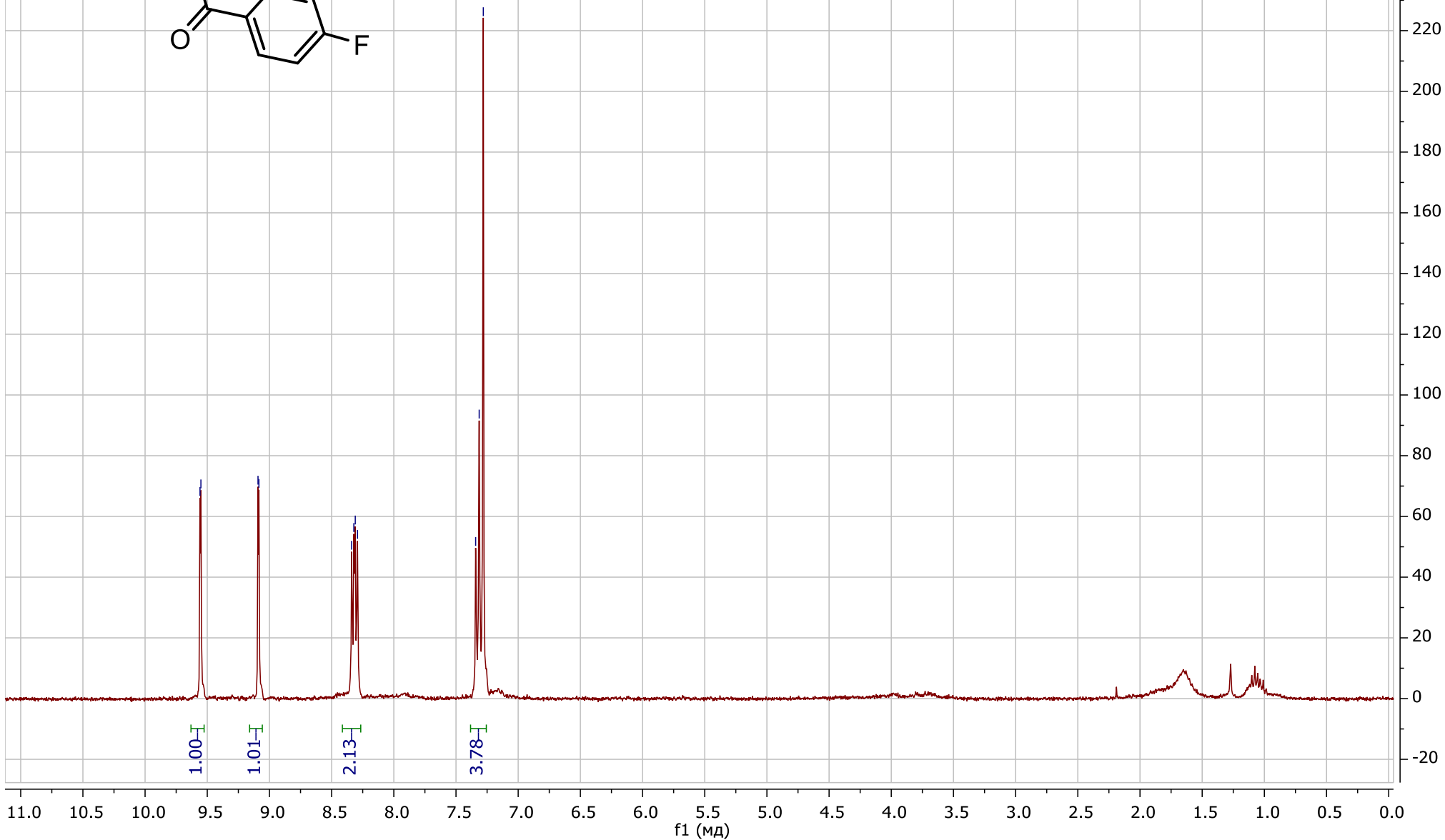
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Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



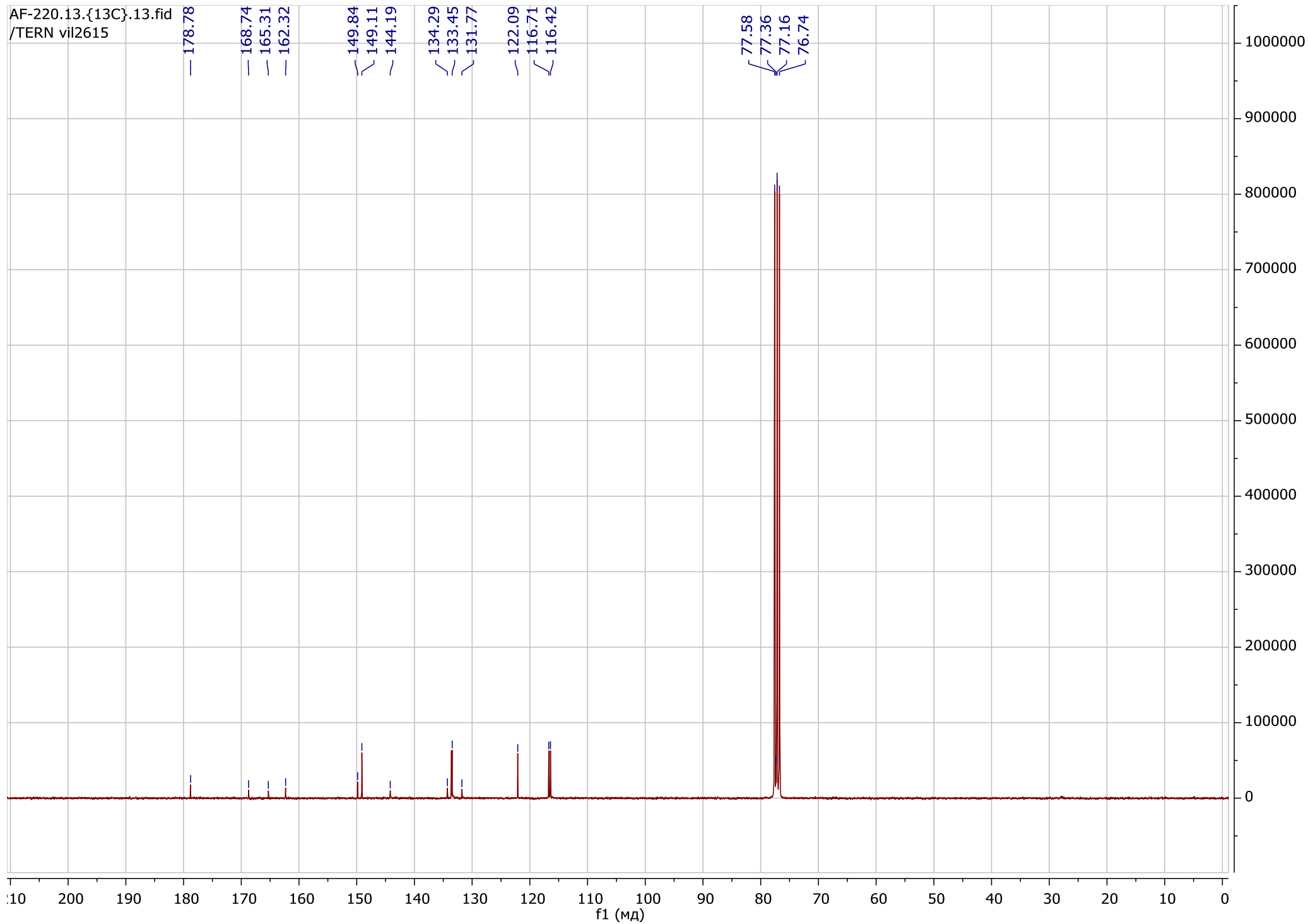
AF-220.1.{1H}.1.fid
/TERN IVYAR2303



9.56
9.55
9.09
9.08
8.34
8.32
8.31
8.29
7.34
7.31
7.28



AF-220.13.{13C}.13.fid
/TERN vil2615



Display Report

Analysis Info

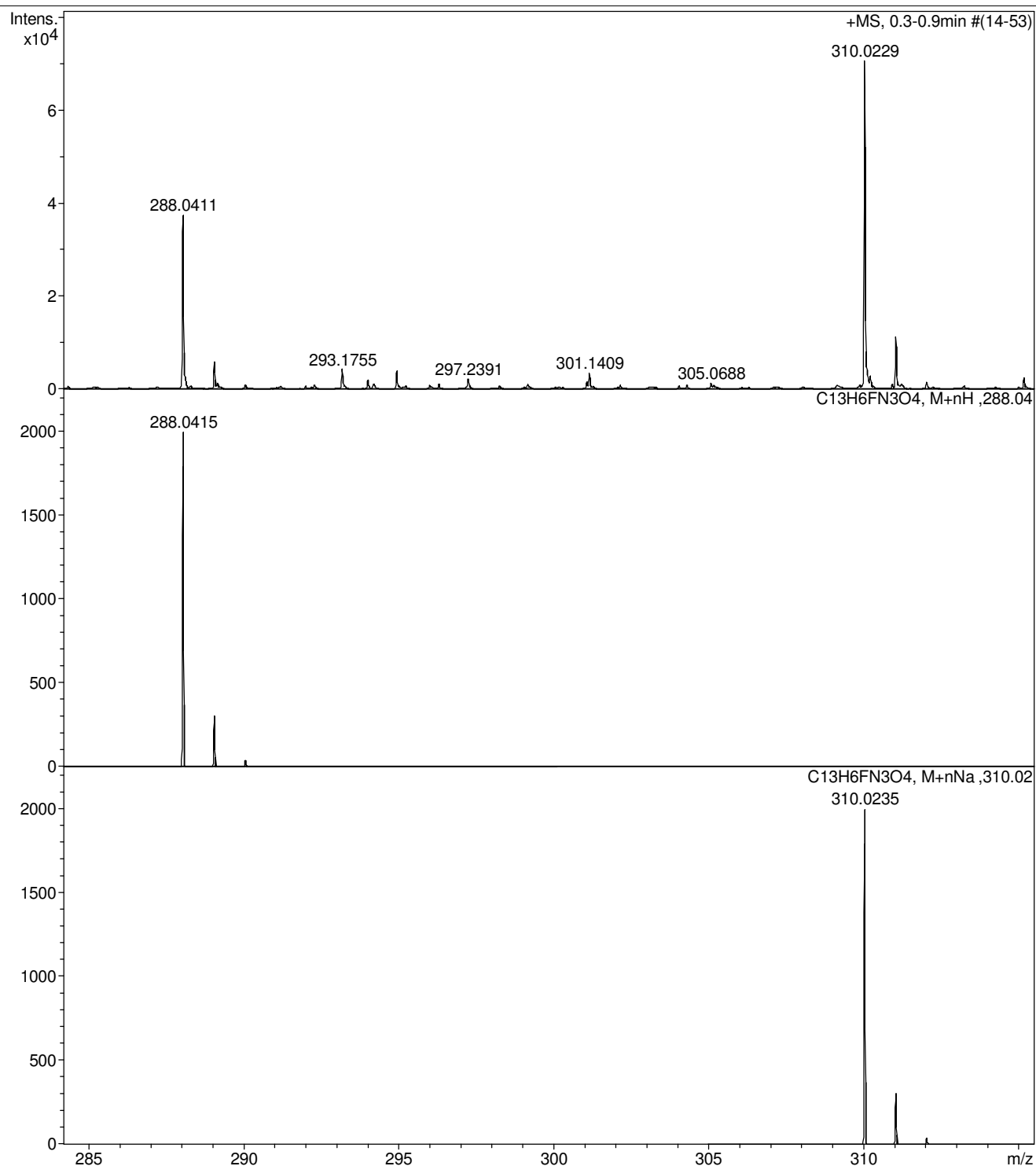
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0326039.d
Method tune_50-1600.m
Sample Name /LPIK AF-220
Comment C13H6FN3O4 mH 288.0415 calibrant added CH3CN

Acquisition Date 26.03.2019 18:58:20

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



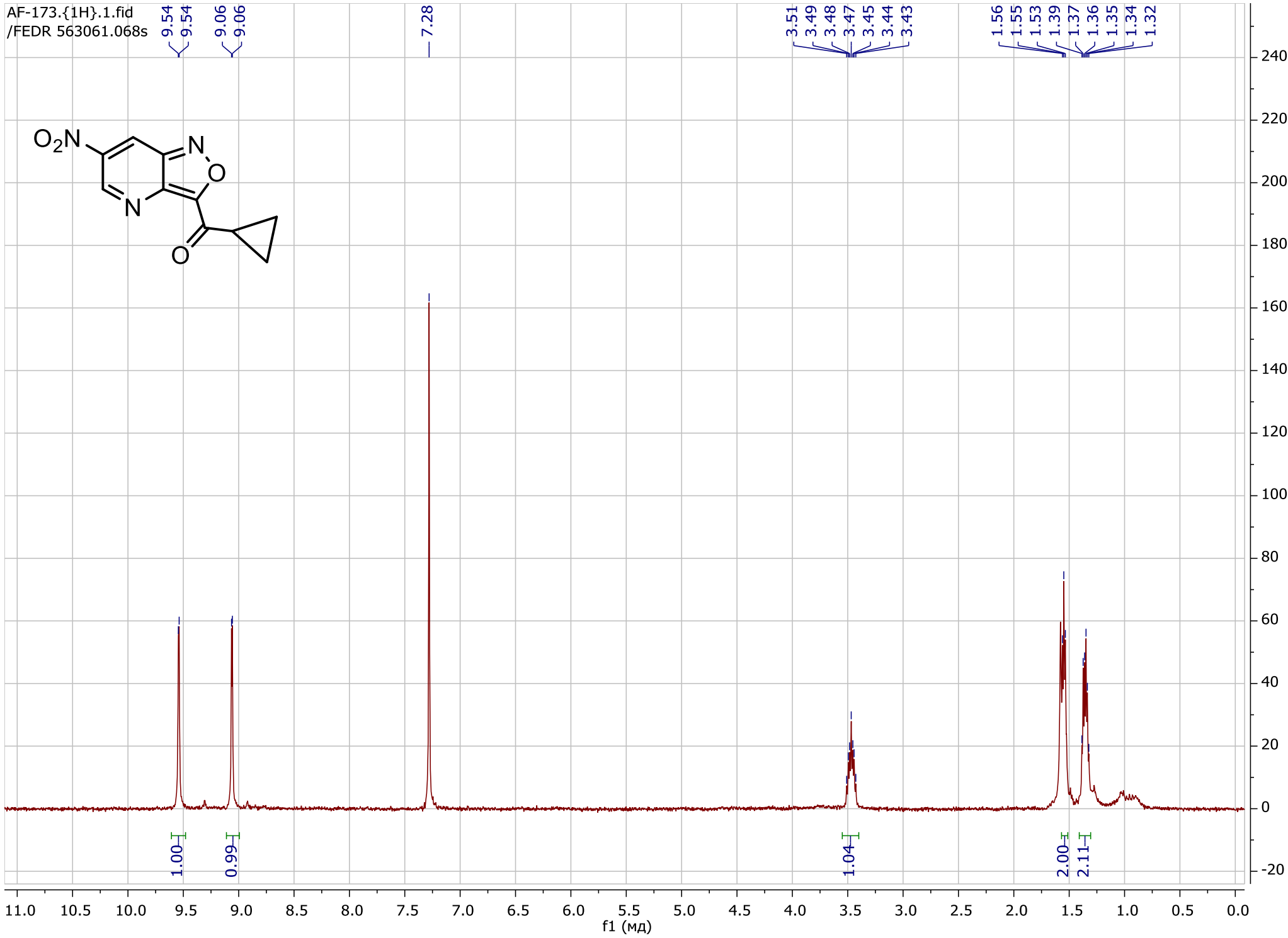
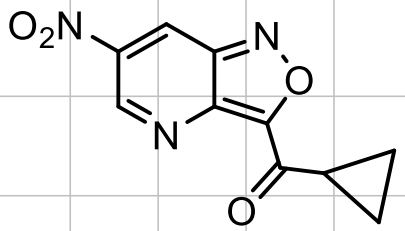
AF-173_{1H}.1.fid
/FEDR 563061.068s

9.54
9.54
9.06
9.06

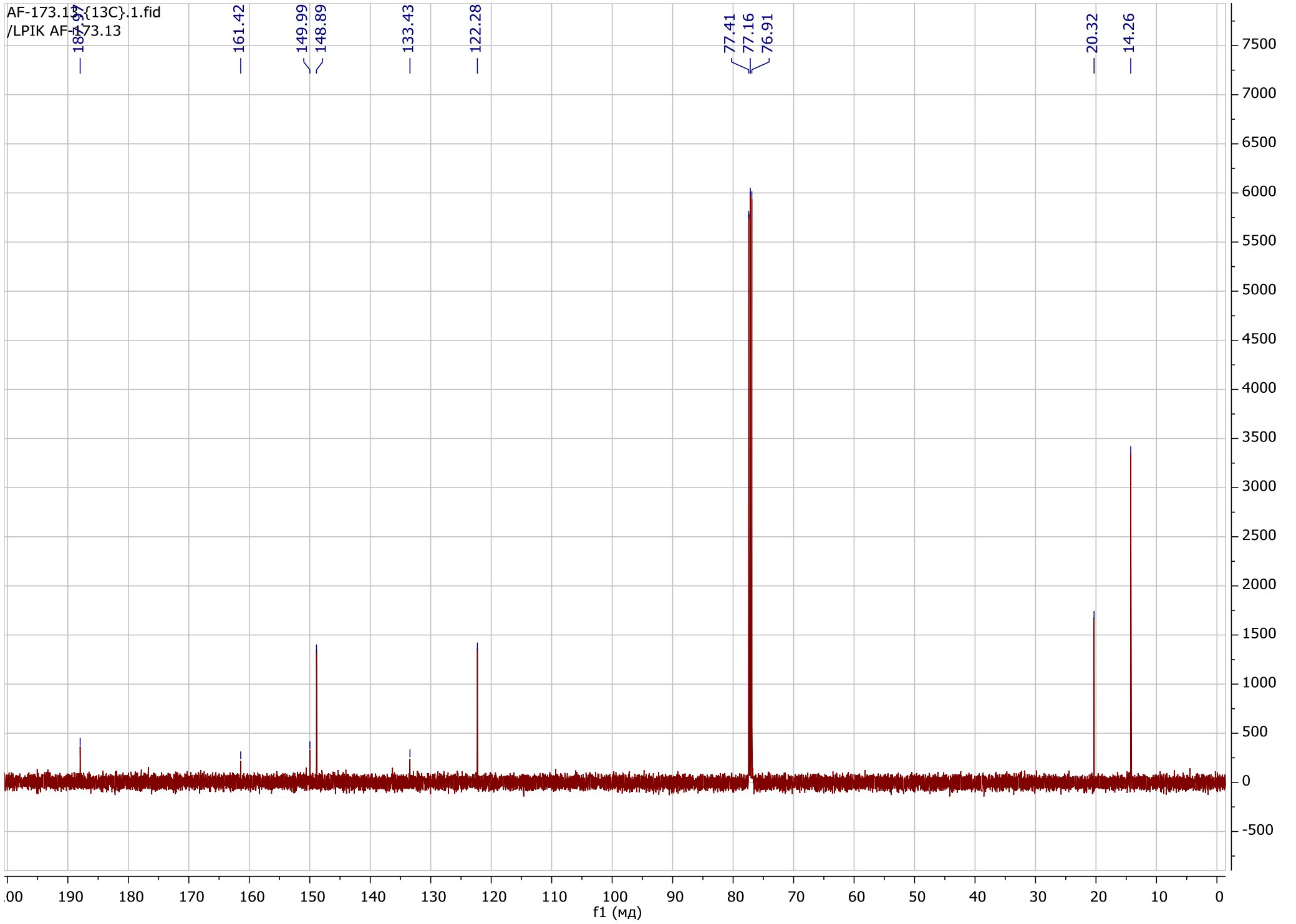
7.28

3.51
3.49
3.48
3.47
3.45
3.44
3.43

1.56
1.55
1.53
1.39
1.37
1.36
1.35
1.34
1.32



AF-173.14 {13C}.1.fid
/LPIK AF-173.13



Display Report

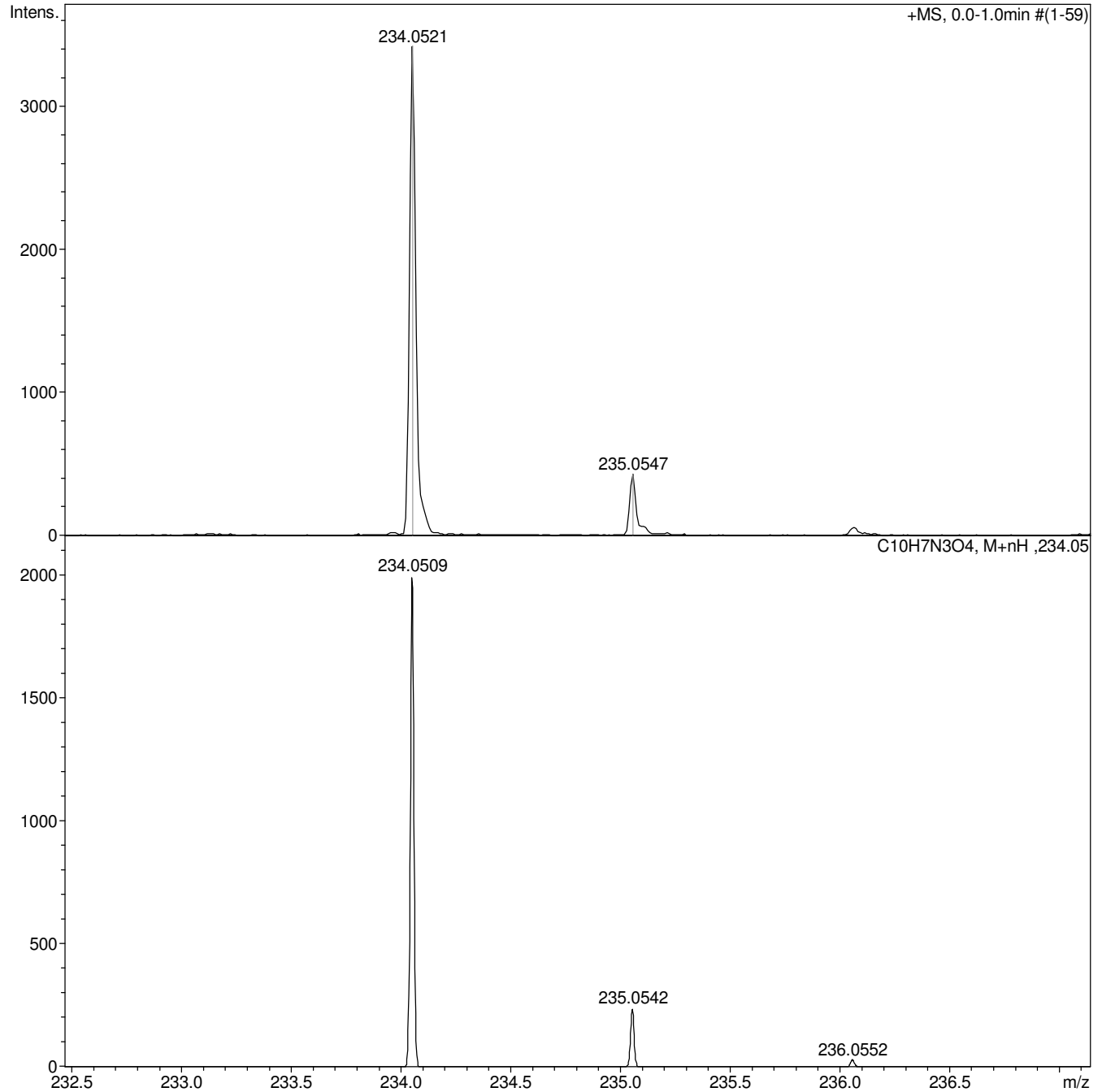
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2014\Bastrakov\0415017.d
Method tune_low.m
Sample Name /LPIK KA-12
Comment C10H7N3O4 mw 233 in CH3CN calibrant added

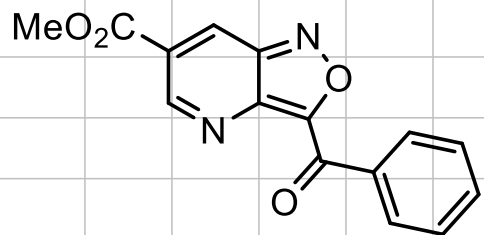
Acquisition Date 15.04.2014 16:15:34
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

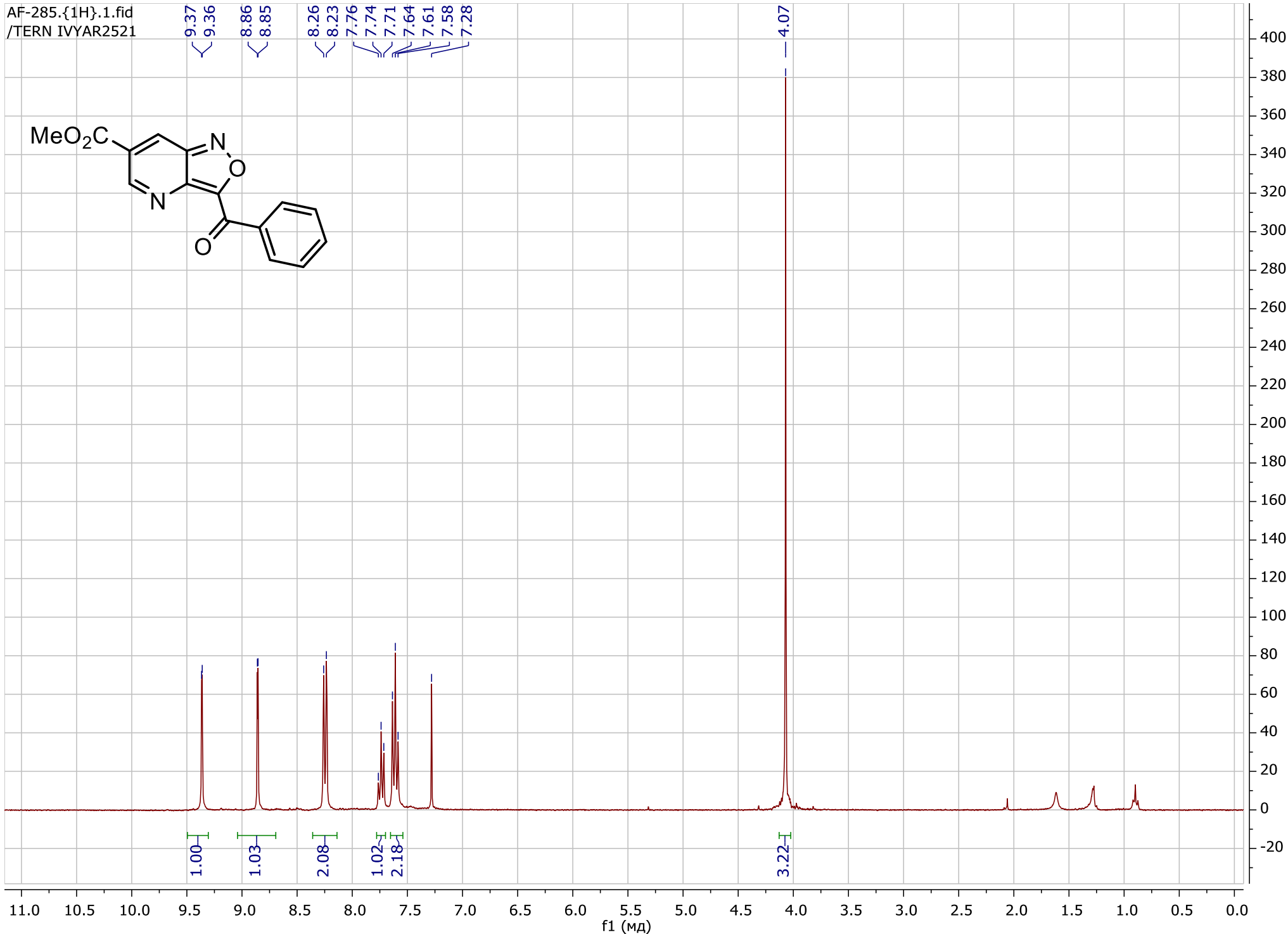
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



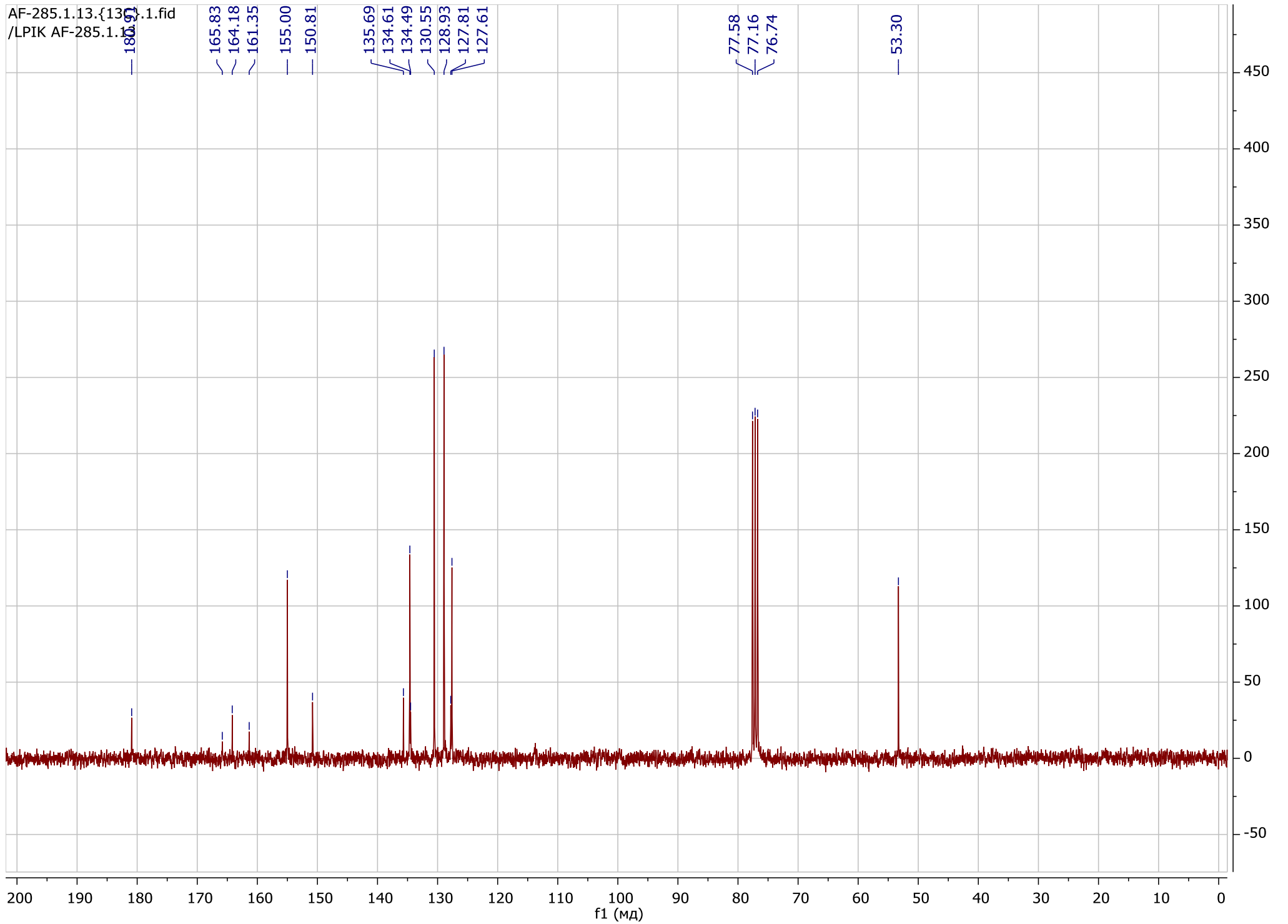
AF-285-¹H}.1.fid
/TERN IVYAR2521



9.37
9.36
8.86
8.85
8.26
8.23
7.76
7.74
7.71
7.64
7.61
7.58
7.28



AF-285.1.13.{13C}.1.fid
/LPIK AF-285.1.1



Display Report

Analysis Info

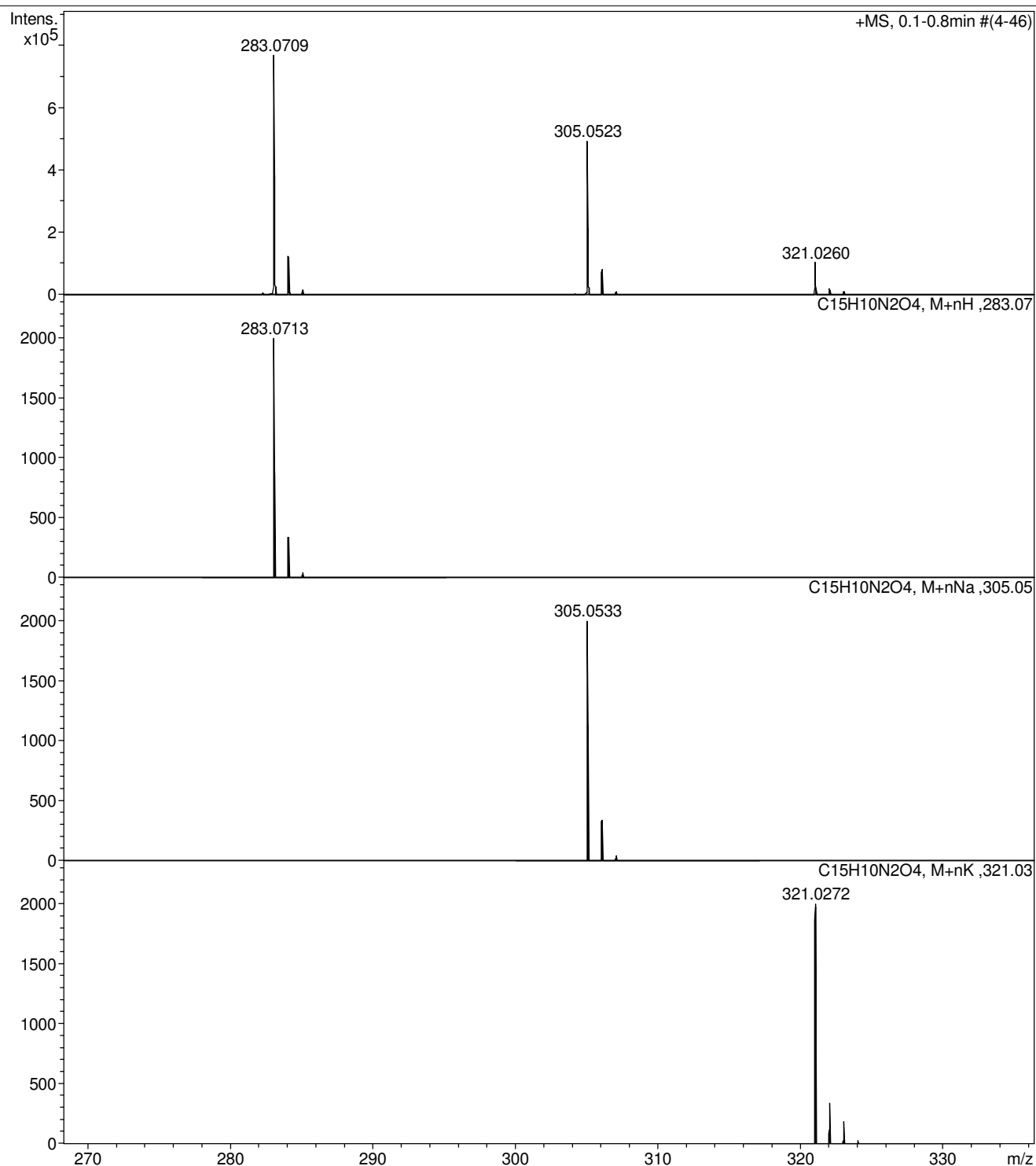
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0423025.d
Method tune_50-1600.m
Sample Name /LPIK AF-285
Comment C15H10N2O4 mH 283.0713 calibrant added

Acquisition Date 23.04.2019 12:50:10

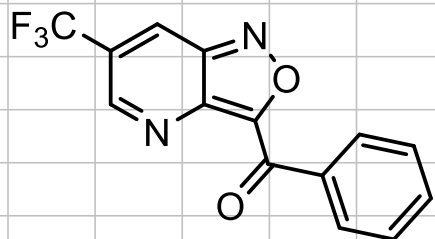
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

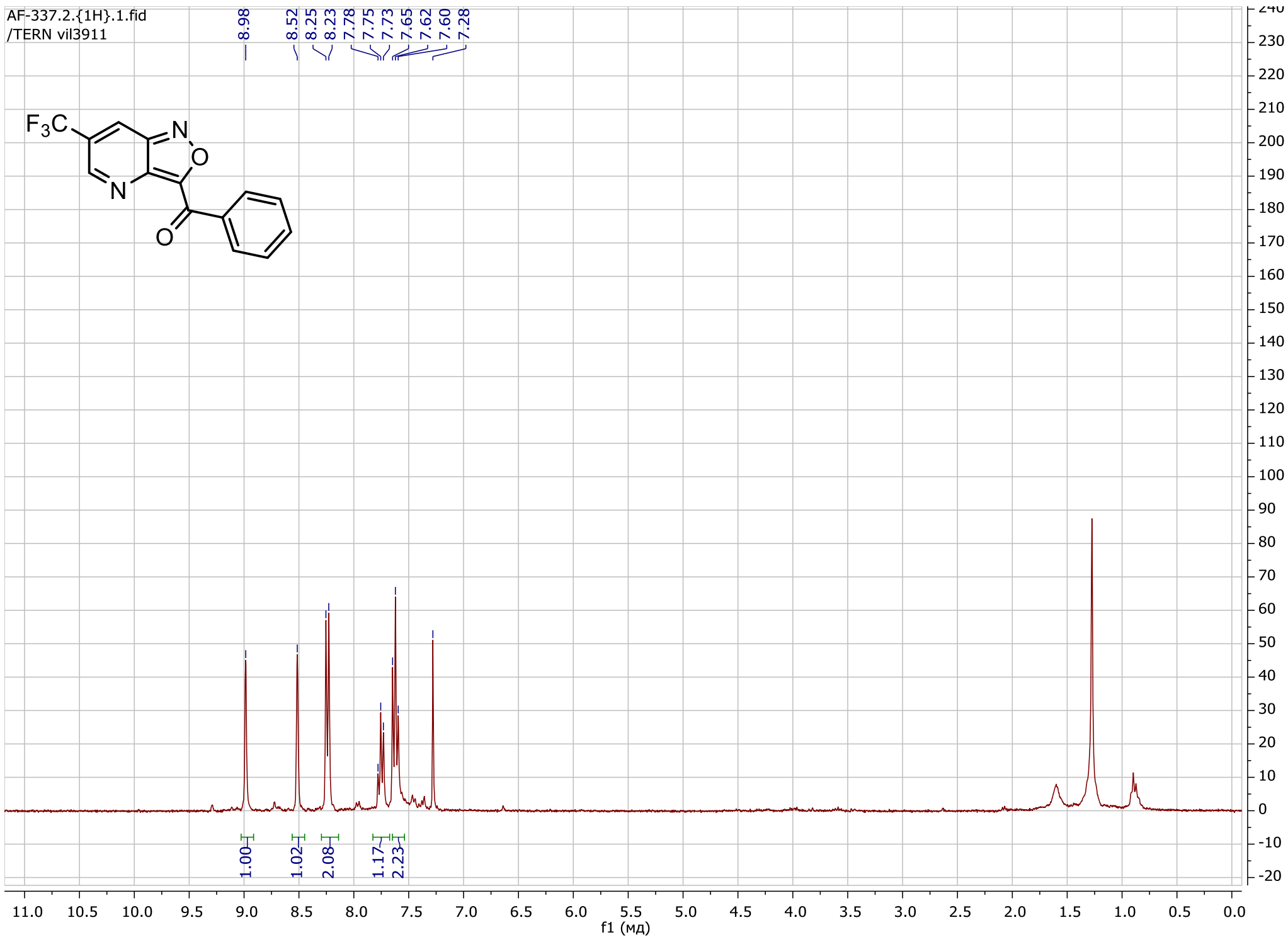
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



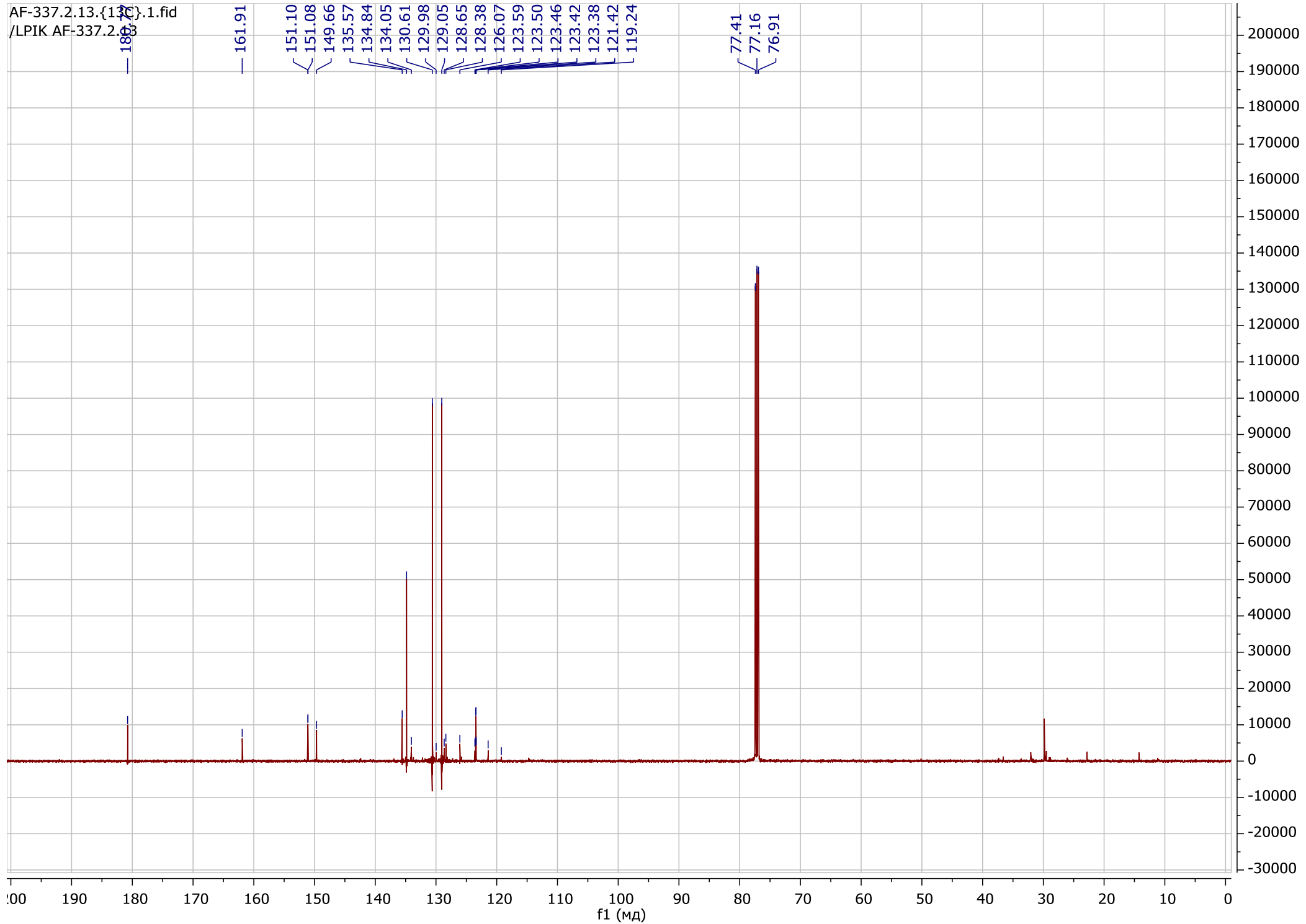
AF-337.2.{1H}.1.fid
/TERN vil3911



8.98
8.52
8.25
8.23
7.78
7.75
7.73
7.65
7.62
7.60
7.28



AF-337.2.13.{13C}.1.fid
/LPIK AF-337.2.13



Display Report

Analysis Info

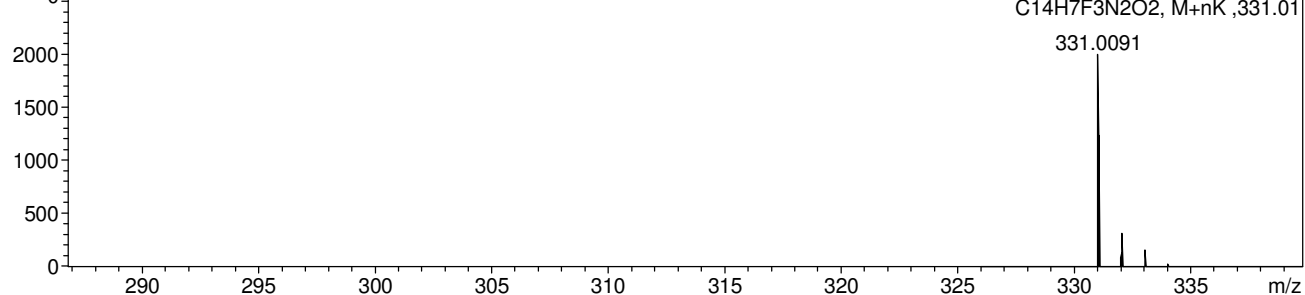
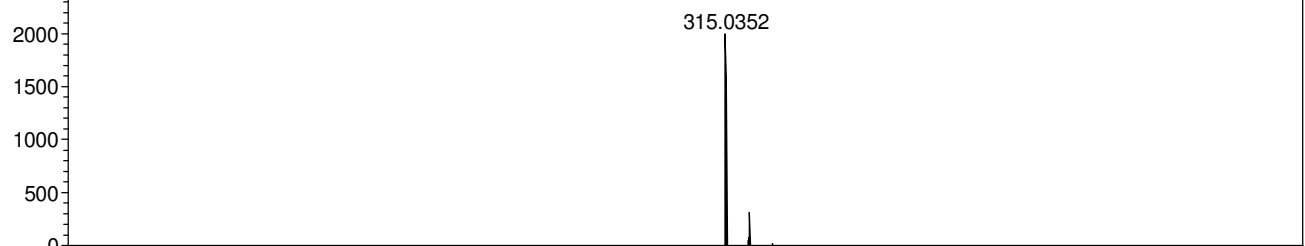
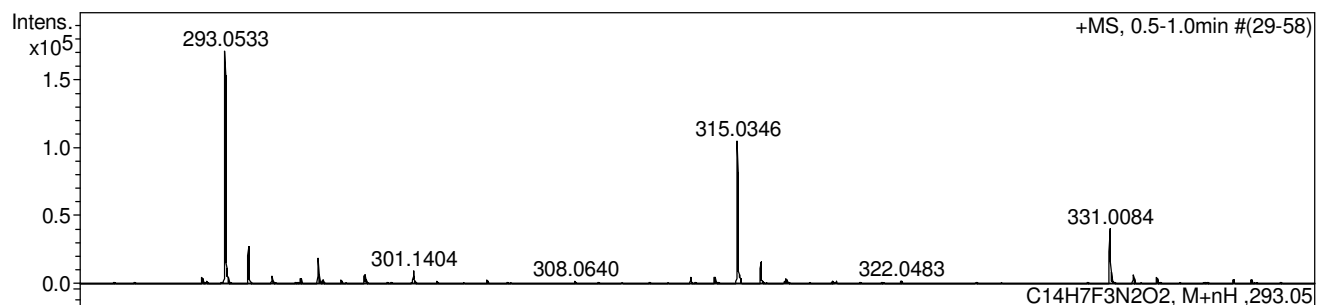
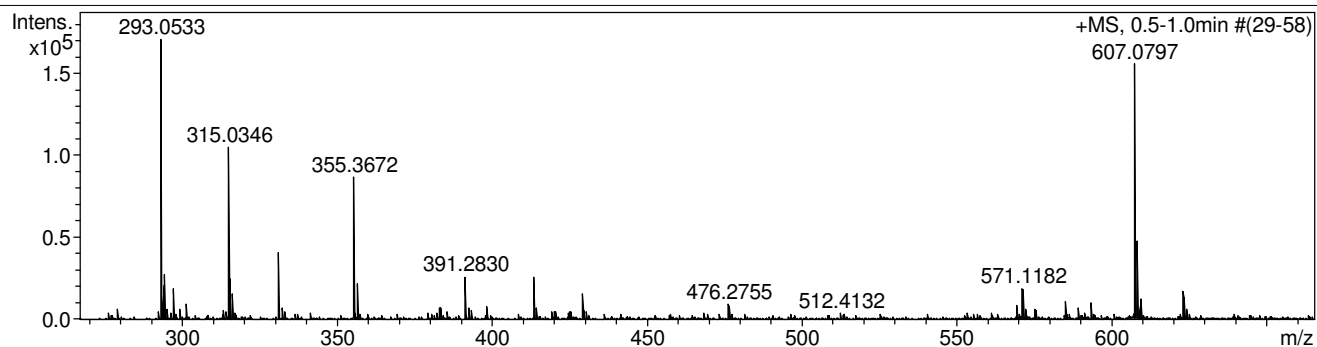
Analysis Name D:\Data\Kolotyrykina\2019\Bastrakov\1127009.d
Method tune_50-1600.m
Sample Name /LPIK AF-337.2
Comment C14H7F3N2O2 mH 293.0532 calibrant added

Acquisition Date 27.11.2019 15:40:50

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

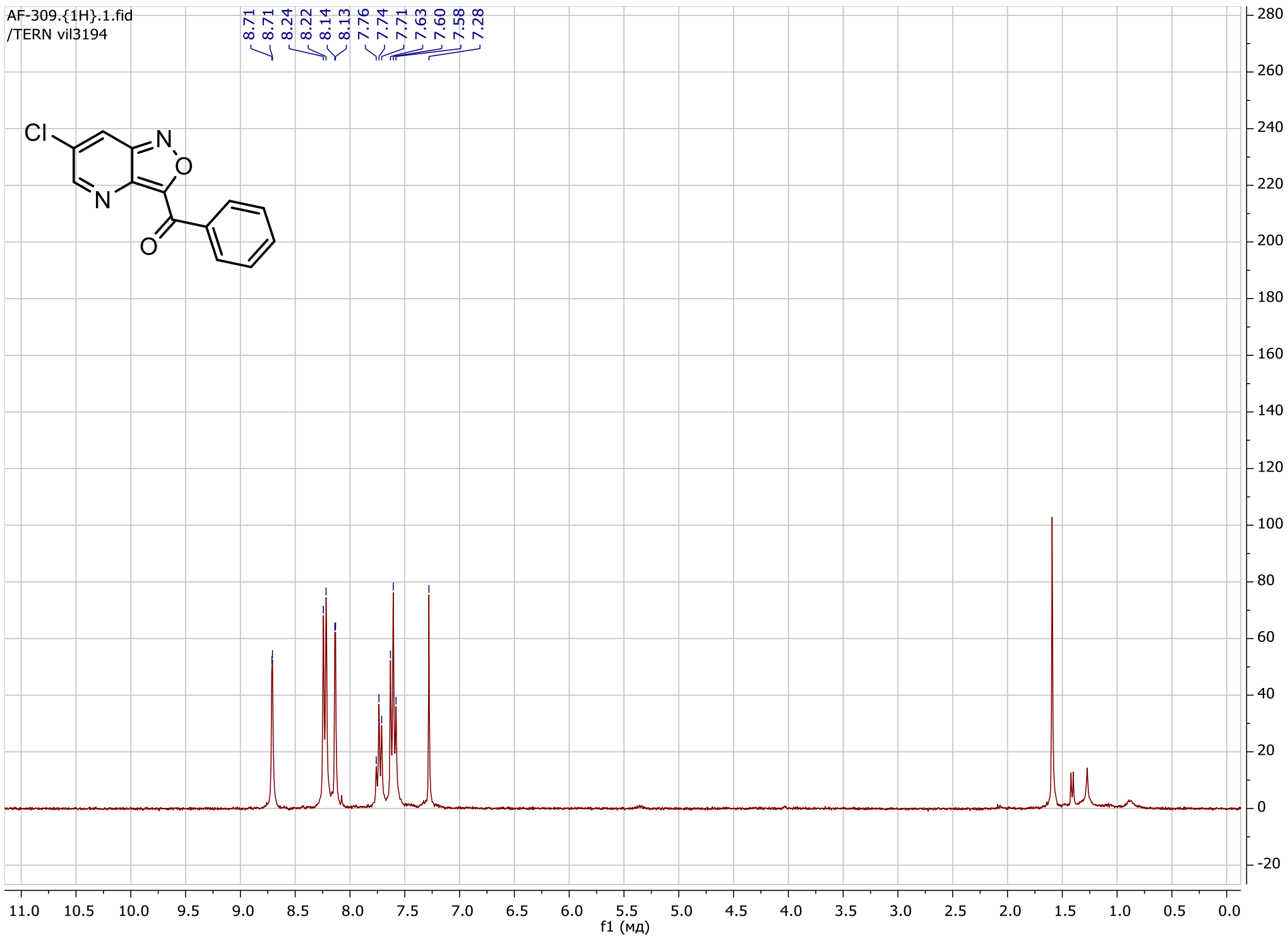
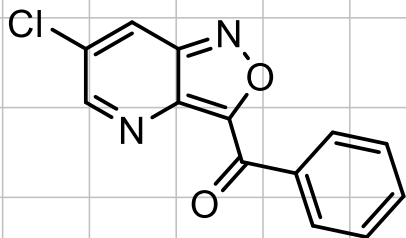
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

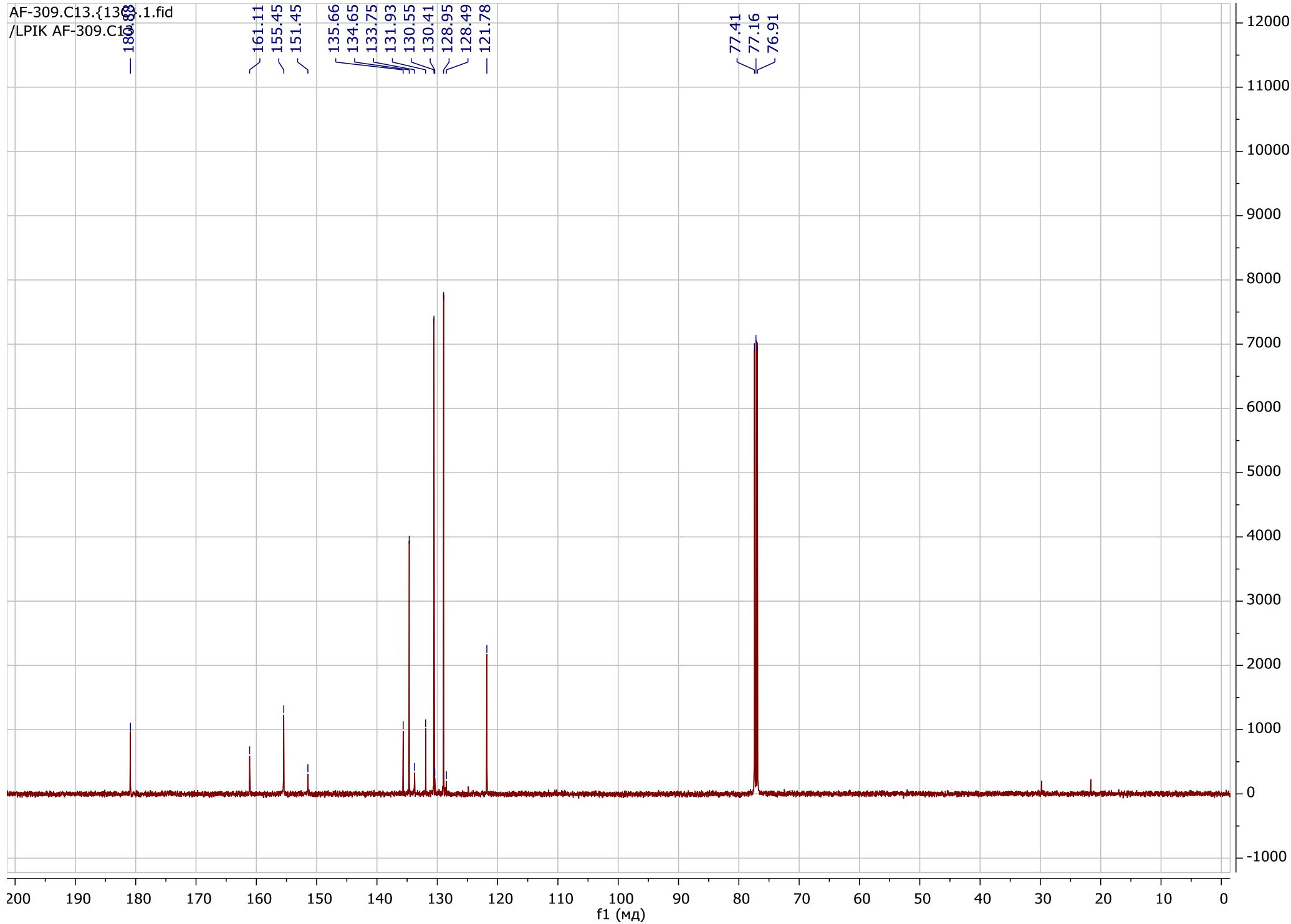


AF-309-¹H}.1.fid
/TERN vil3194

8.71
8.71
8.24
8.22
8.14
8.13
7.76
7.74
7.71
7.63
7.60
7.58
7.28



AF-309.C13.{133}.1.fid
/LPIK AF-309.C13



Display Report

Analysis Info

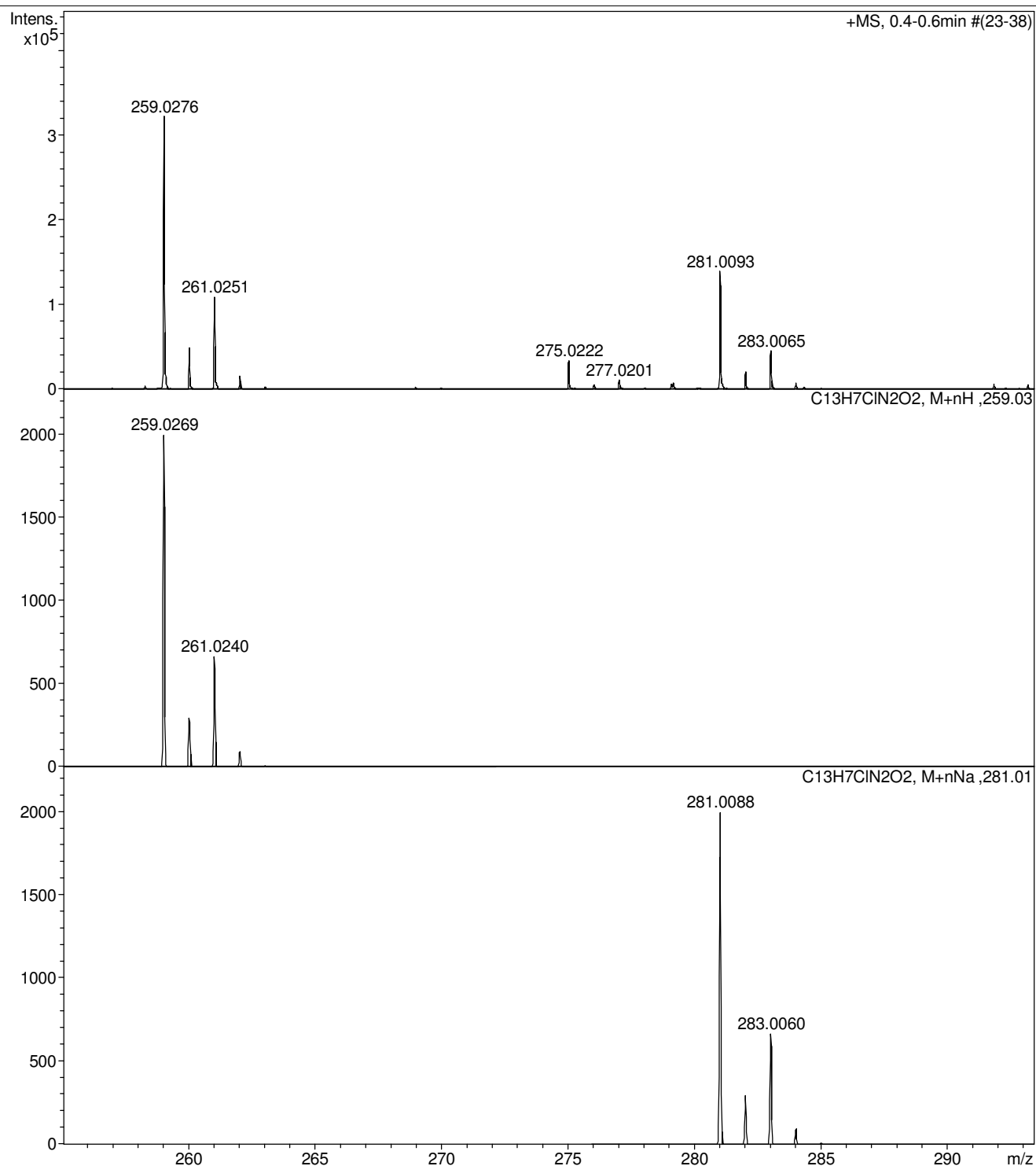
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0925006.d
Method tune_50-1600.m
Sample Name /LPIK AF-309
Comment C13H7CIN2O2 mH 259.0268 calibrant added

Acquisition Date 25.09.2019 12:43:56

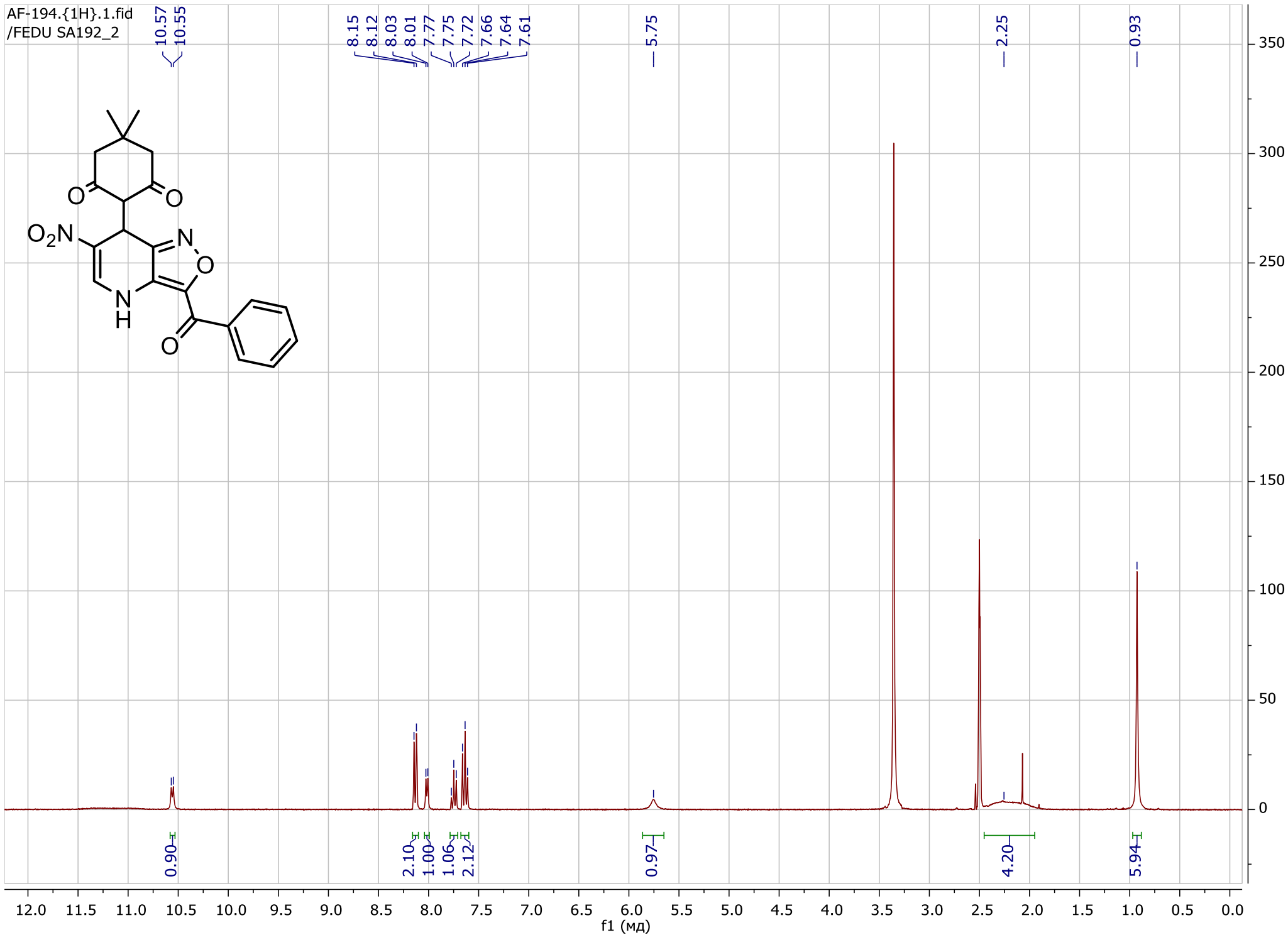
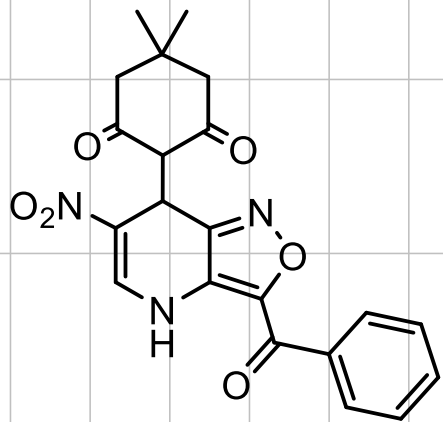
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

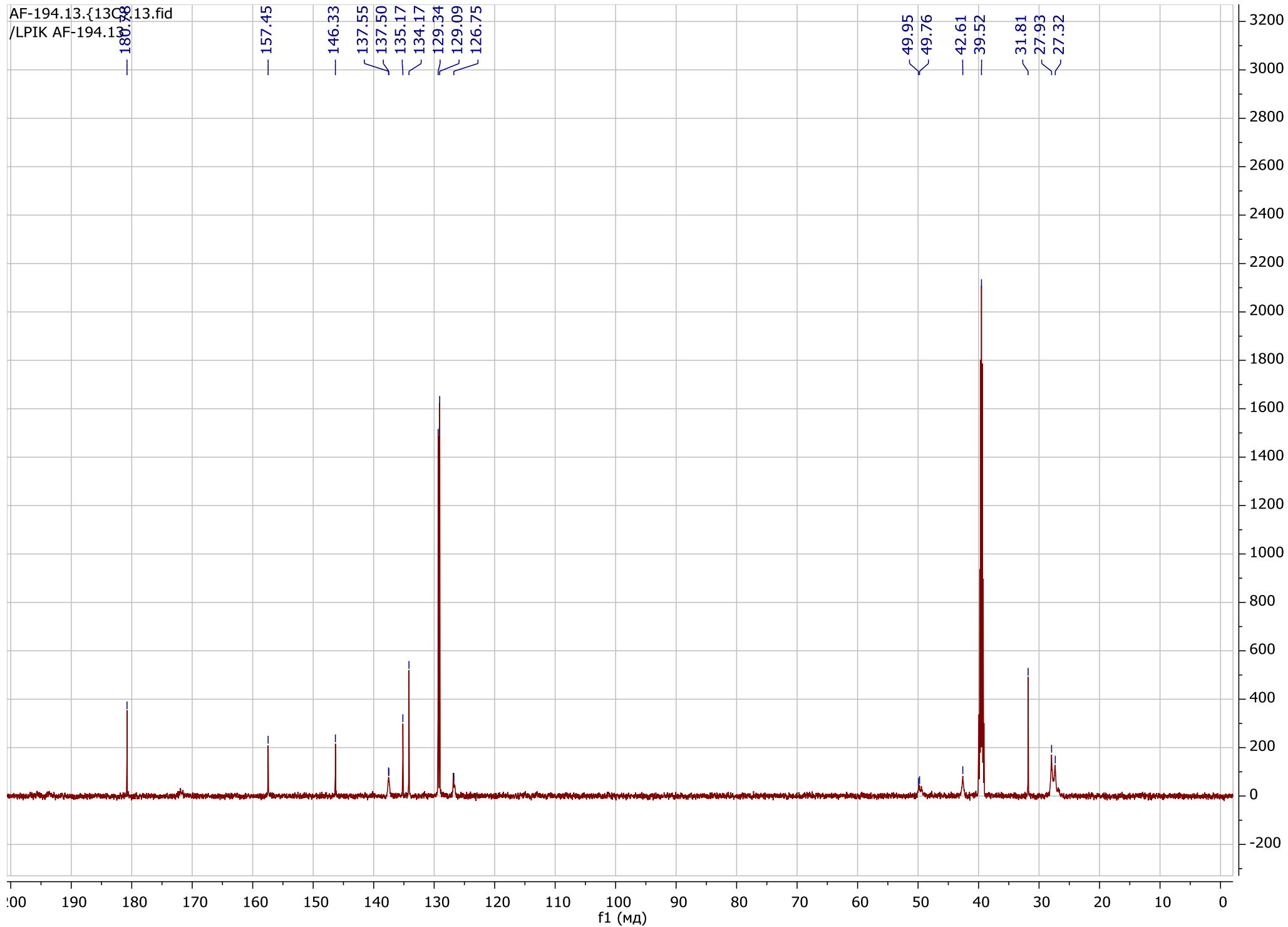
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-194.{1H}.1.fid
/FEDU SA192_2



AF-194.13.{13C}.13.fid
/LPIK AF-194.13



Display Report

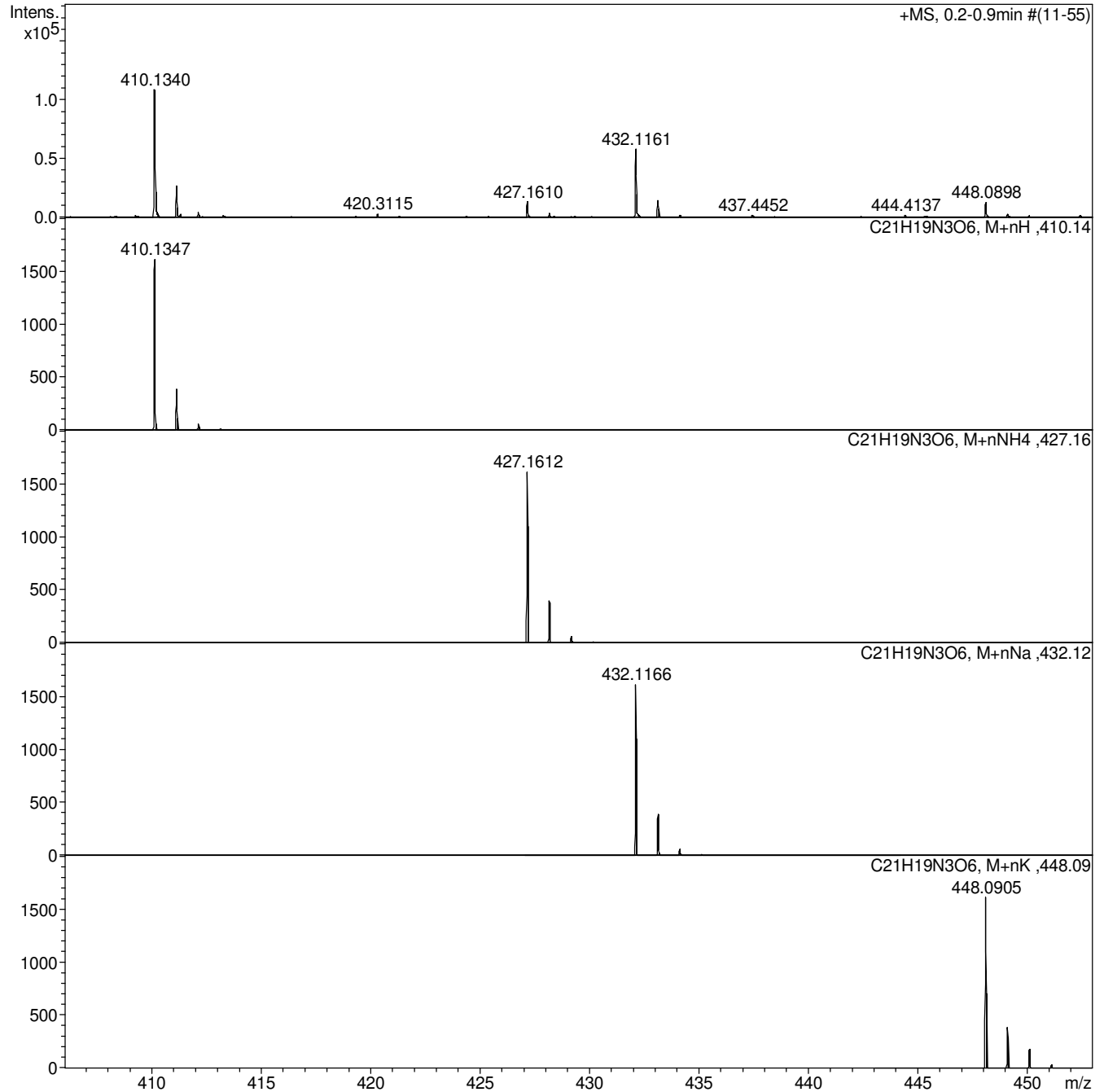
Analysis Info

Analysis Name D:\Data\Kolotyrykina\2018\Bastrakov\1113014.d
Method tune_50-1600.m
Sample Name /LPIK AF-194
Comment C21H19N3O6 mH 410.1346 calibrant added

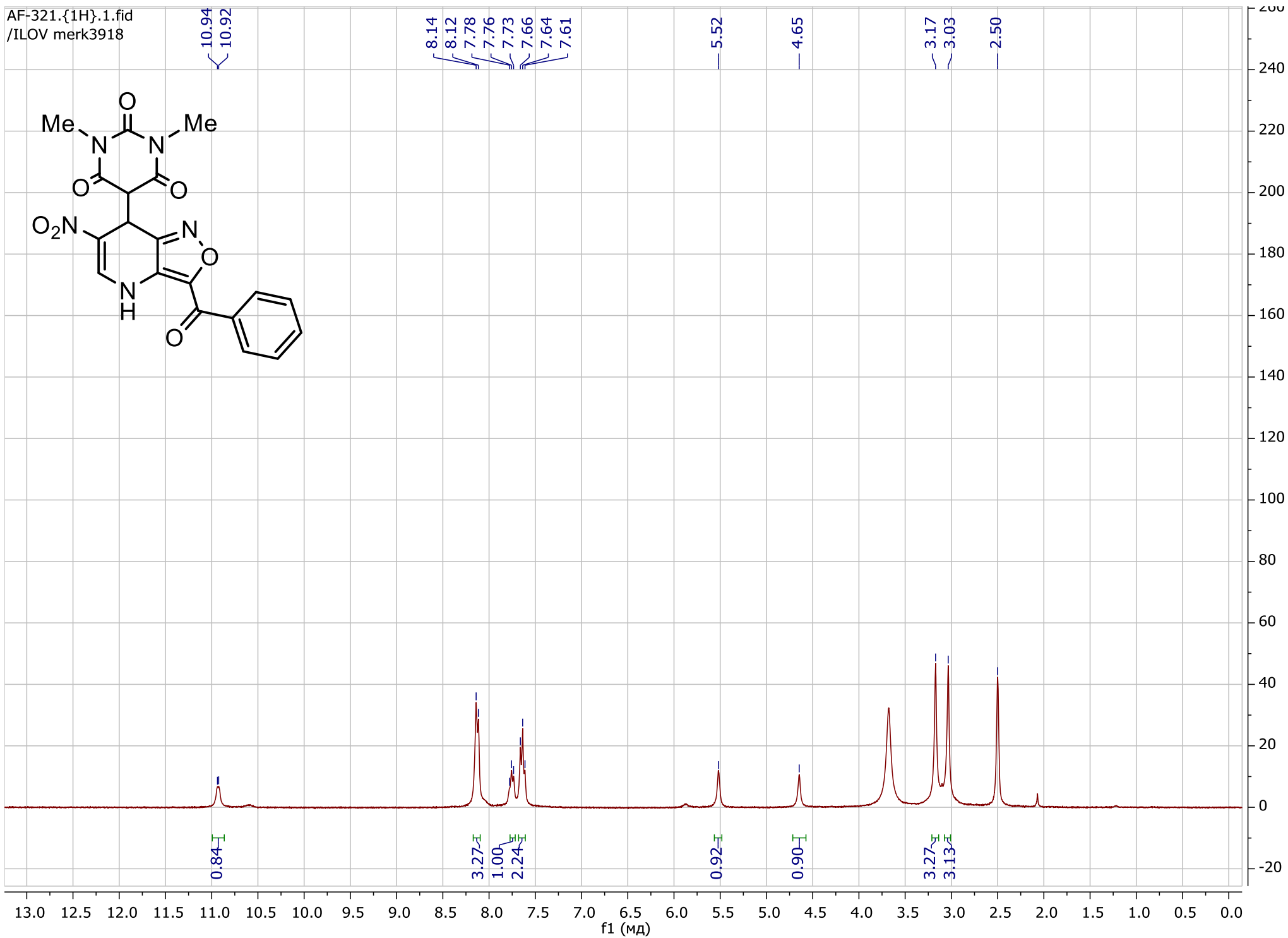
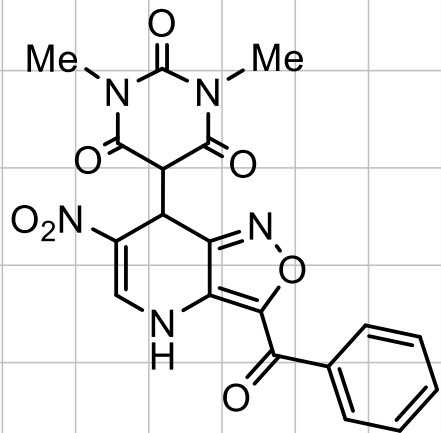
Acquisition Date 13.11.2018 11:04:52
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

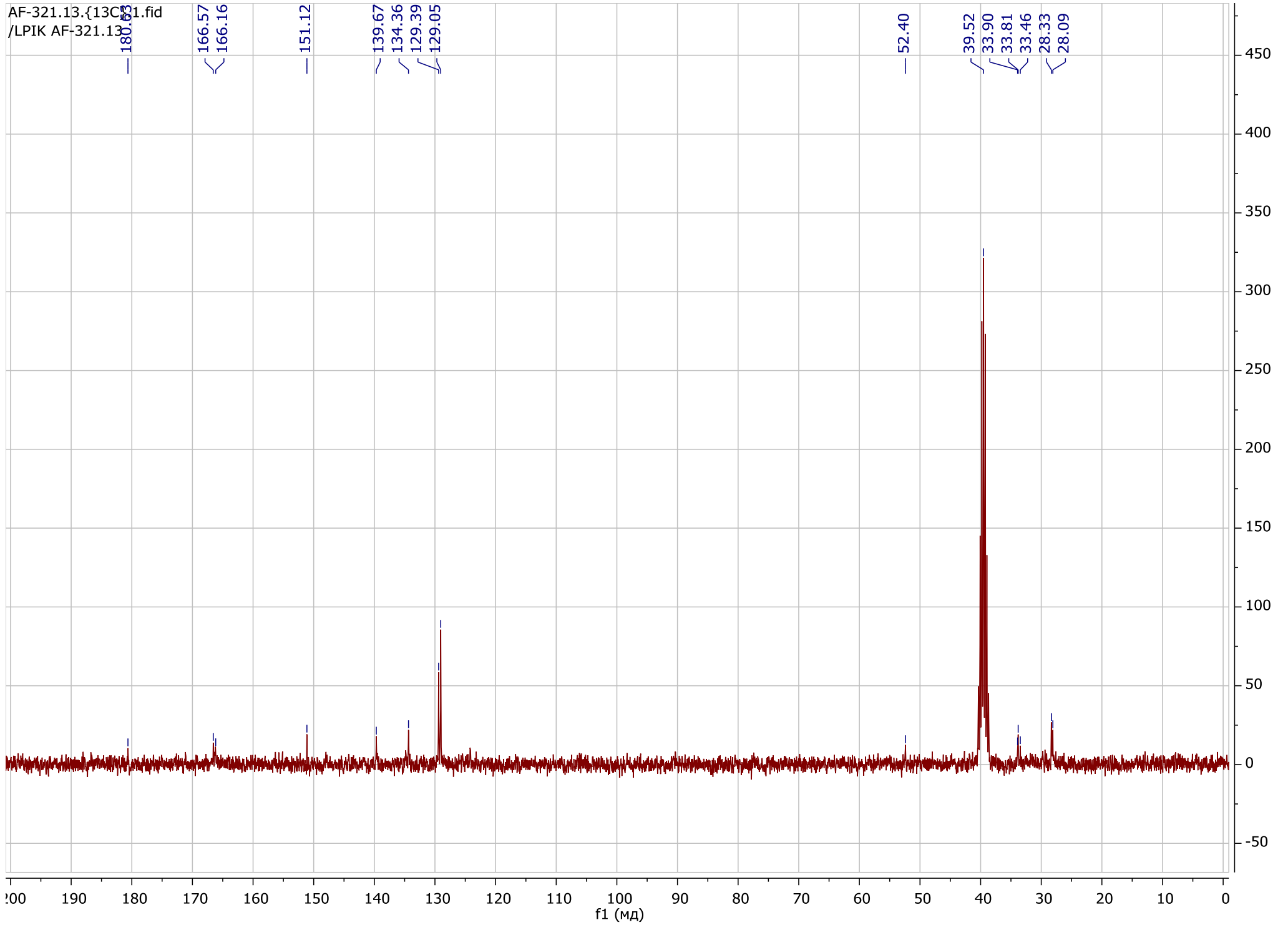
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-321.{1H}.1.fid
/ILOV merk3918



AF-321.13.{13C}.1.fid
/LPIK AF-321.13



Display Report

Analysis Info

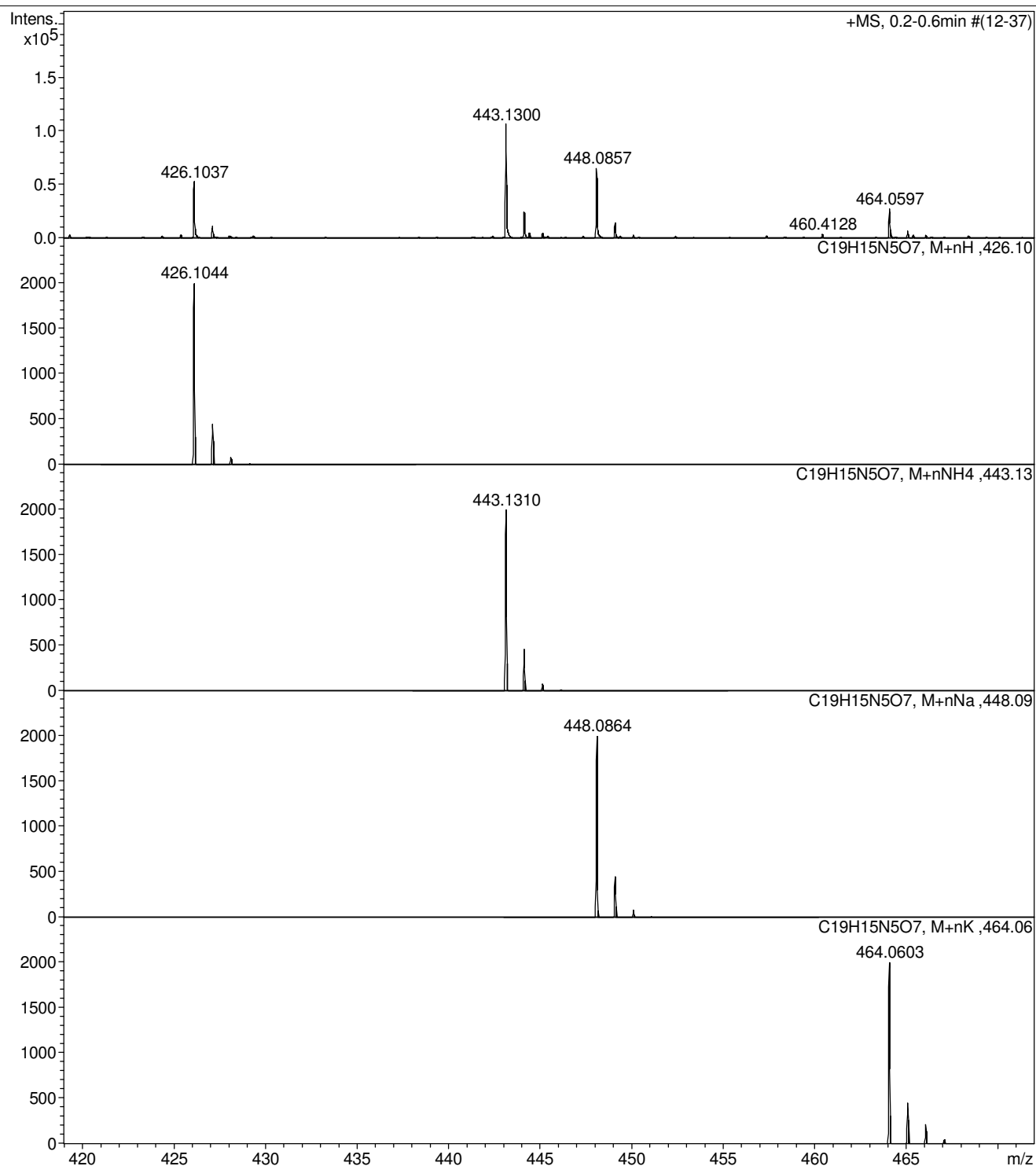
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0925009.d
Method tune_50-1600.m
Sample Name /LPIK AF-321
Comment C19H15N5O7 mH 426.1044 calibrant added

Acquisition Date 25.09.2019 13:01:51

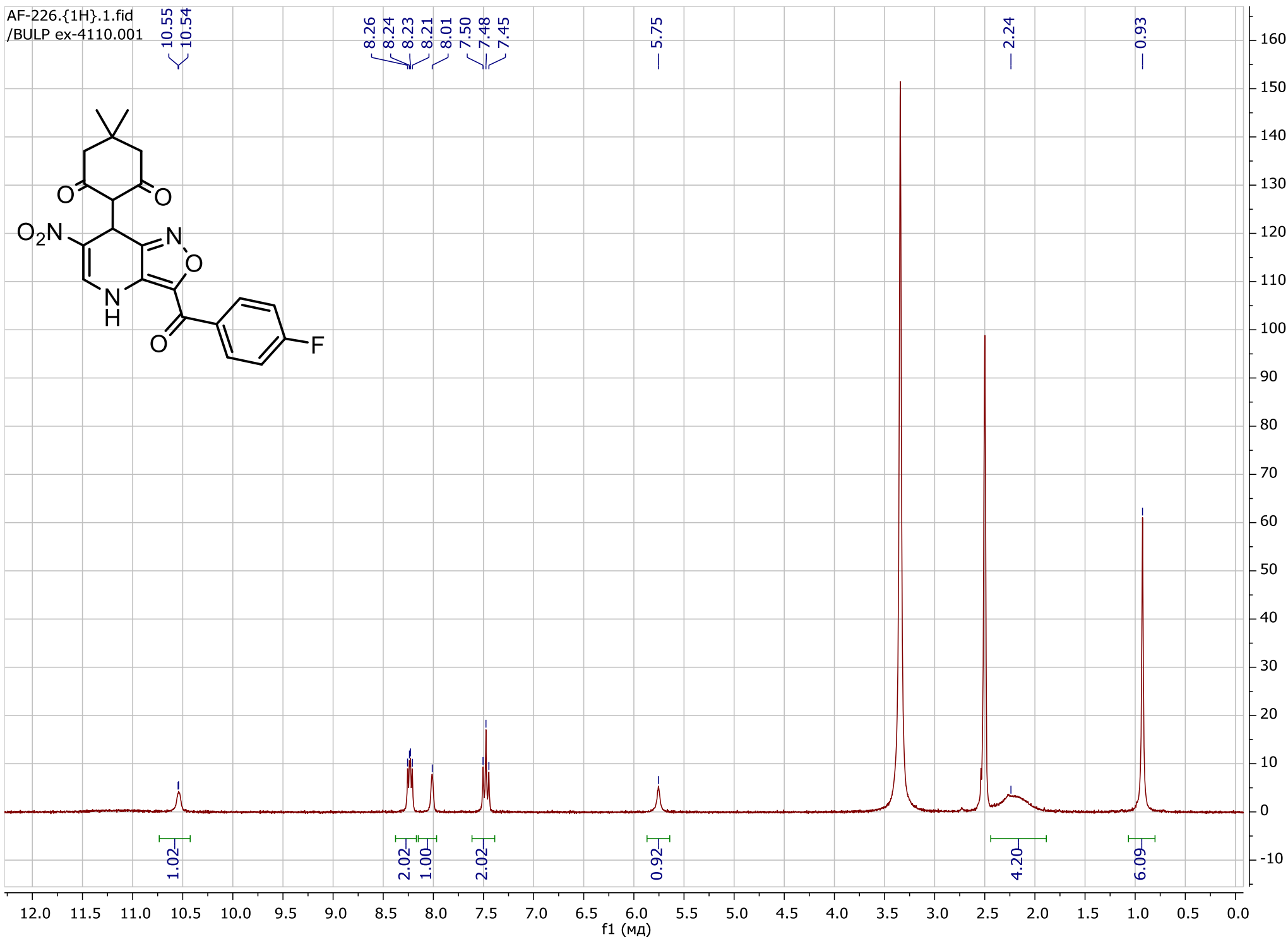
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

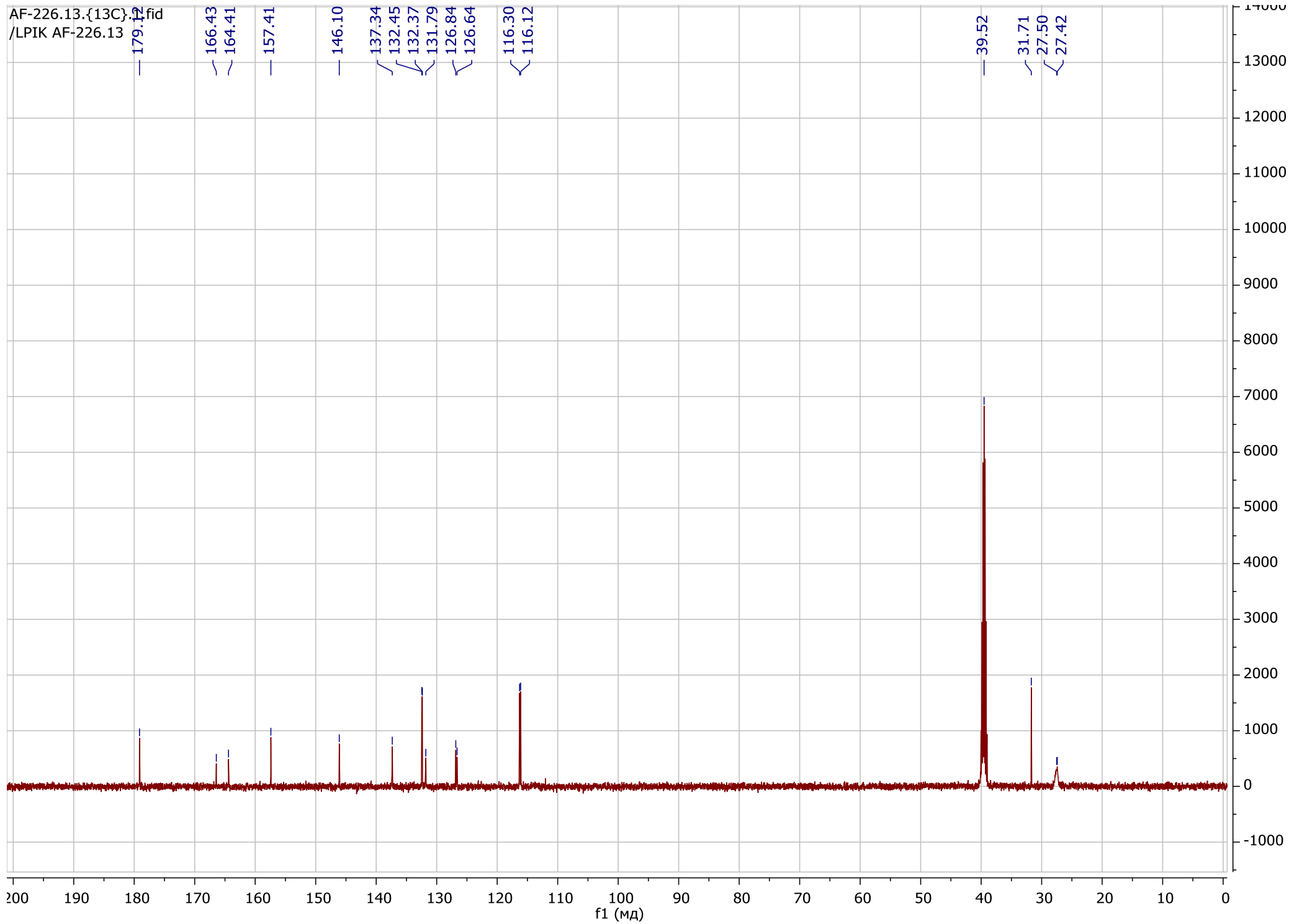
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-226.{1H}.1.fid
/BULP ex-4110.001



AF-226.13.{13C}.fid
/LPIK AF-226.13



Display Report

Analysis Info

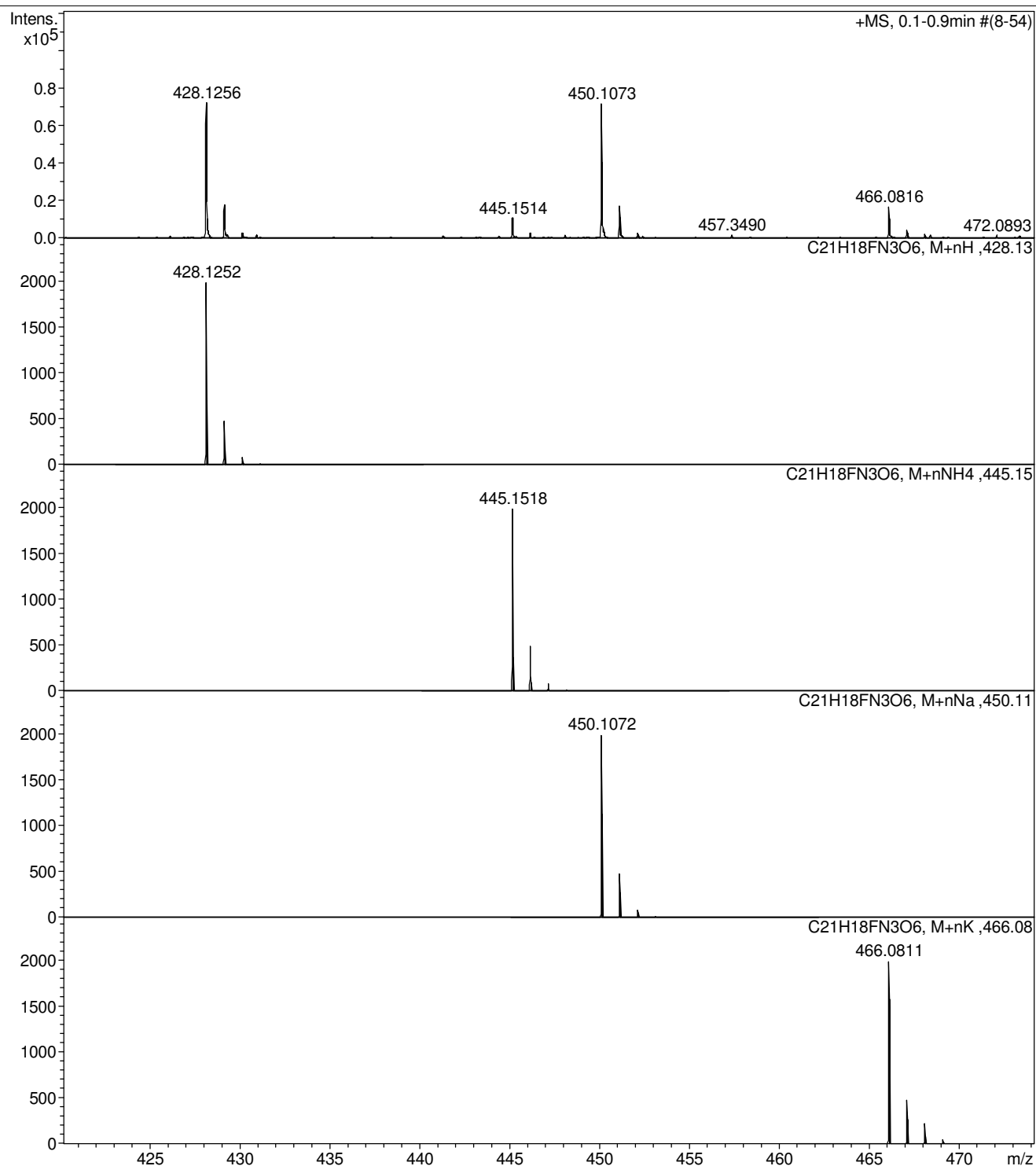
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0326040.d
Method tune_50-1600.m
Sample Name /LPIK AF-226
Comment C21H18FN3O6 mH 428.1252 calibrant added CH3CN

Acquisition Date 26.03.2019 19:03:42

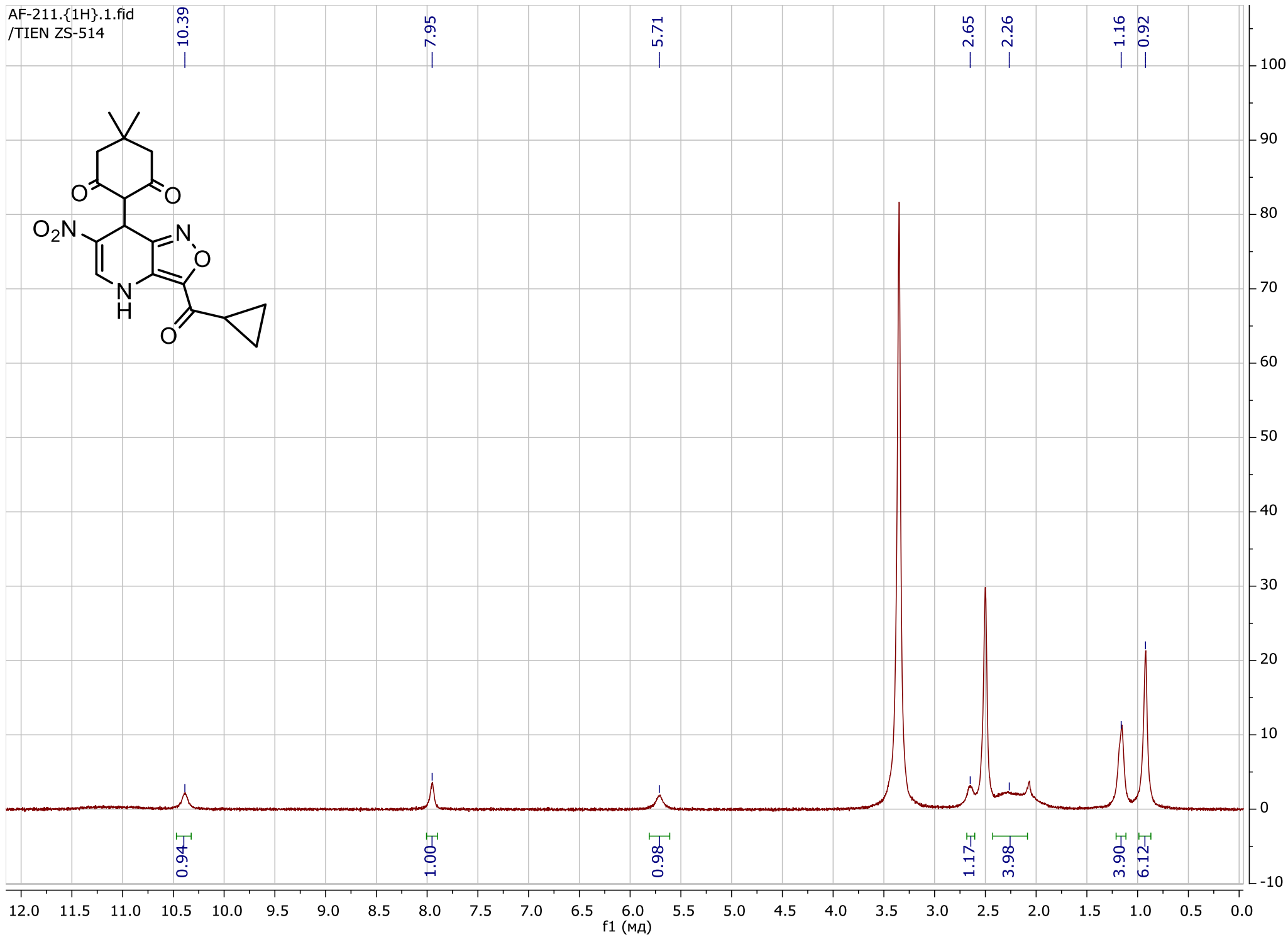
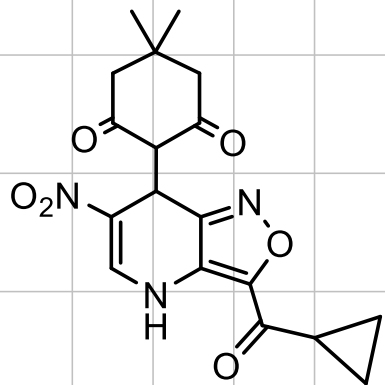
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

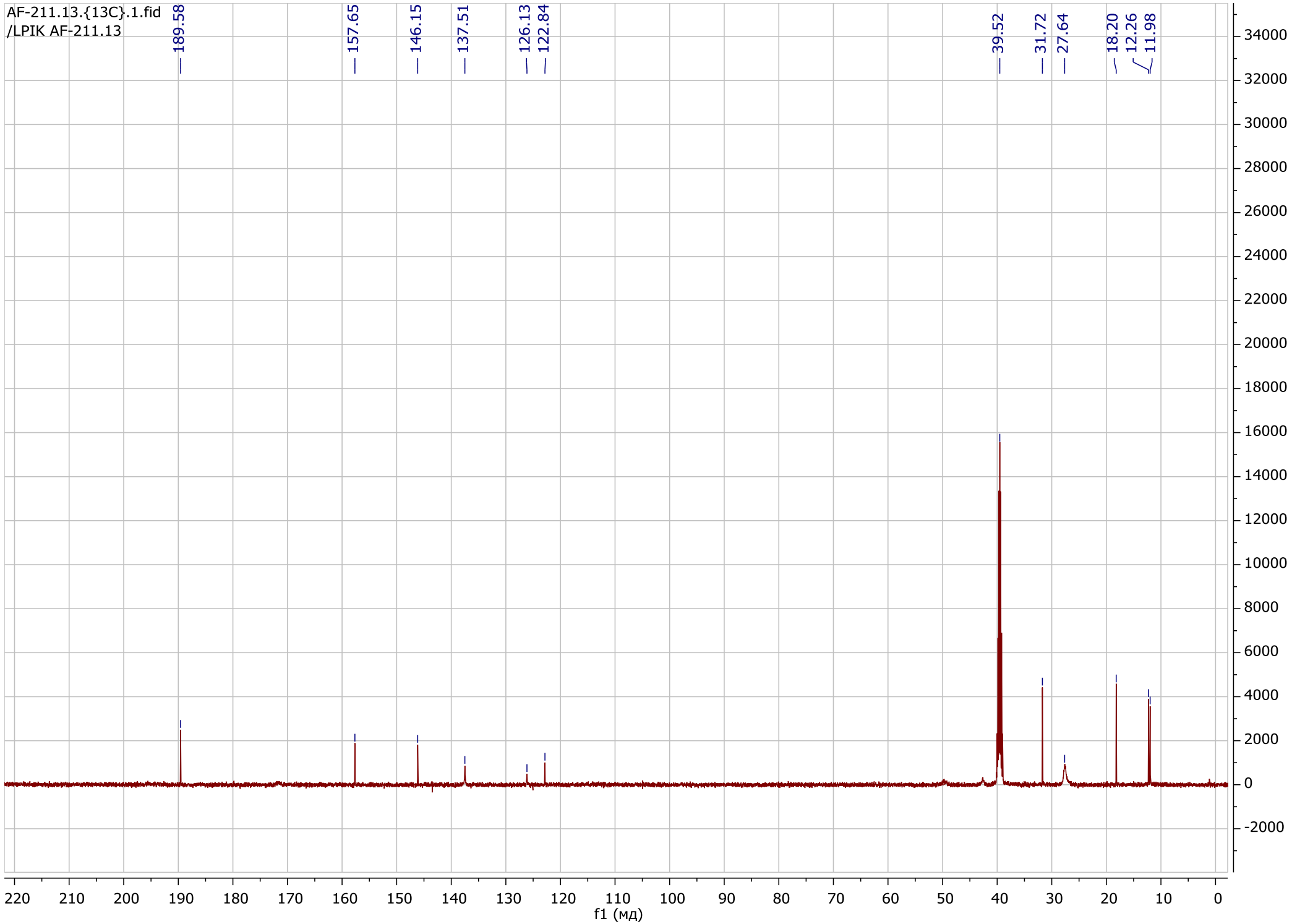
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-211.{1H}.1.fid
/TIEN ZS-514



AF-211.13.{13C}.1.fid
/LPIK AF-211.13



Display Report

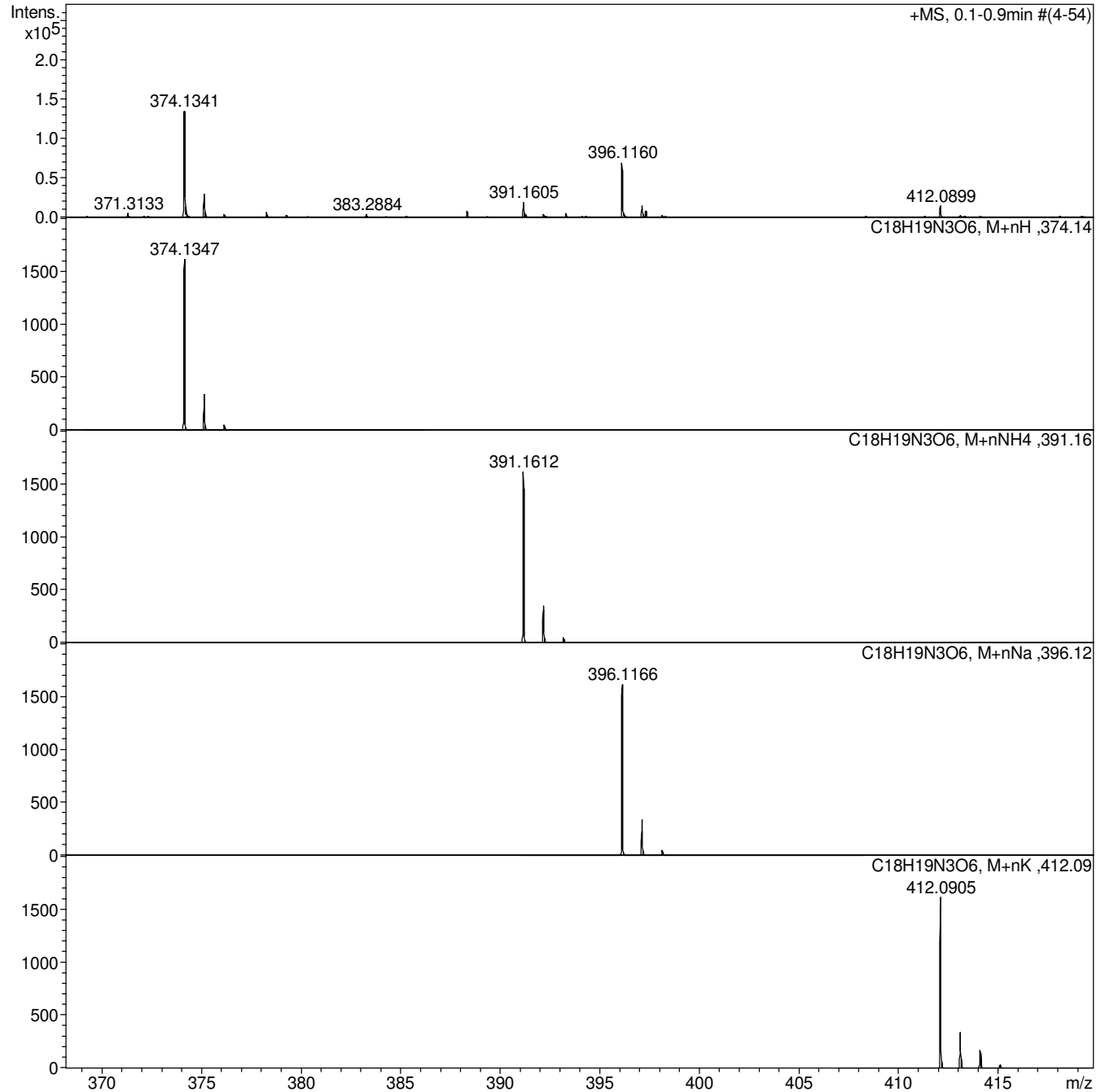
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2018\Bastrakov\1113015.d
Method tune_50-1600.m
Sample Name /LPIK AF-211
Comment C18H19N3O6 mH 374.1346 calibrant added

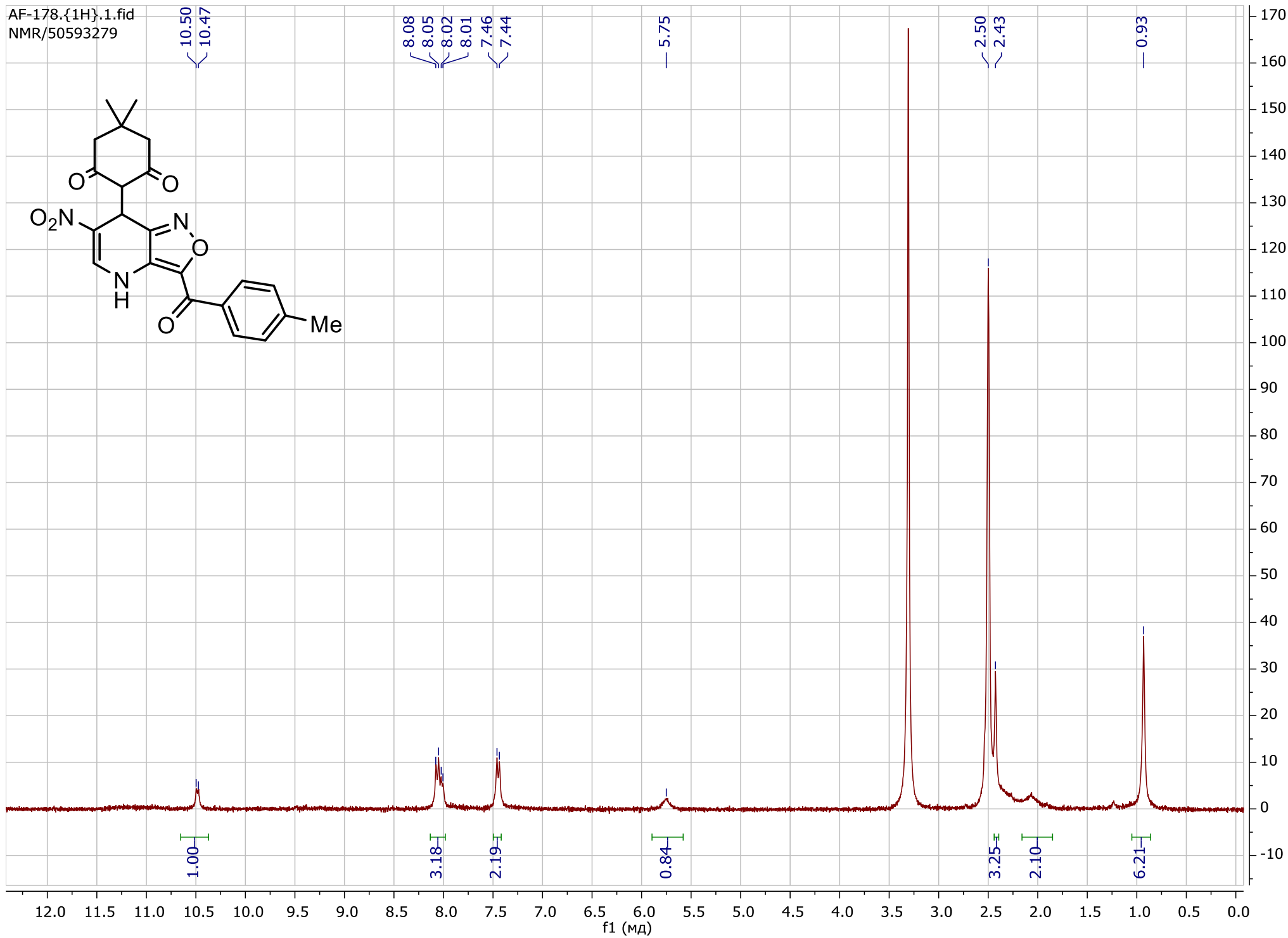
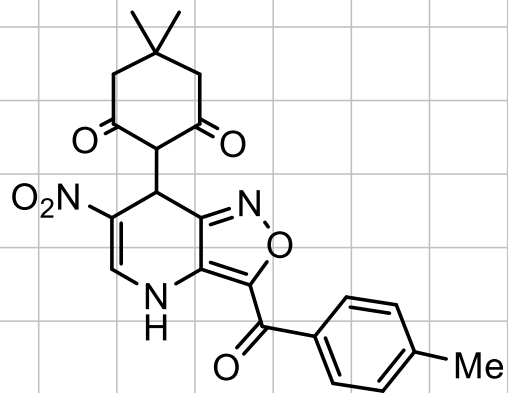
Acquisition Date 13.11.2018 11:09:49
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

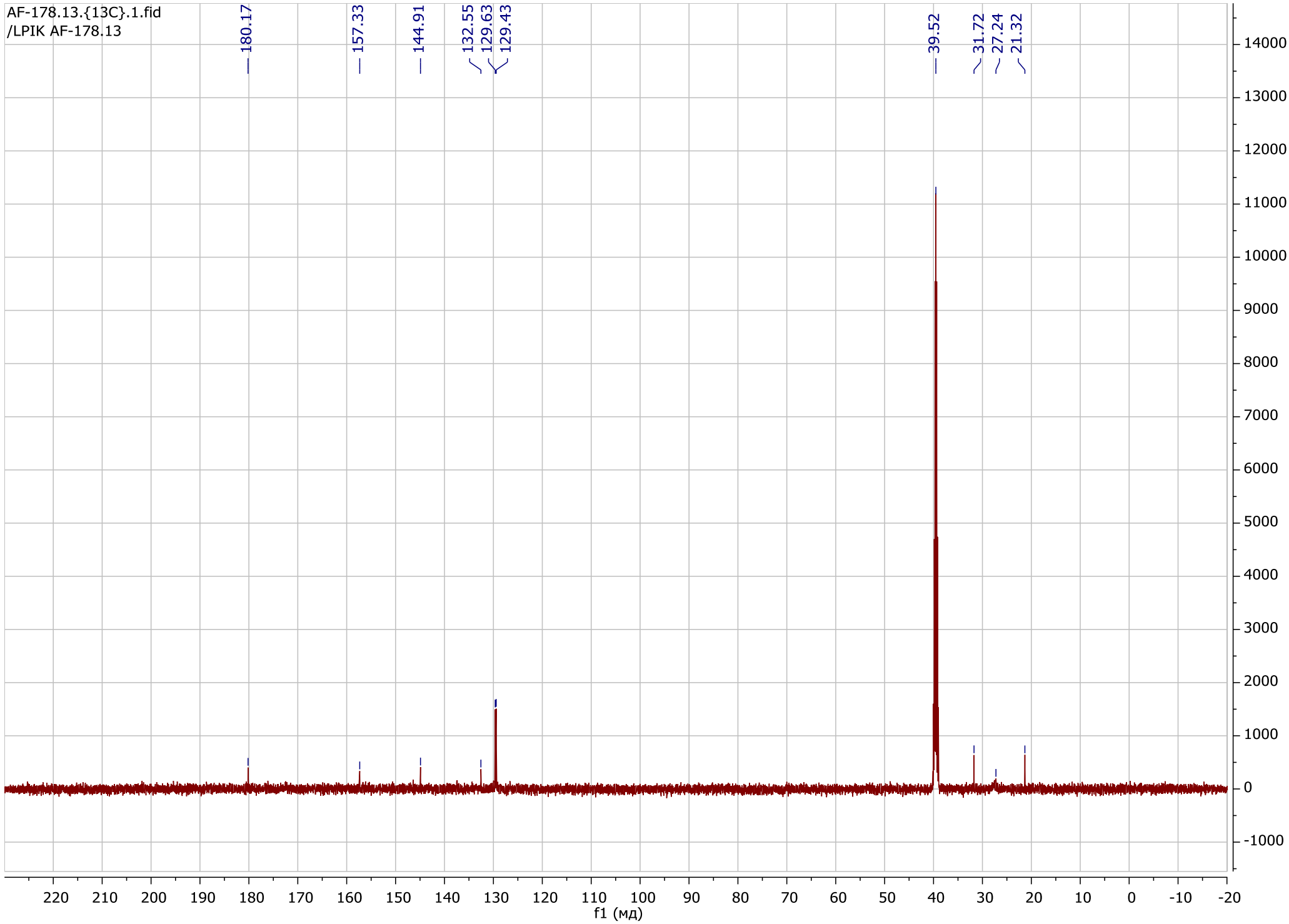
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-178.{1H}.1.fid
NMR/50593279



AF-178.13.{13C}.1.fid
/LPIK AF-178.13



Display Report

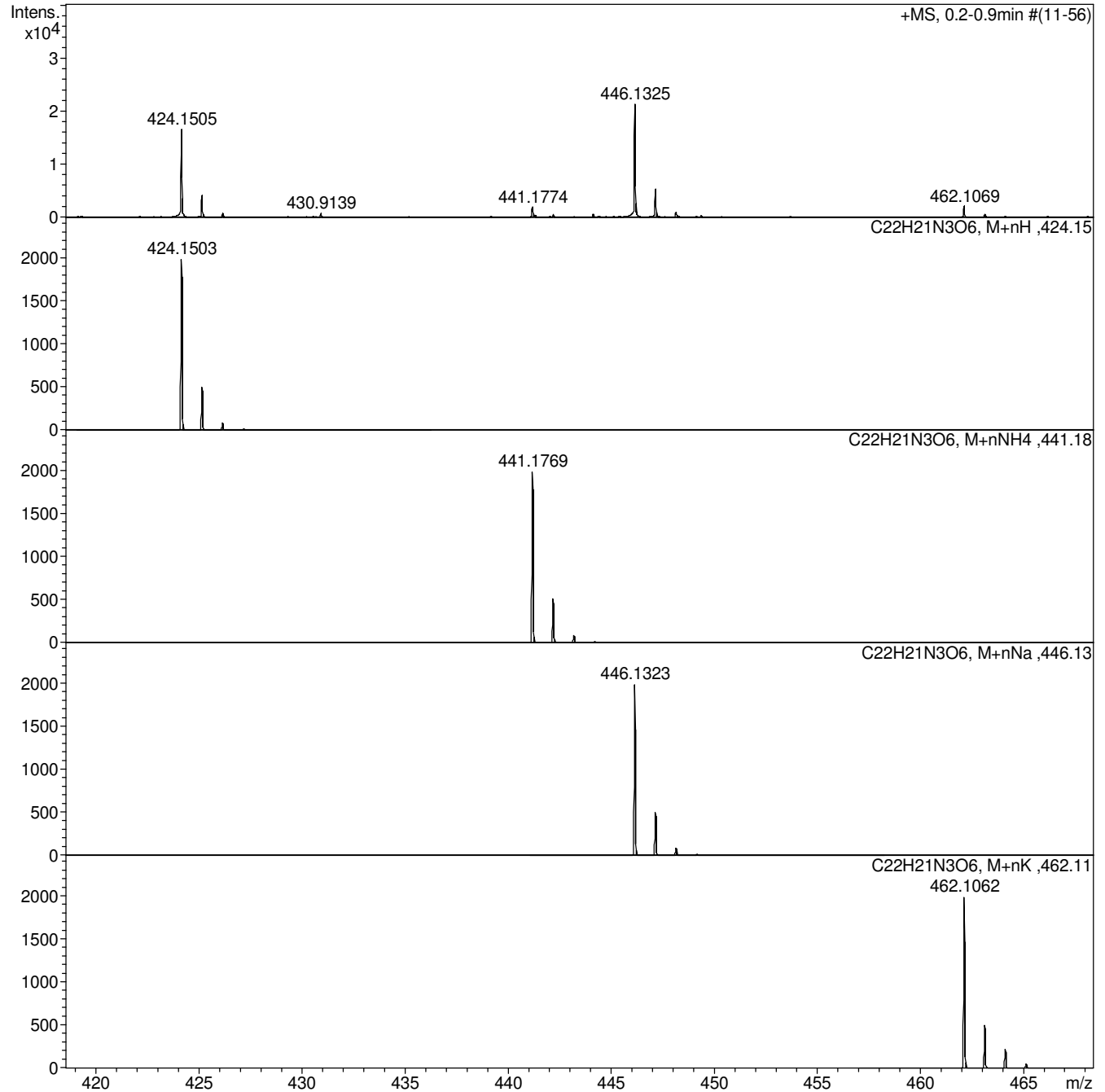
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2018\Bastrakov\0703003.d
Method tune_50-1600.m
Sample Name /LPIK AF-178
Comment C22H21N3O6 mH 424.1503 calibrant added

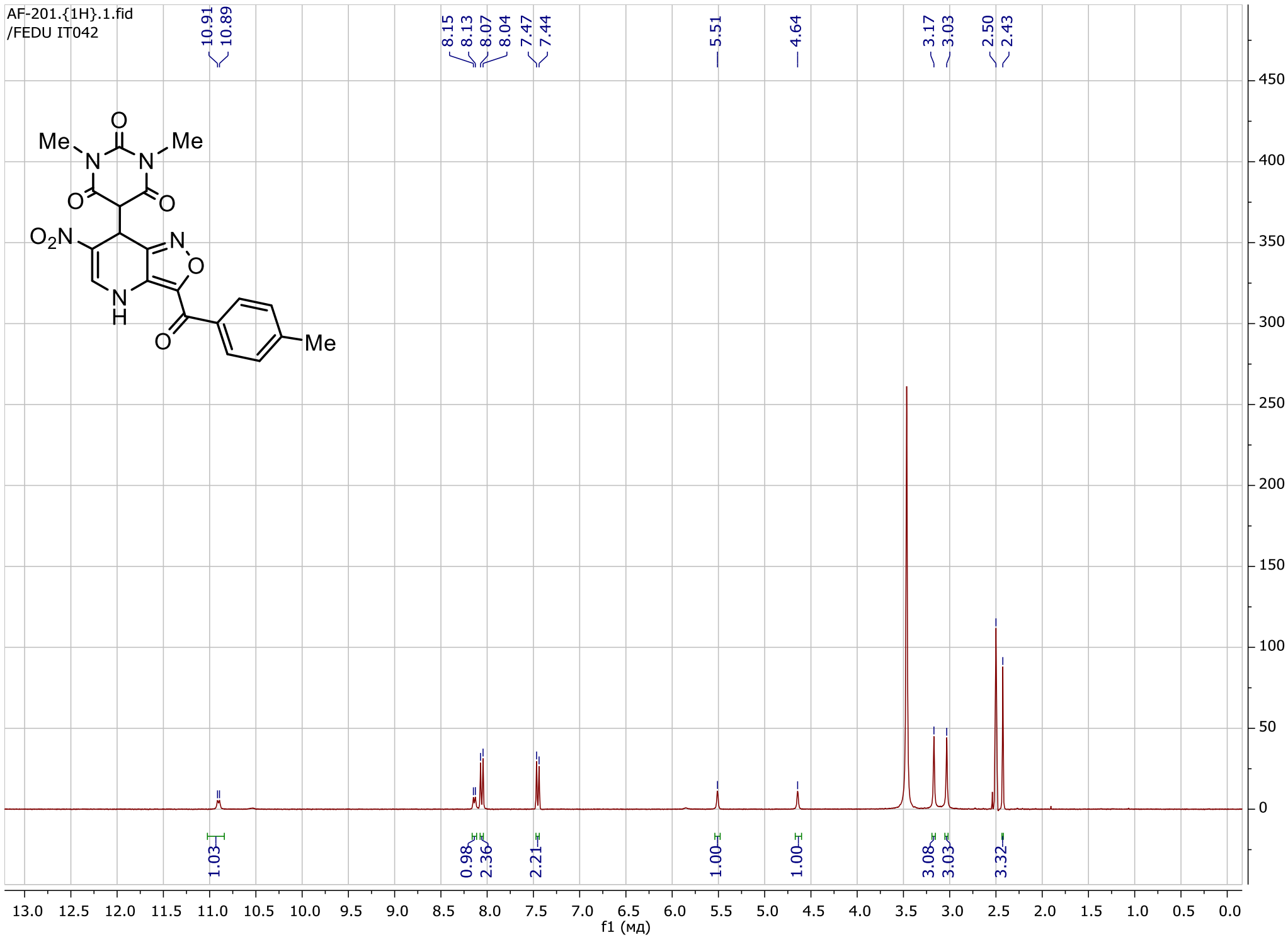
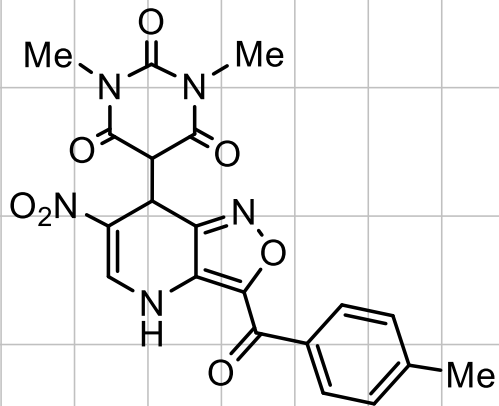
Acquisition Date 03.07.2018 10:43:38
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

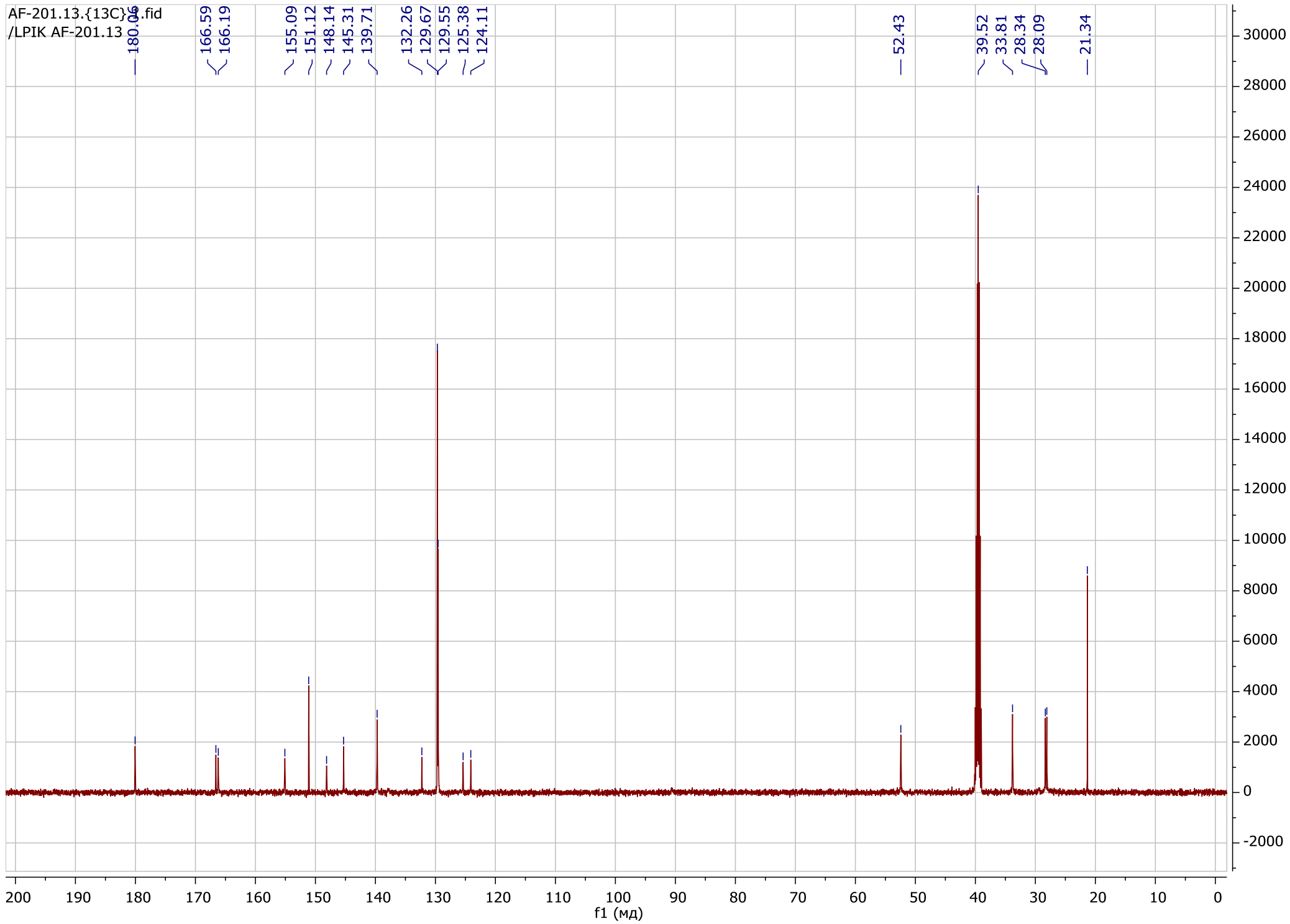
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-201.{1H}.1.fid
/FEDU IT042



AF-201.13.{13C}.fid
/LPIK AF-201.13



Display Report

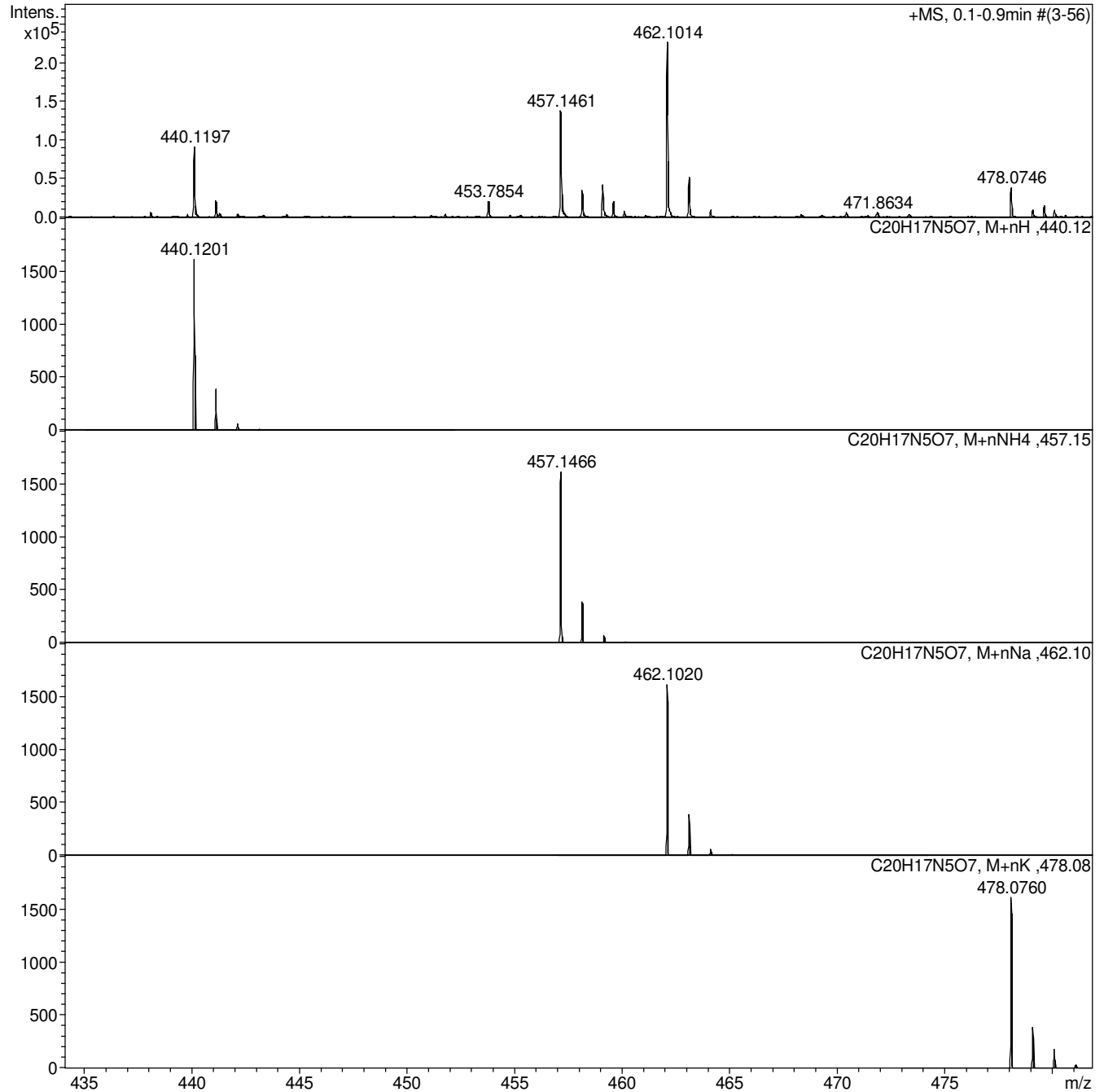
Analysis Info

Analysis Name D:\Data\Kolotyrykina\2018\Bastrakov\1113025.d
Method tune_50-1600.m
Sample Name /LPIK AF-201
Comment C20H17N5O7 mH 440.1201 calibrant added

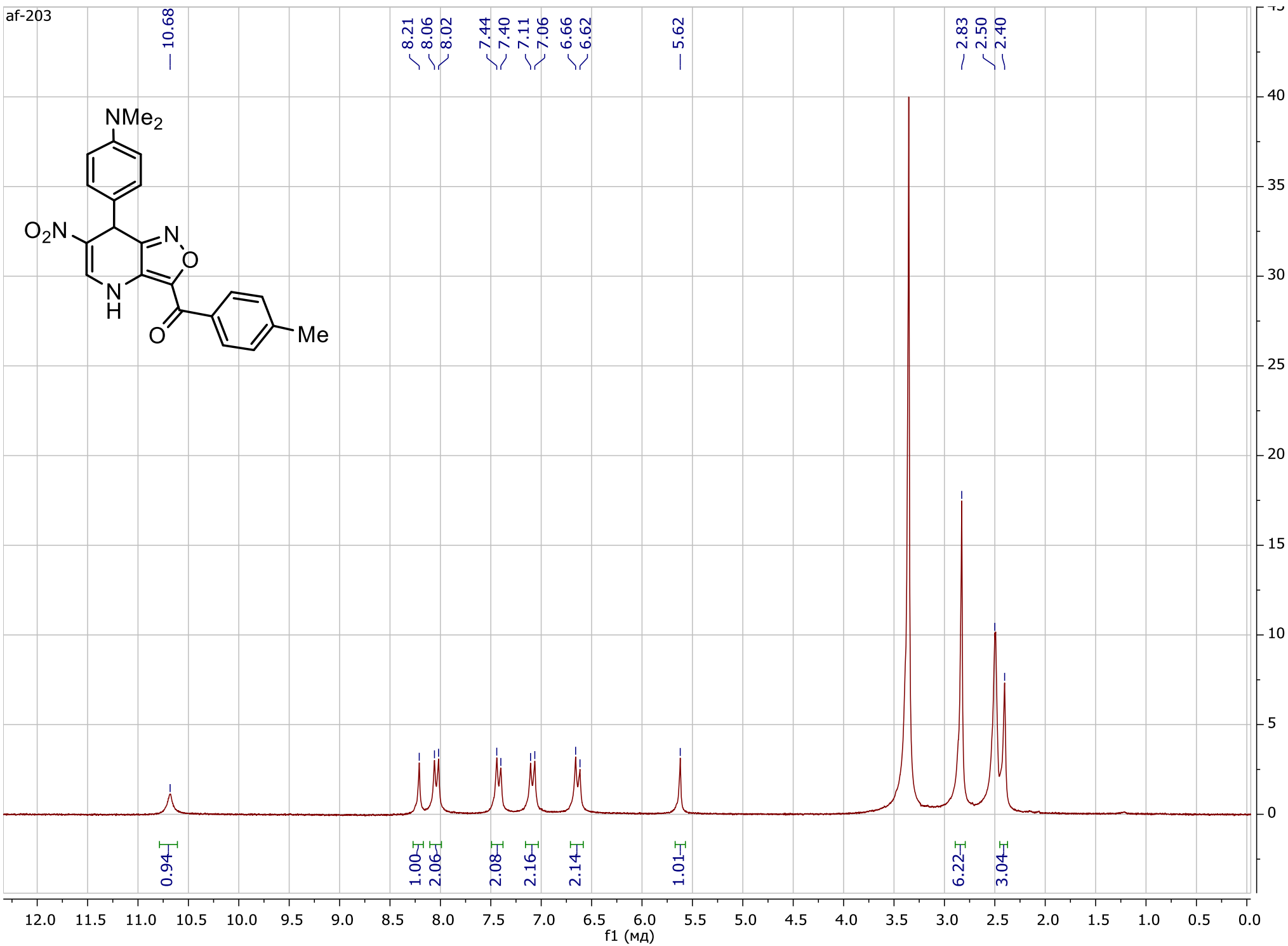
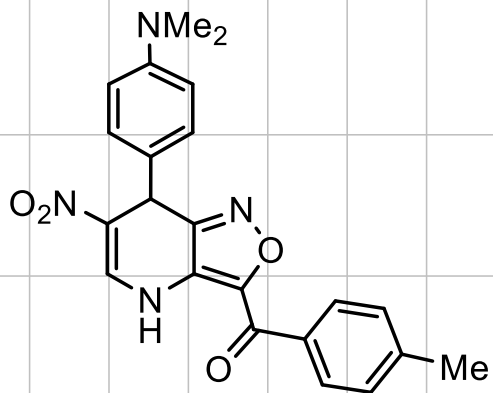
Acquisition Date 13.11.2018 12:52:08
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

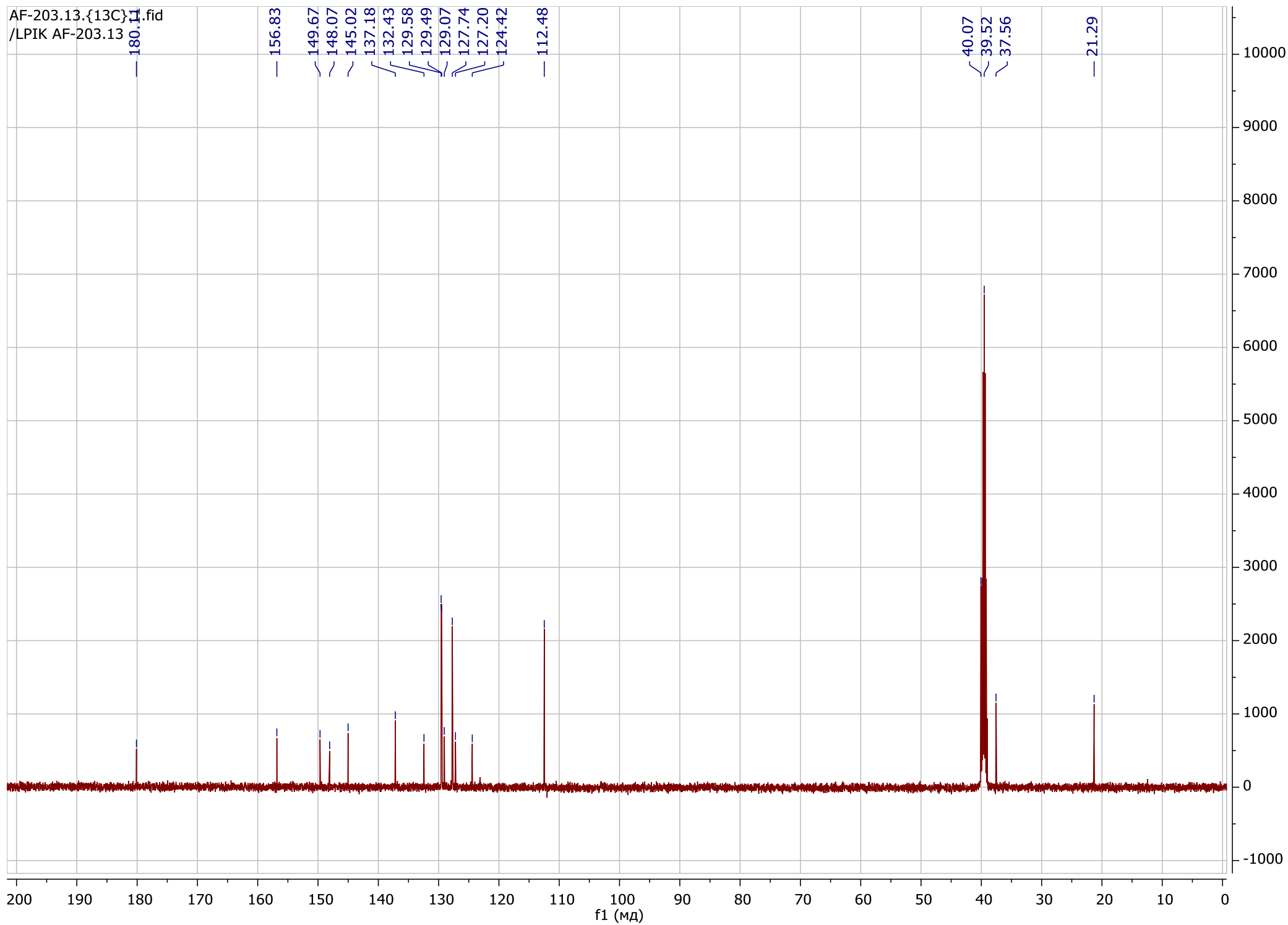
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



af-203



AF-203.13.{13C}.fid
/LPIK AF-203.13



Display Report

Analysis Info

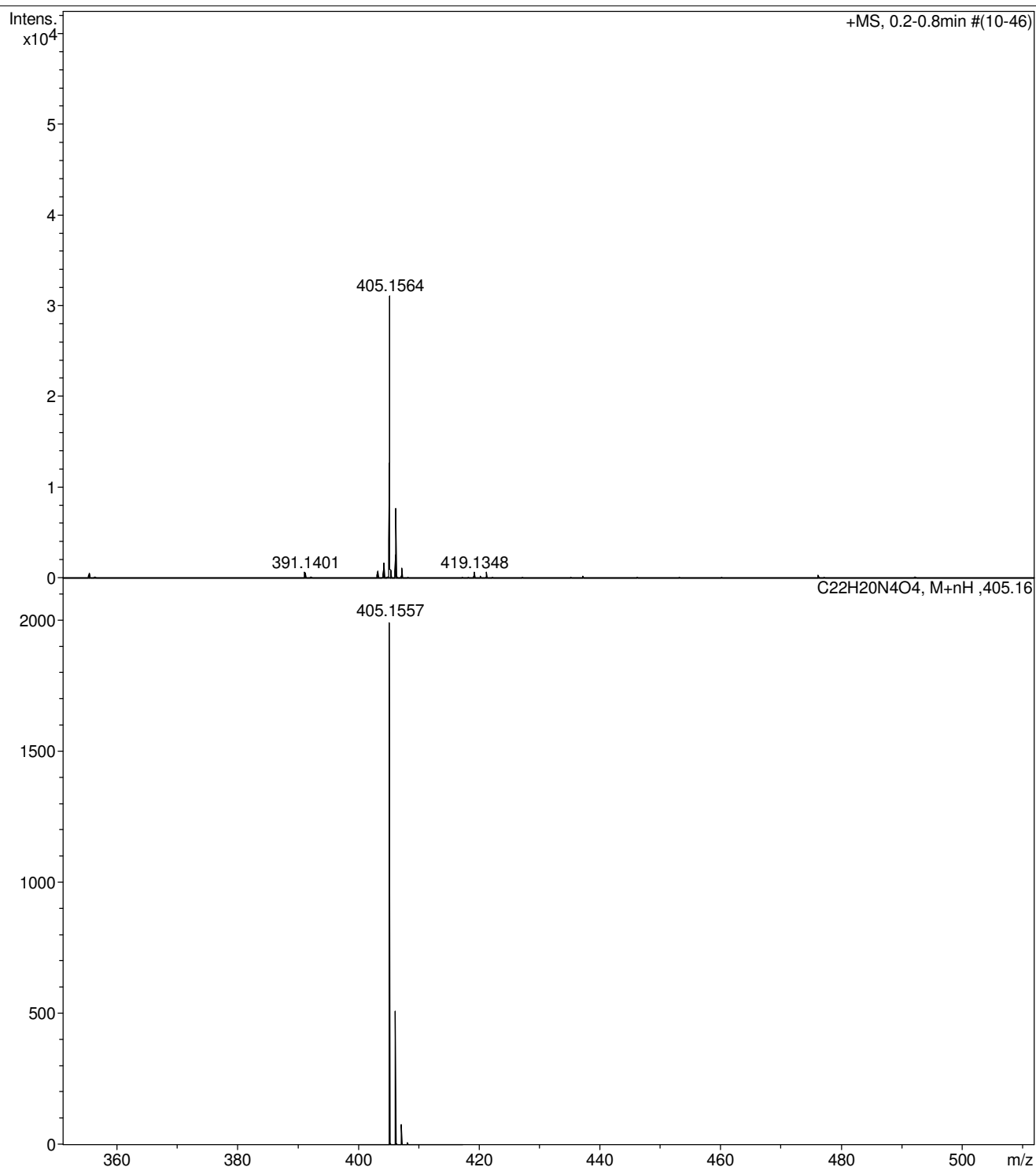
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0326047.d
Method tune_50-1600.m
Sample Name /LPIK AF-203
Comment C22H20N4O4 mH 405.1557 calibrant added CH3CN

Acquisition Date 26.03.2019 20:00:38

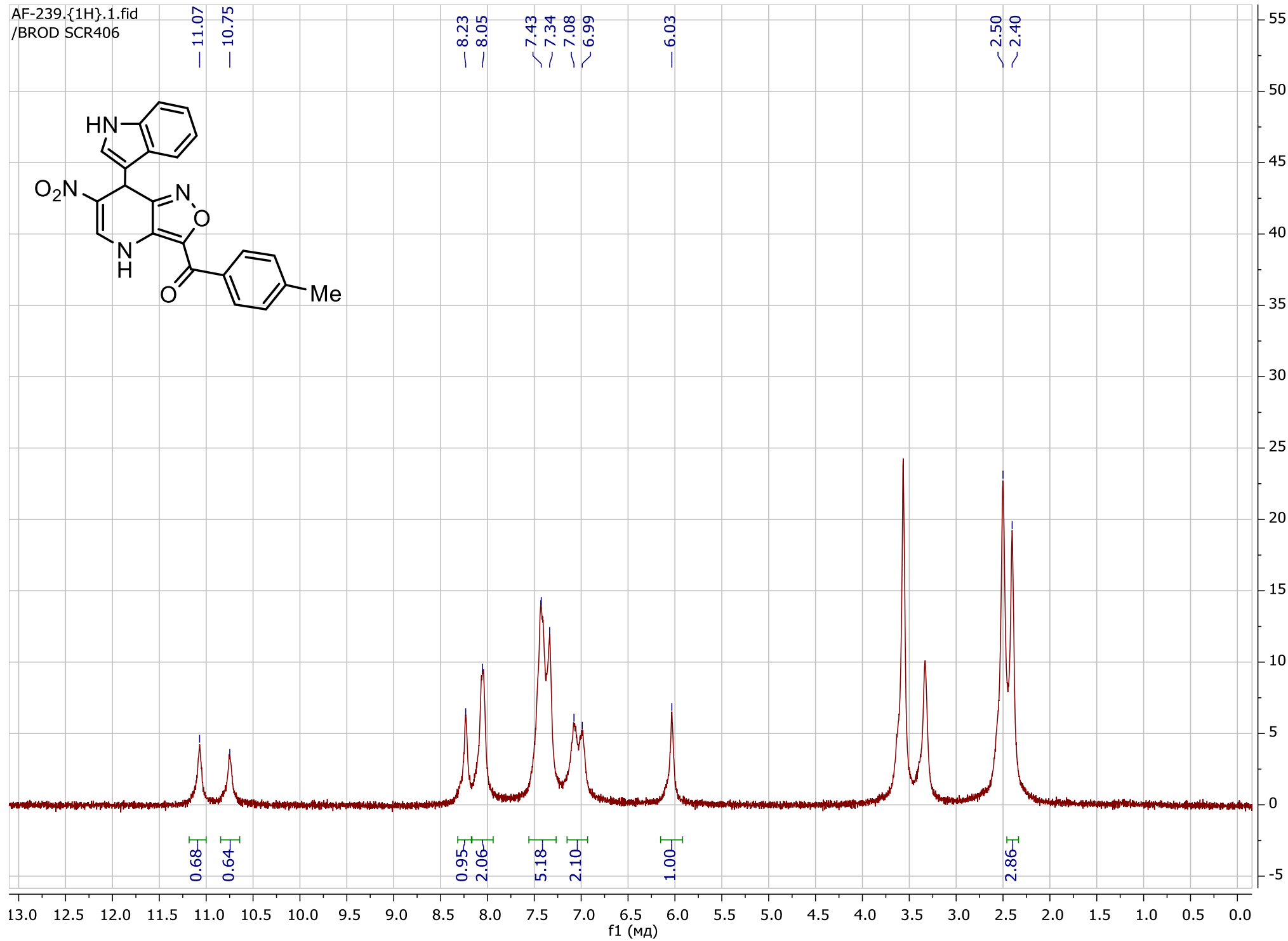
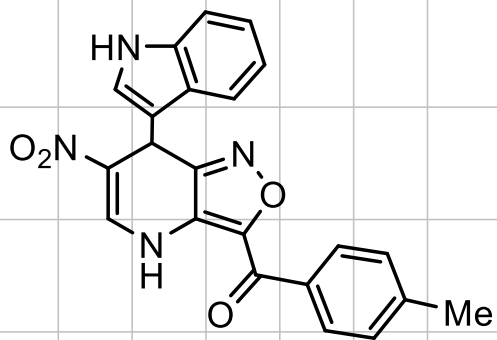
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

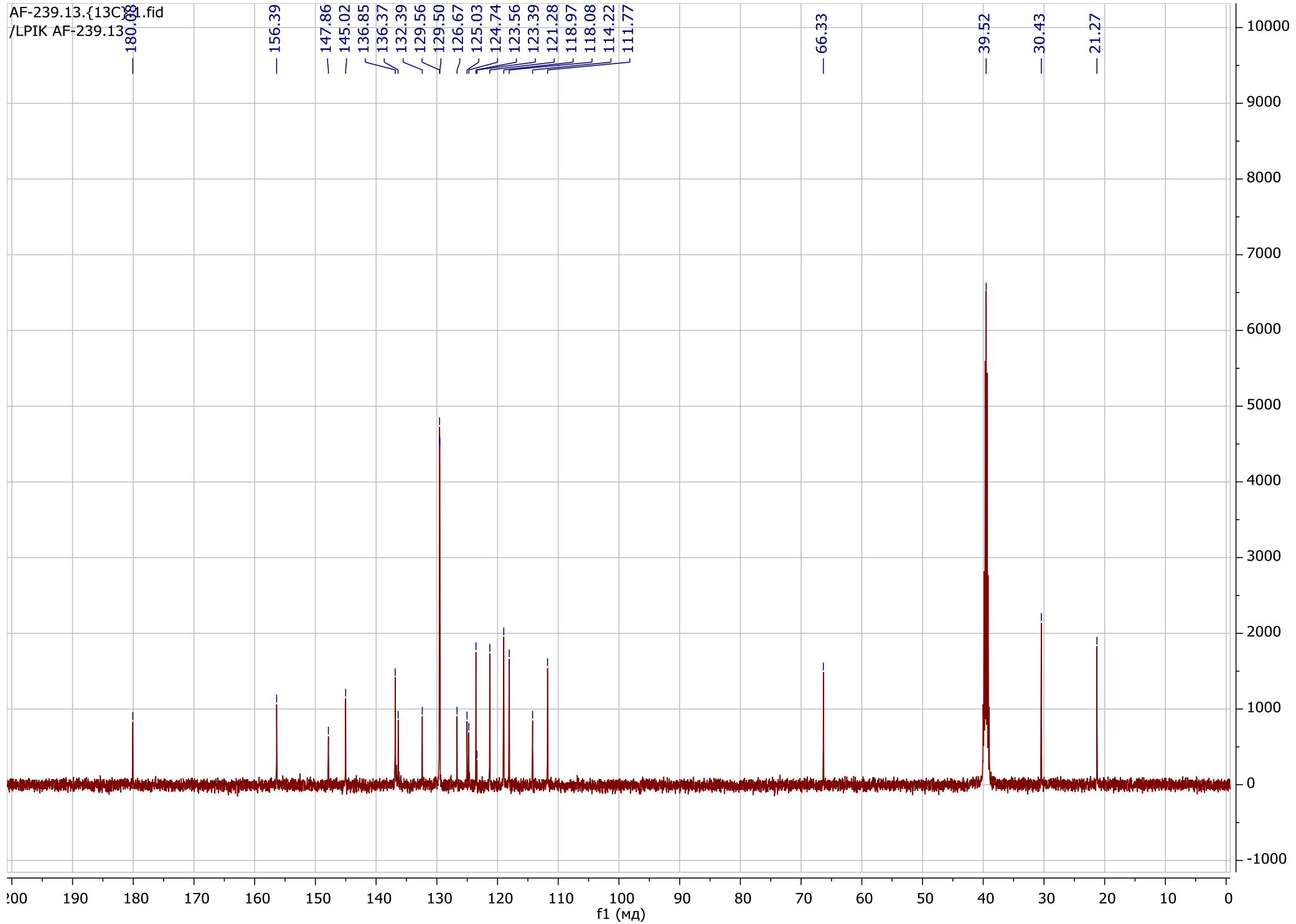
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-239_{1H}.1.fid
/BROD SCR406



AF-239.13.{13C}.fid
/LPIK AF-239.13



Display Report

Analysis Info

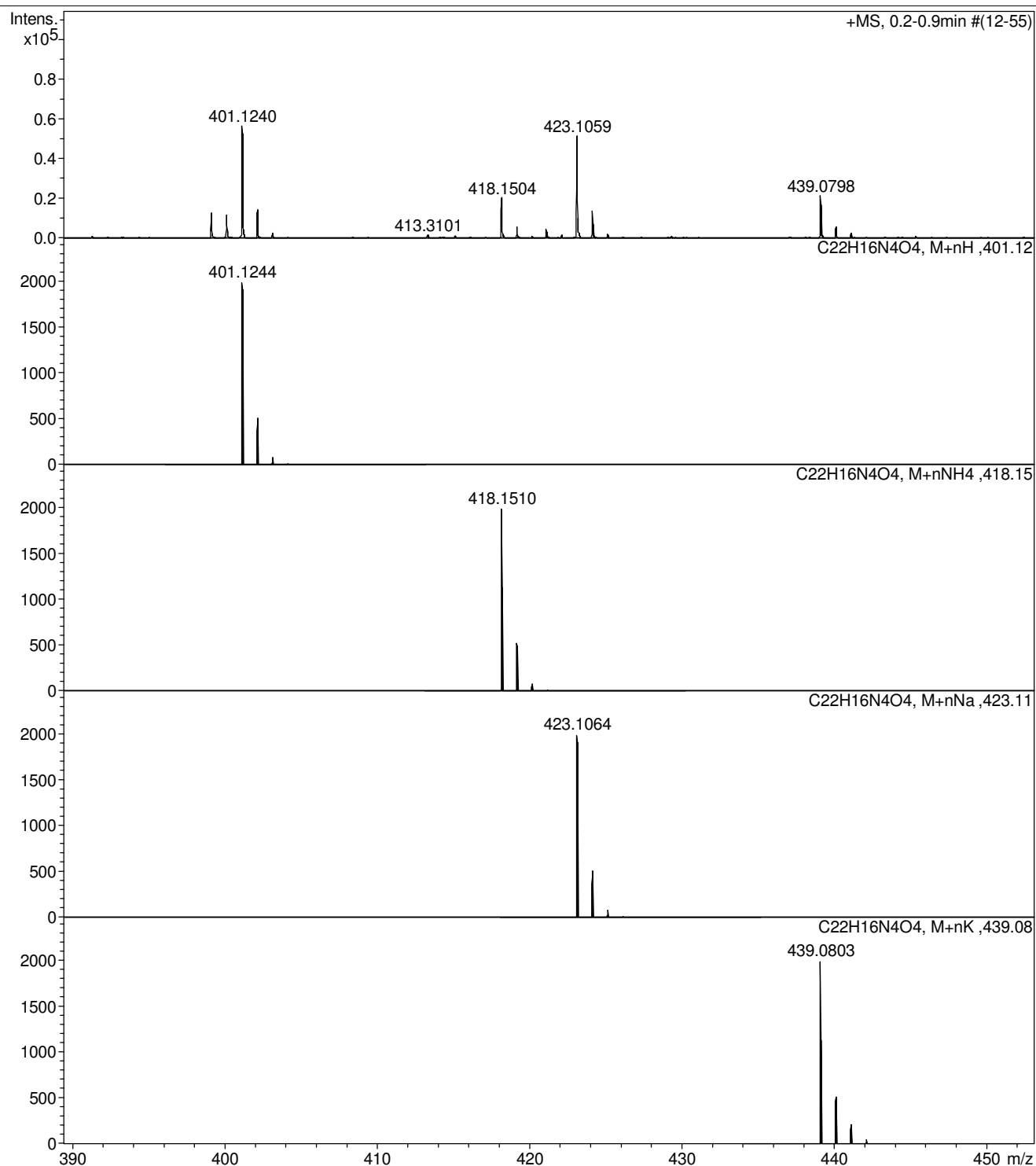
Analysis Name D:\Data\Kolotyrykina\2019\Bastrakov\0326049.d
Method tune_50-1600.m
Sample Name /LPIK AF-239
Comment C22H16N4O4 mH 401.1243 calibrant added CH3CN

Acquisition Date 26.03.2019 20:09:53

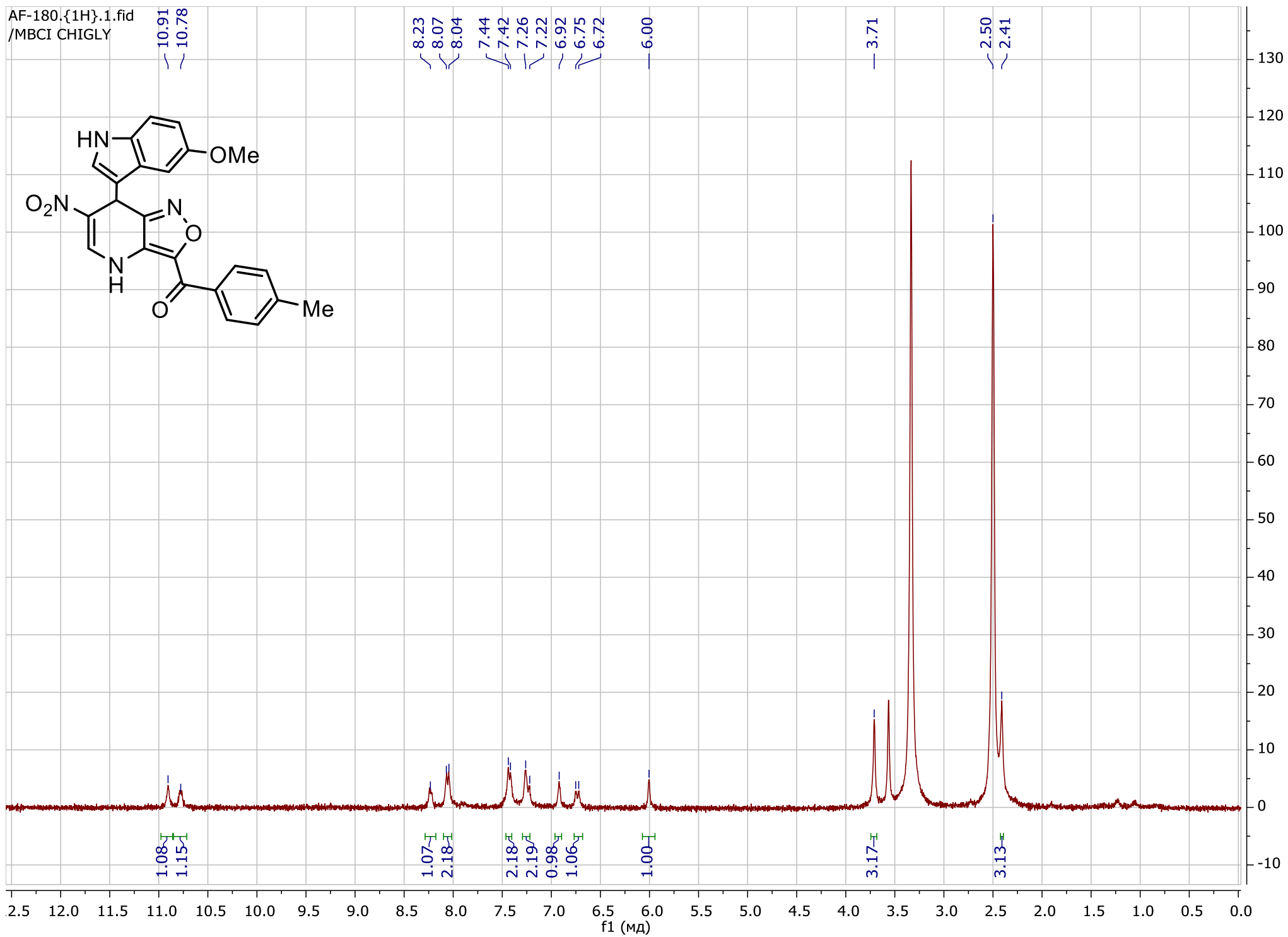
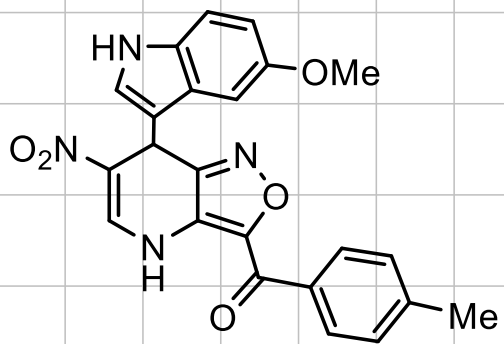
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

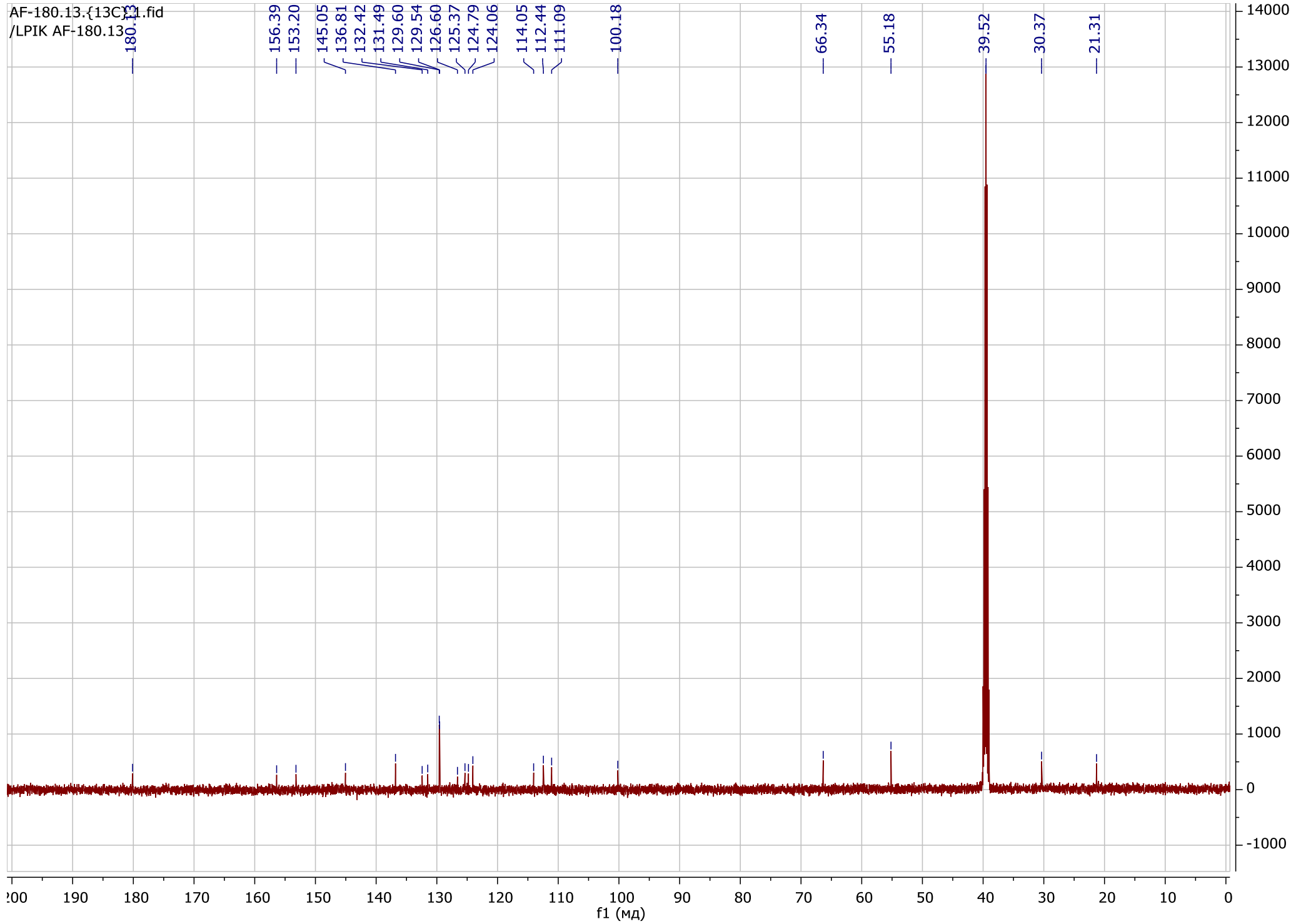
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-180_{1H}.1.fid
/MBCI CHIGLY



AF-180.13-¹³C.fid
/LPIK AF-180.13



Display Report

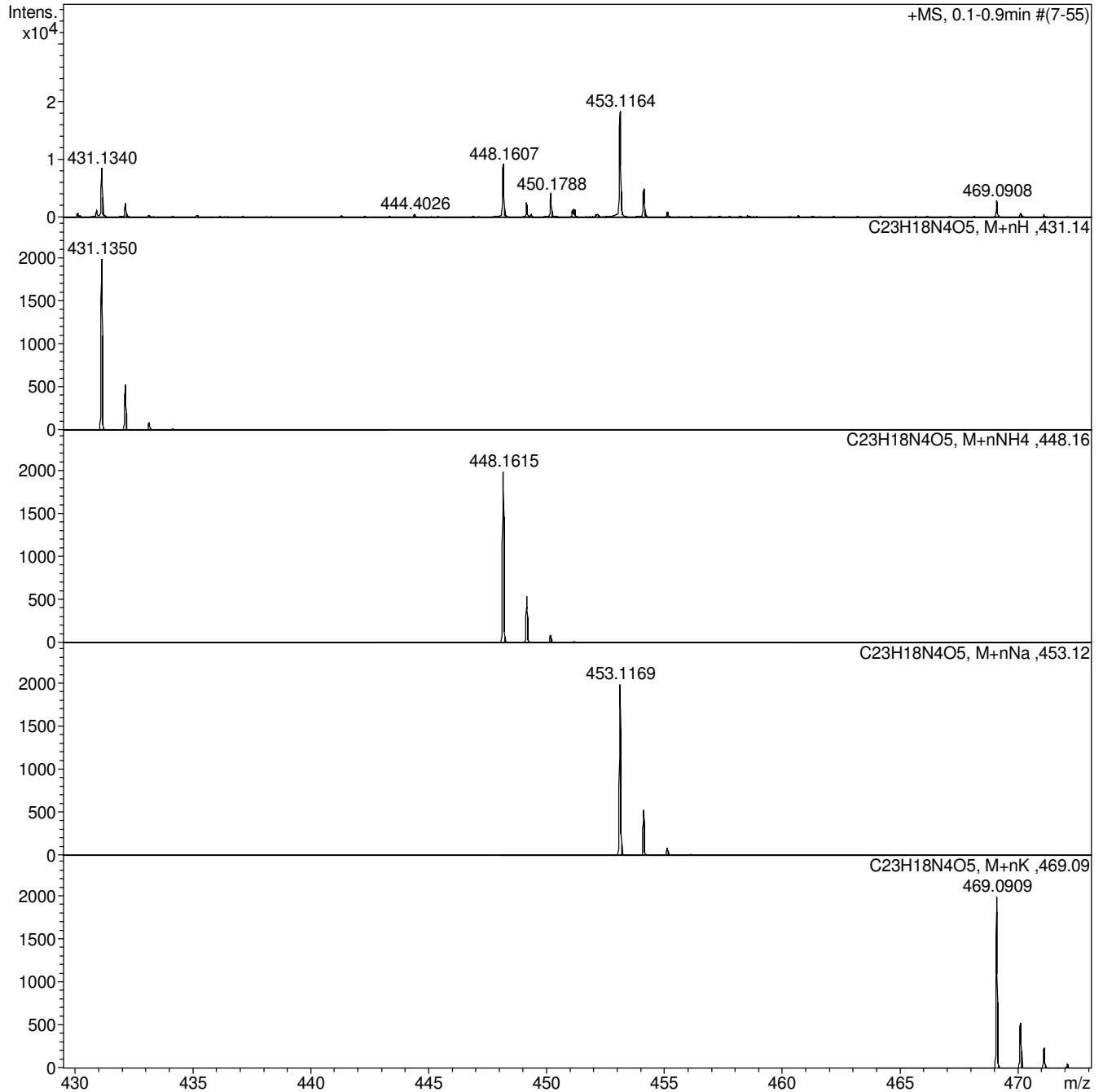
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2018\Bastrakov\0703005.d
Method tune_50-1600.m
Sample Name /LPIK AF-180
Comment C23H18N4O5 mH 431.1349 calibrant added

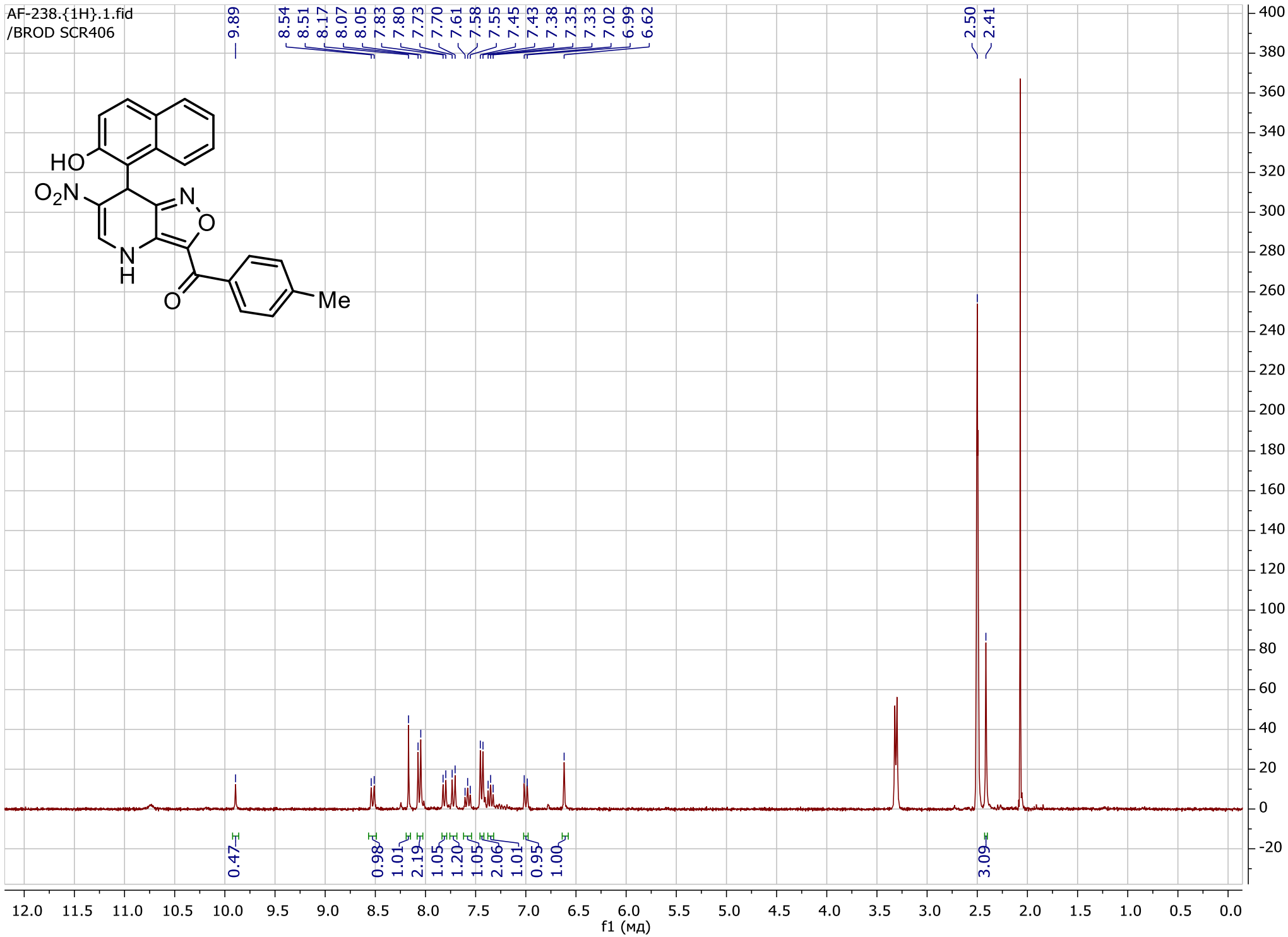
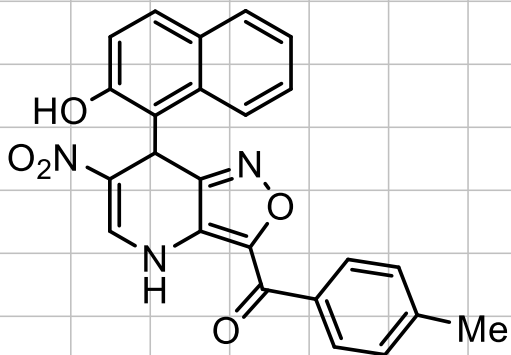
Acquisition Date 03.07.2018 10:59:14
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

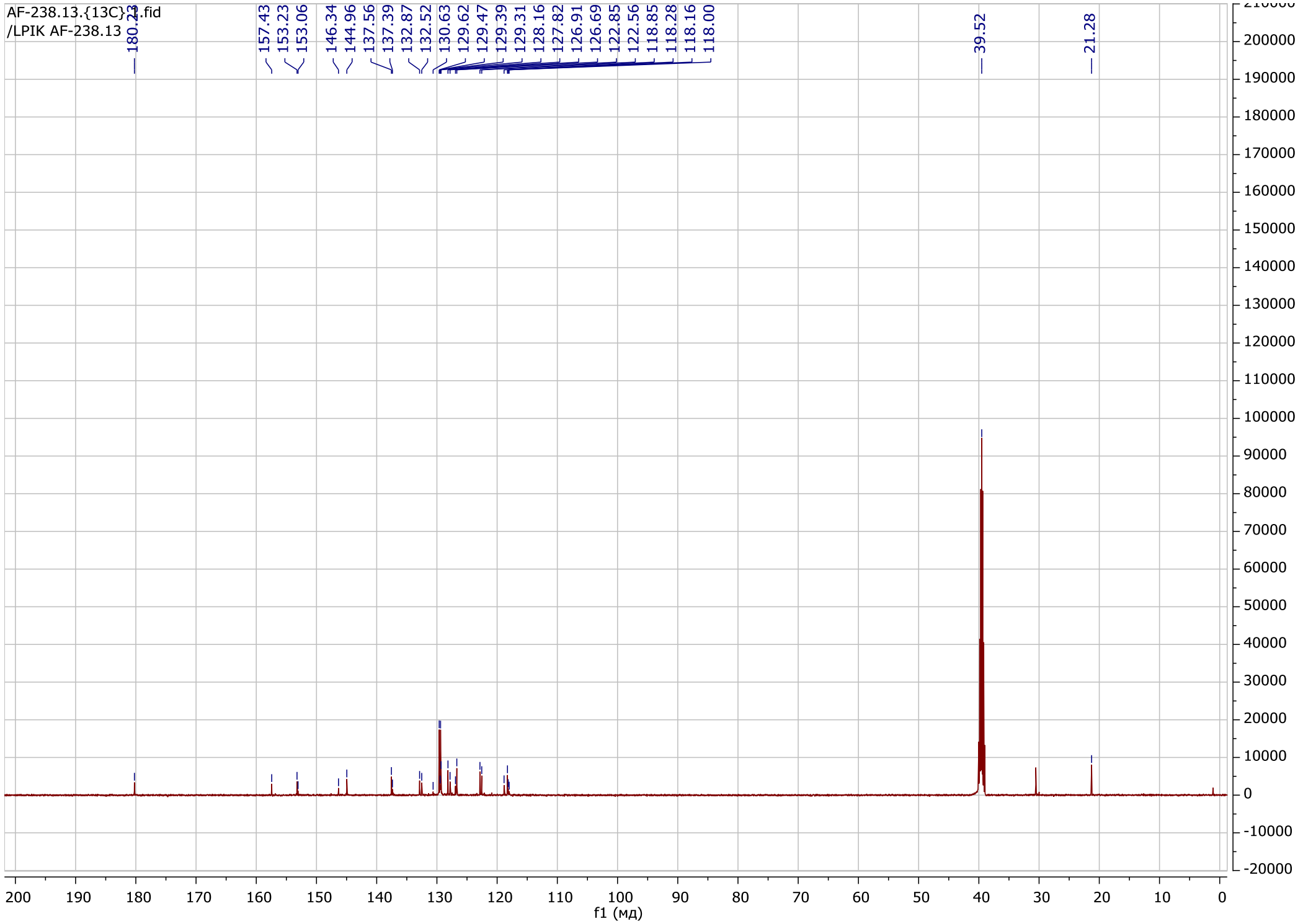
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-238-{1H}.1.fid
/BROD SCR406



AF-238.13.{13C}.fid
/LPIK AF-238.13



Display Report

Analysis Info

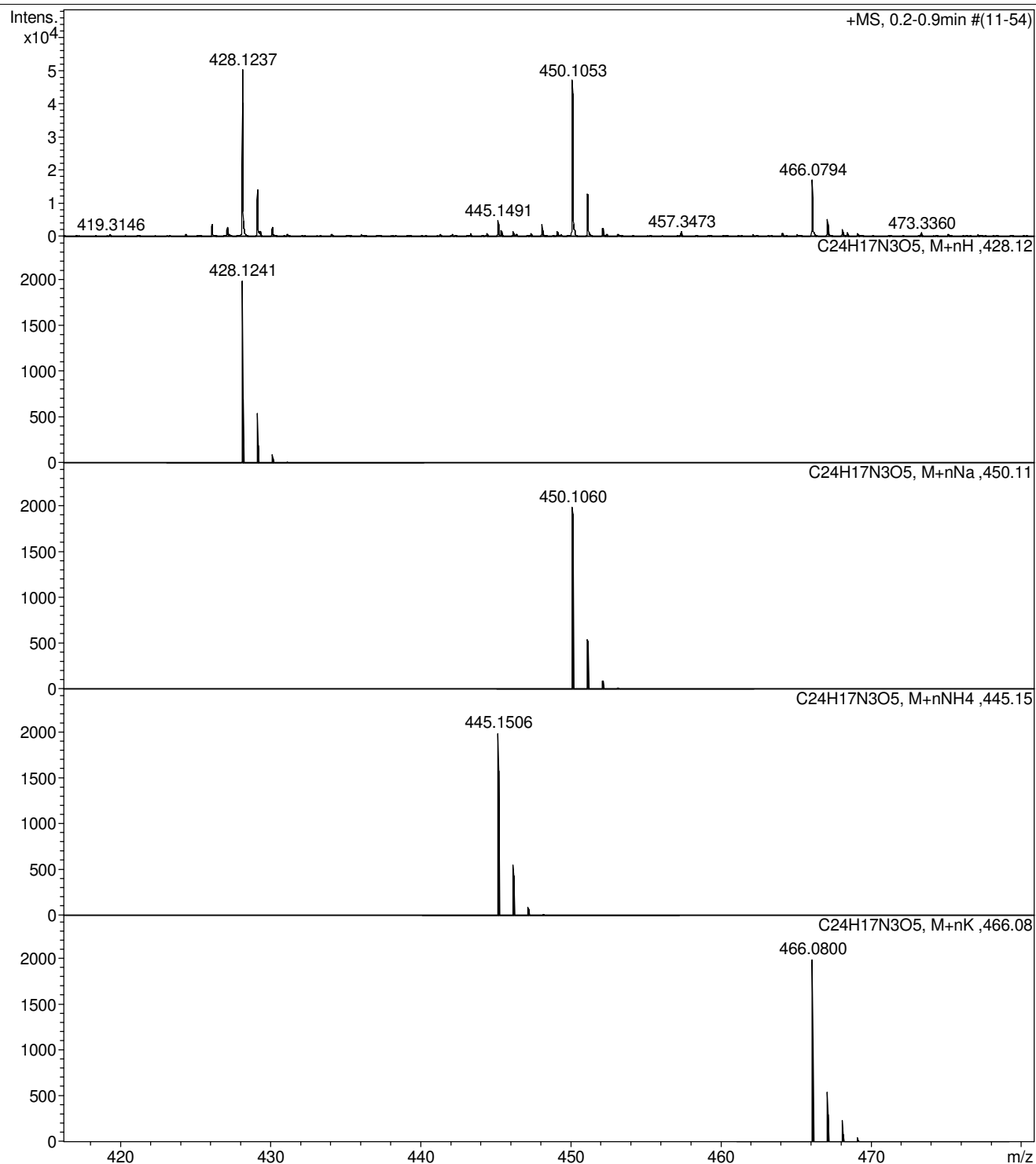
Analysis Name D:\Data\Kolotyrykina\2019\Bastrakov\0326048.d
Method tune_50-1600.m
Sample Name /LPIK AF-238
Comment C24H17N3O5 mH 428.1240 calibrant added CH3CN

Acquisition Date 26.03.2019 20:04:56

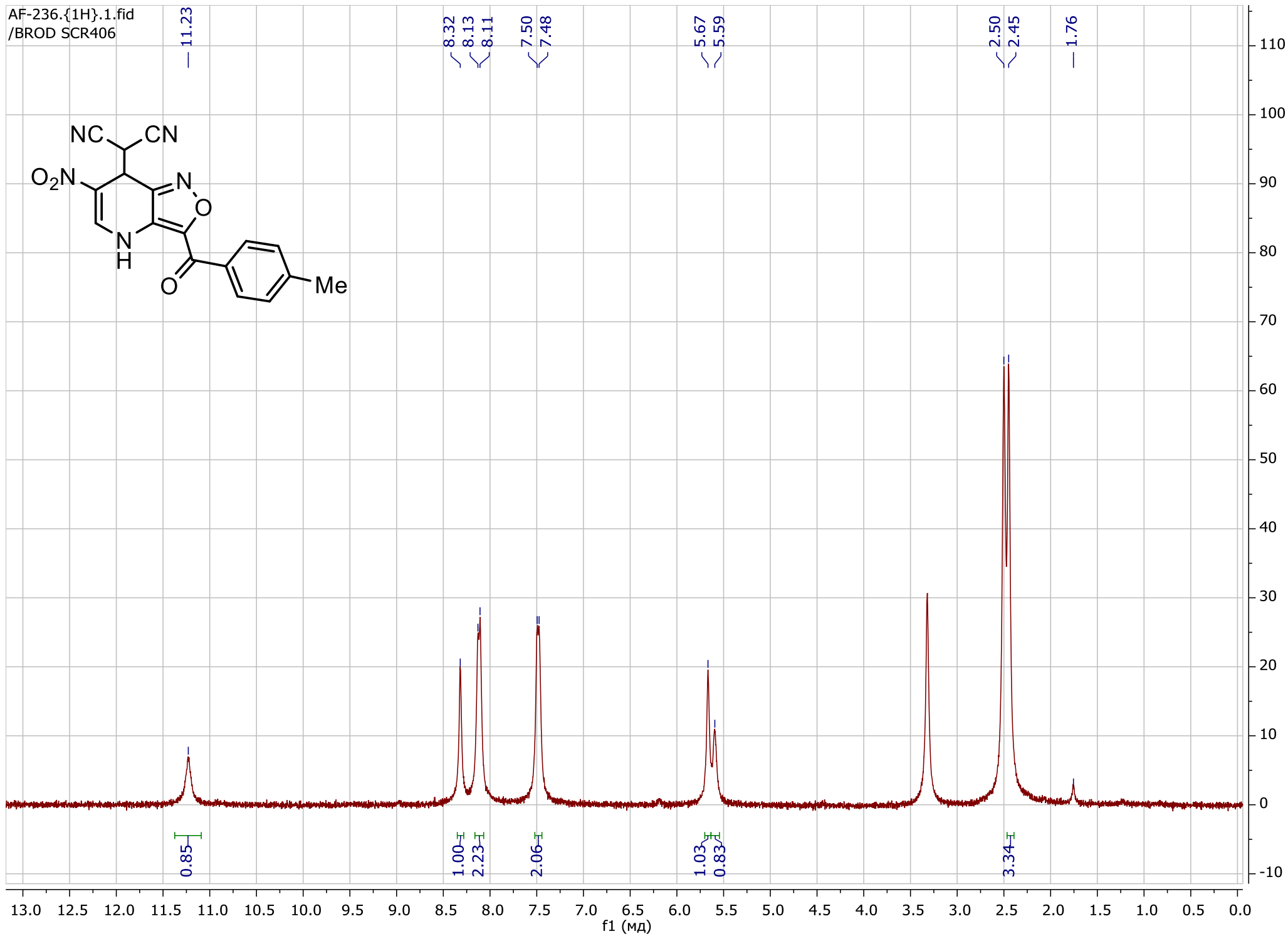
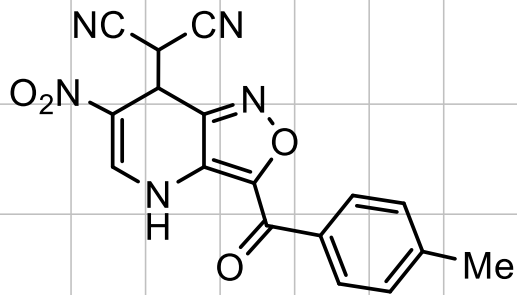
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

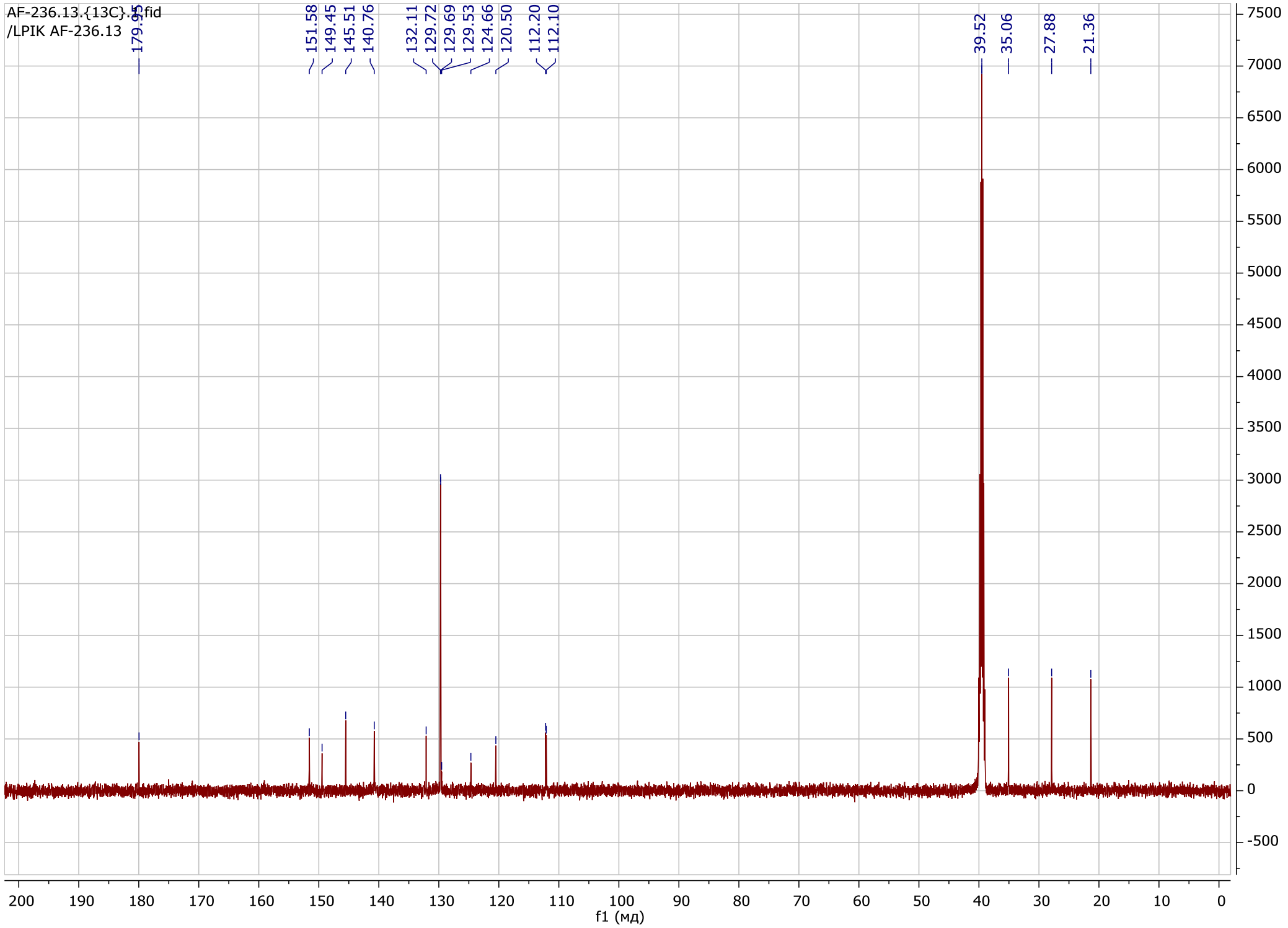
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-236.{1H}.1.fid
/BROD SCR406



AF-236.13.{13C}.fid
/LPIK AF-236.13



Display Report

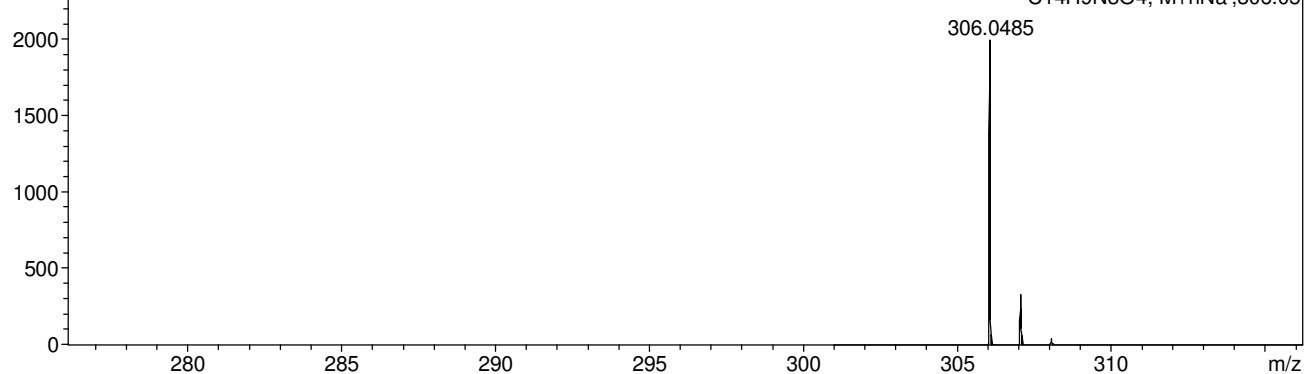
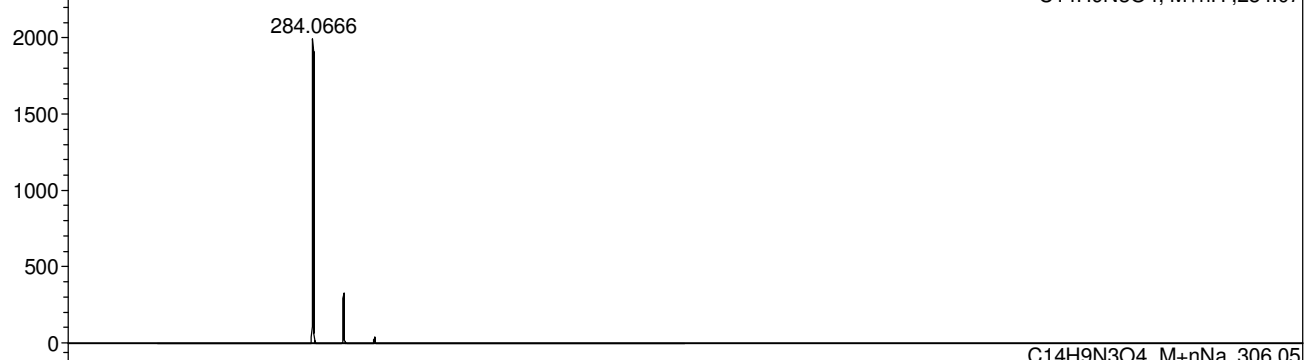
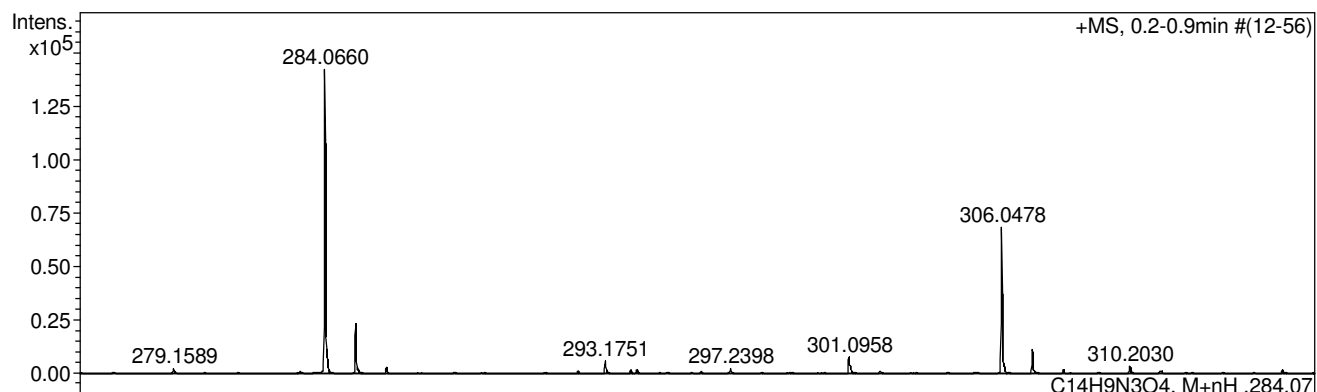
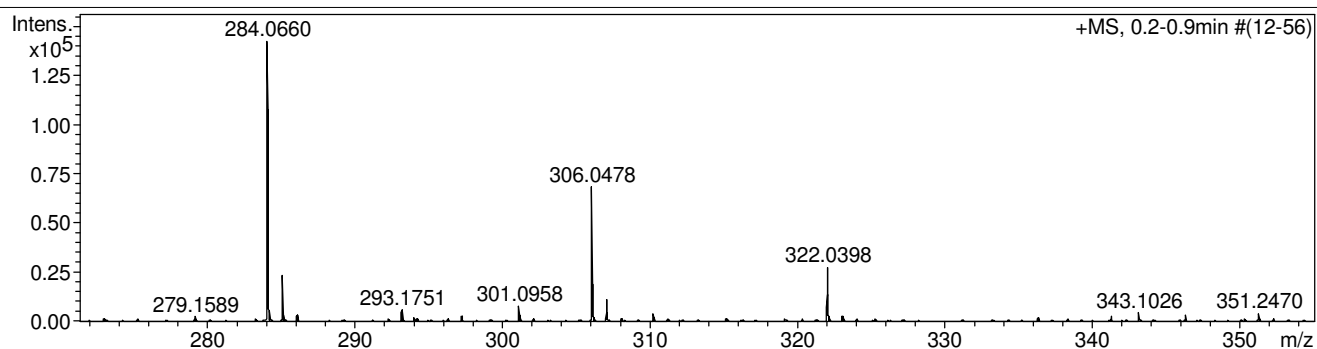
Analysis Info

Analysis Name D:\Data\Kolotyrykina\2019\Bastrakov\0326045.d
Method tune_50-1600.m
Sample Name /LPIK AF-236
Comment C17H11N5O4 mH 350.0883 calibrant added CH3CN

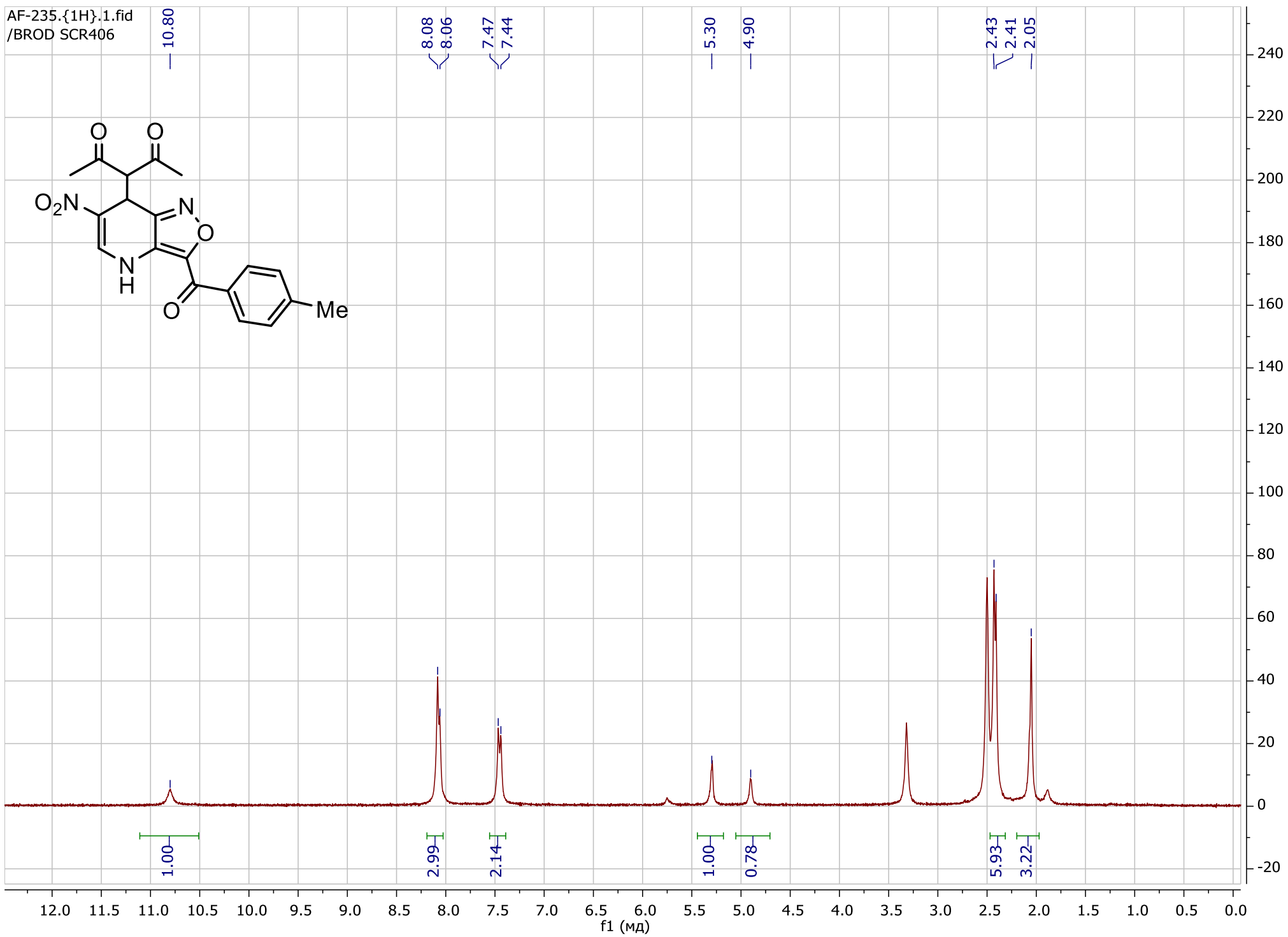
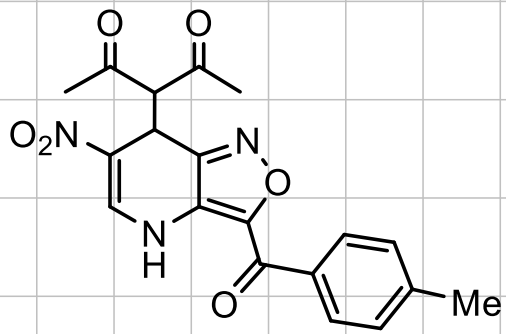
Acquisition Date 26.03.2019 19:47:49
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

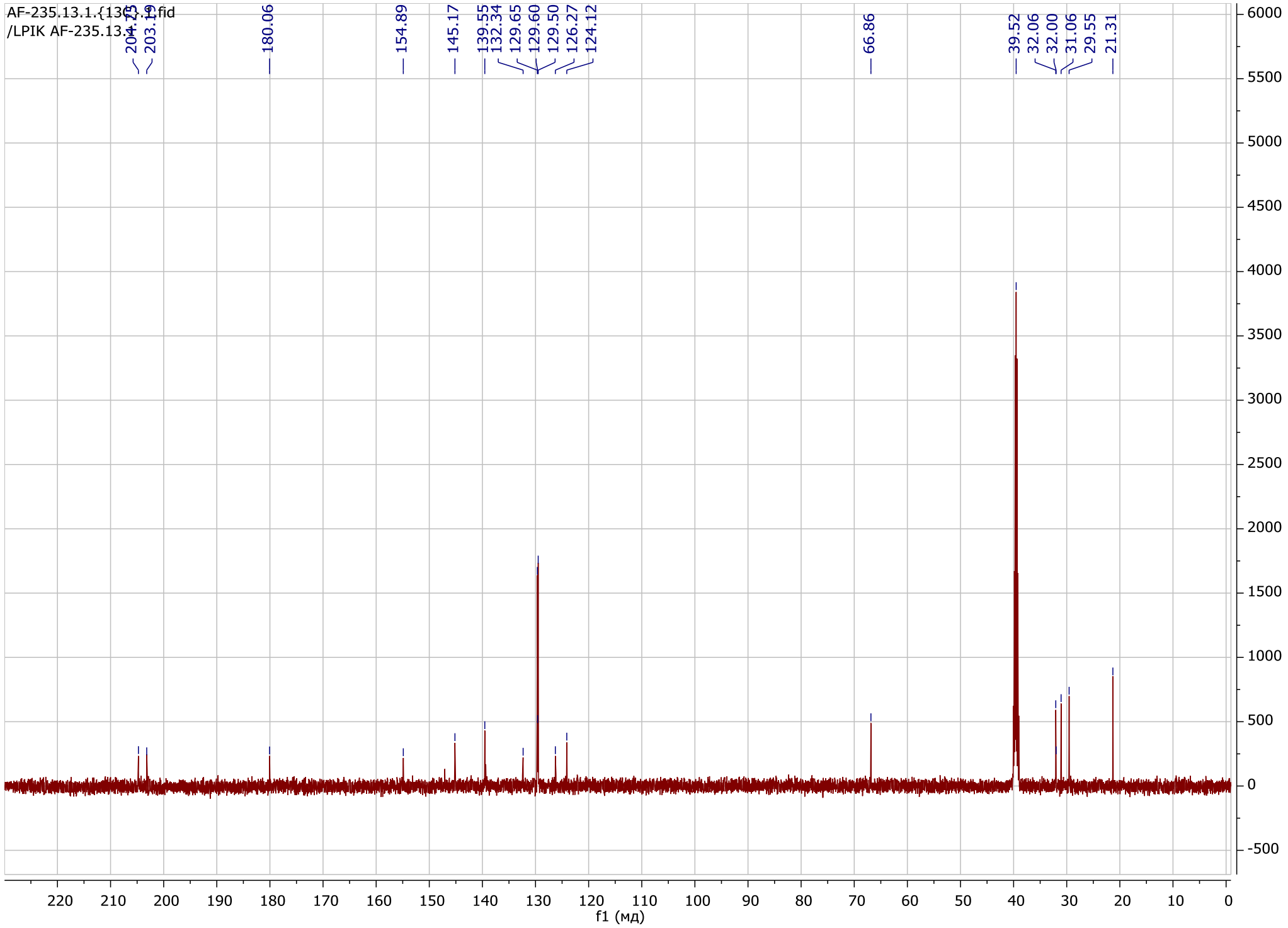
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-235.{1H}.1.fid
/BROD SCR406



AF-235.13.1.{13C}.fid
/LPIK AF-235.13.



Display Report

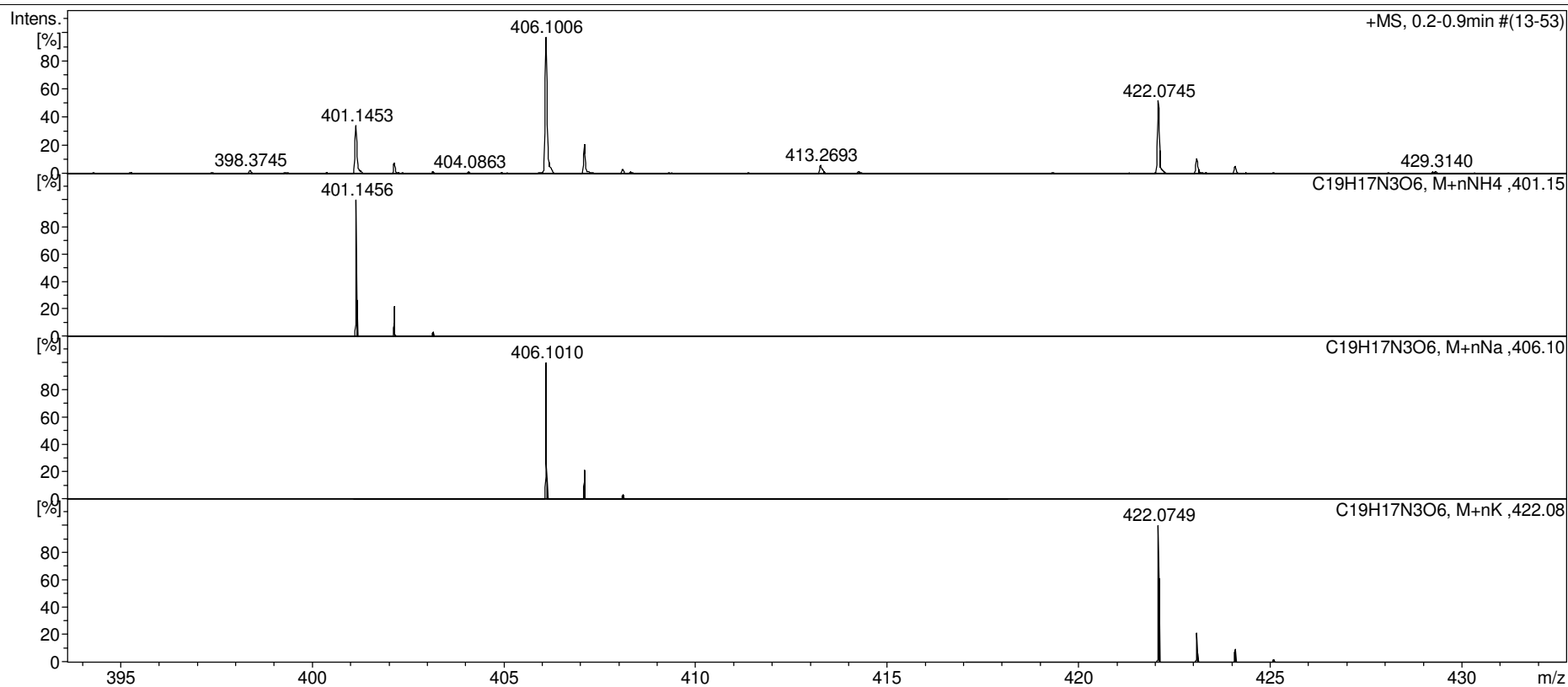
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0326043.d
Method tune_50-1600.m
Sample Name /LPIK AF-235
Comment C19H17N3O6 mH 384.1190 calibrant added CH3CN

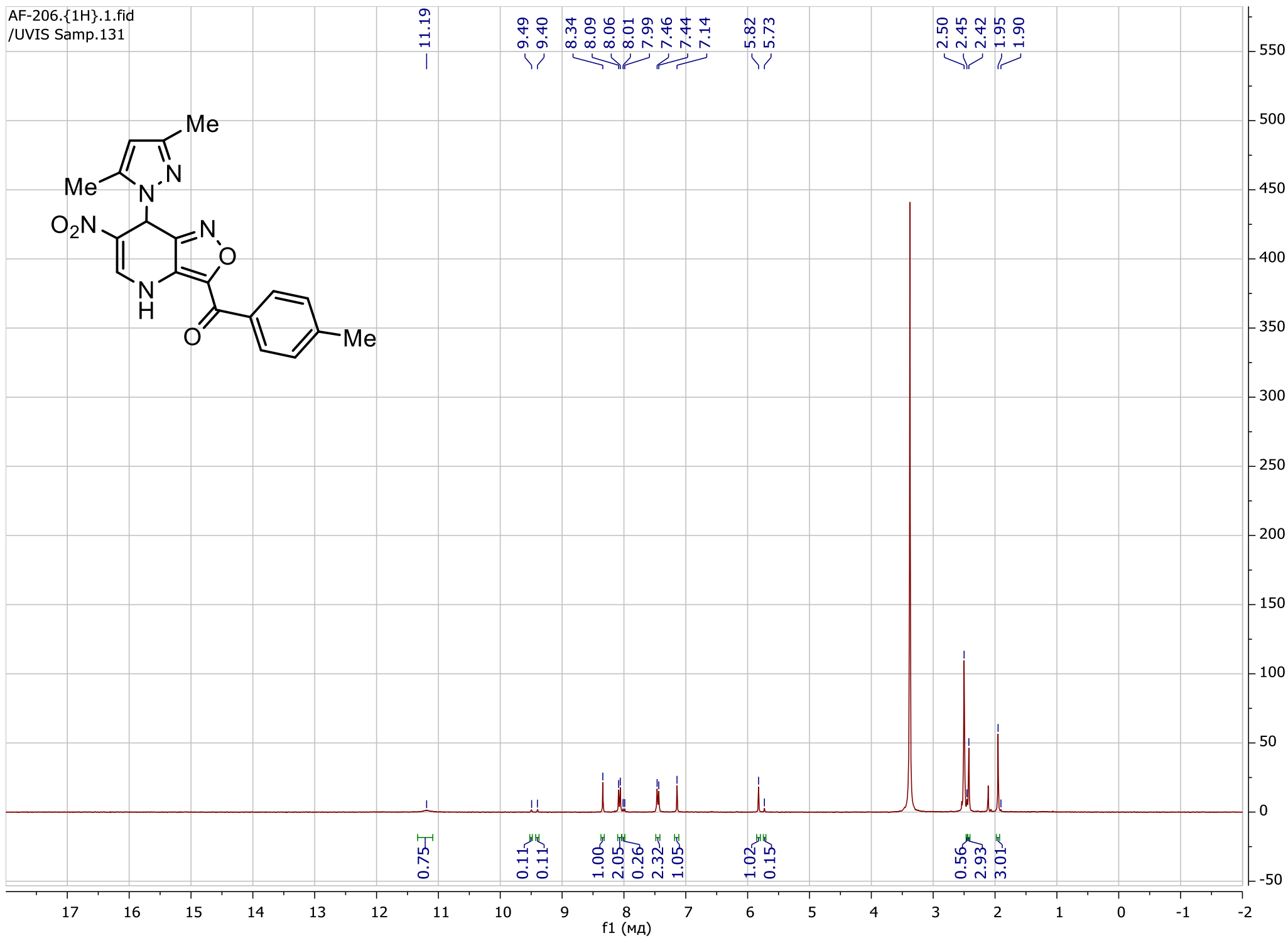
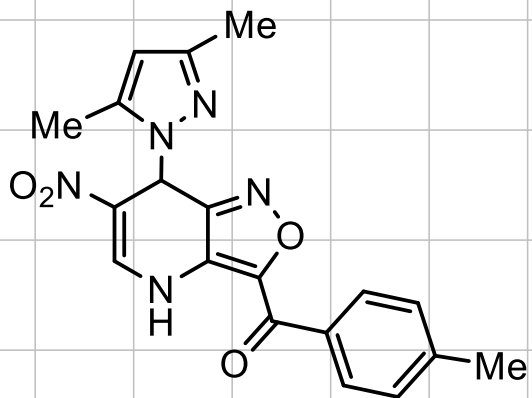
Acquisition Date 26.03.2019 19:37:54
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

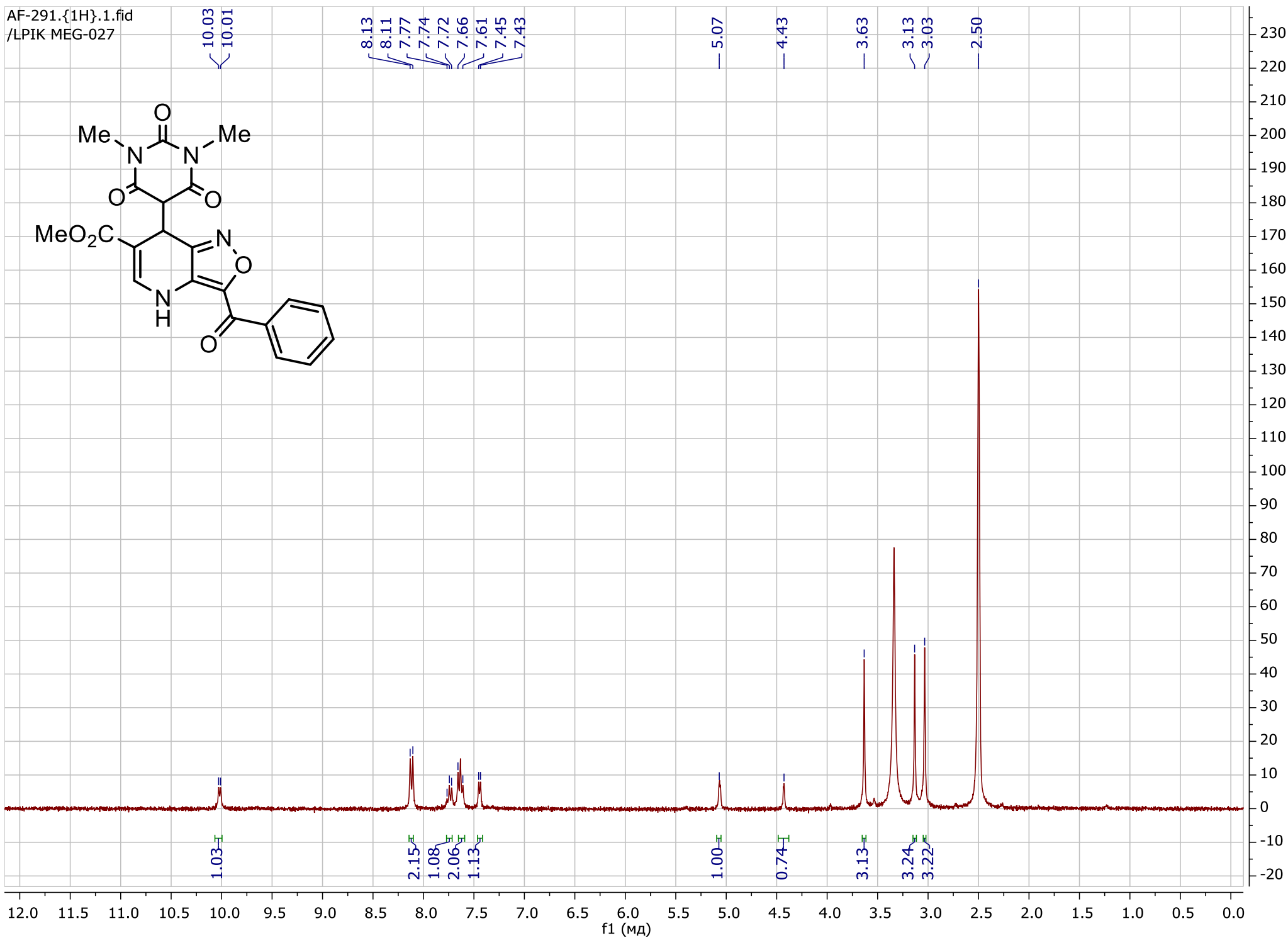
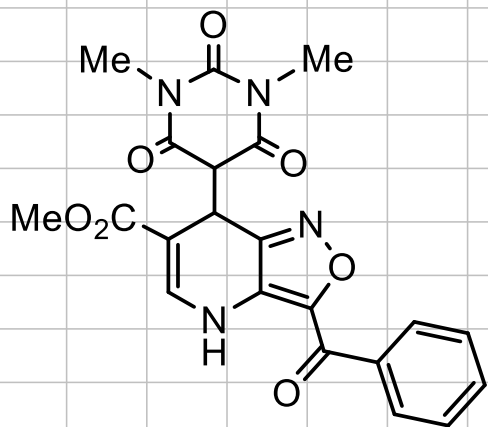
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



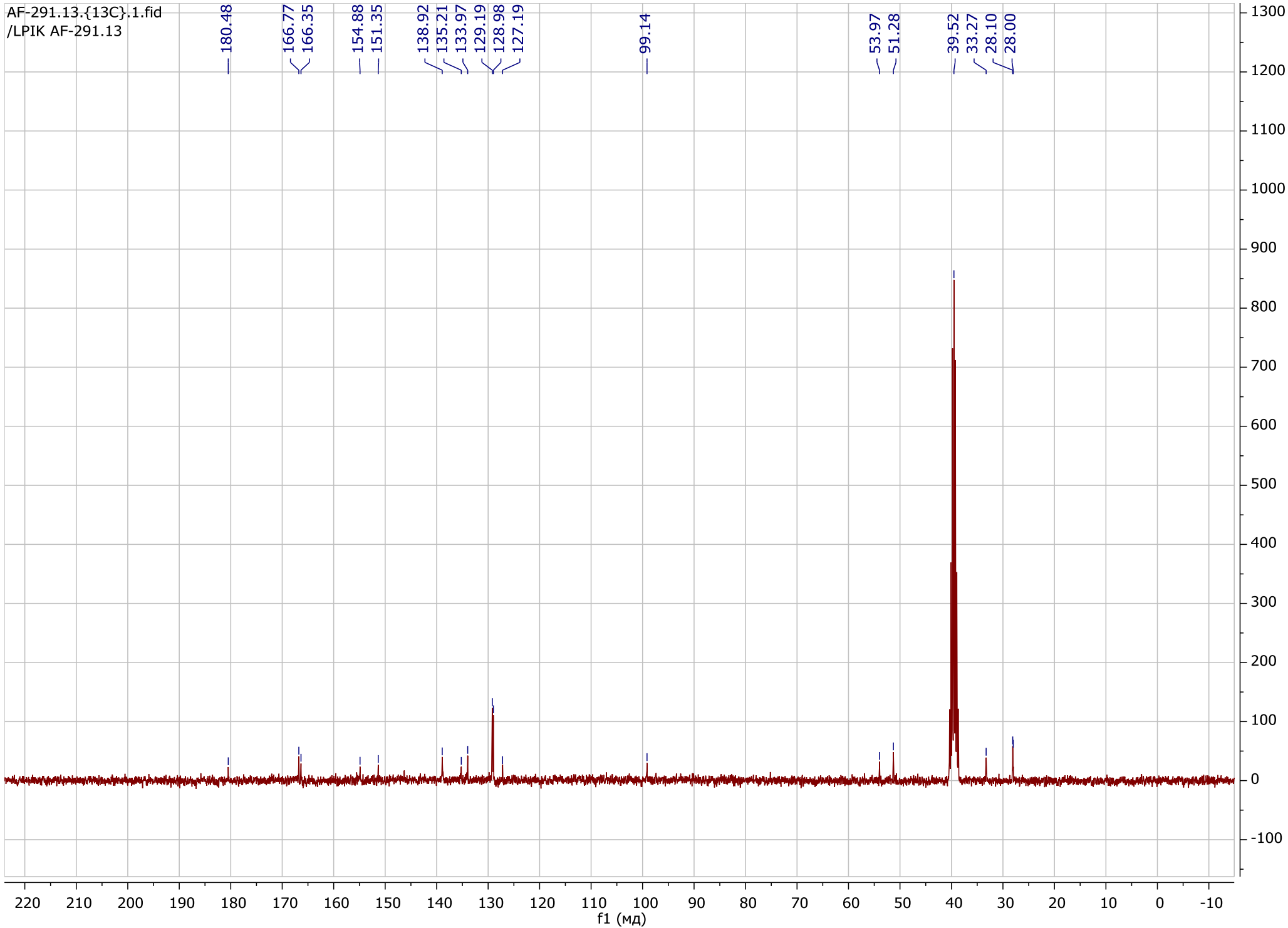
AF-206.{1H}.1.fid
/UVIS Samp.131



AF-291.{1H}.1.fid
/LPIK MEG-027



AF-291.13-¹³C}.1.fid
/LPIK AF-291.13



Display Report

Analysis Info

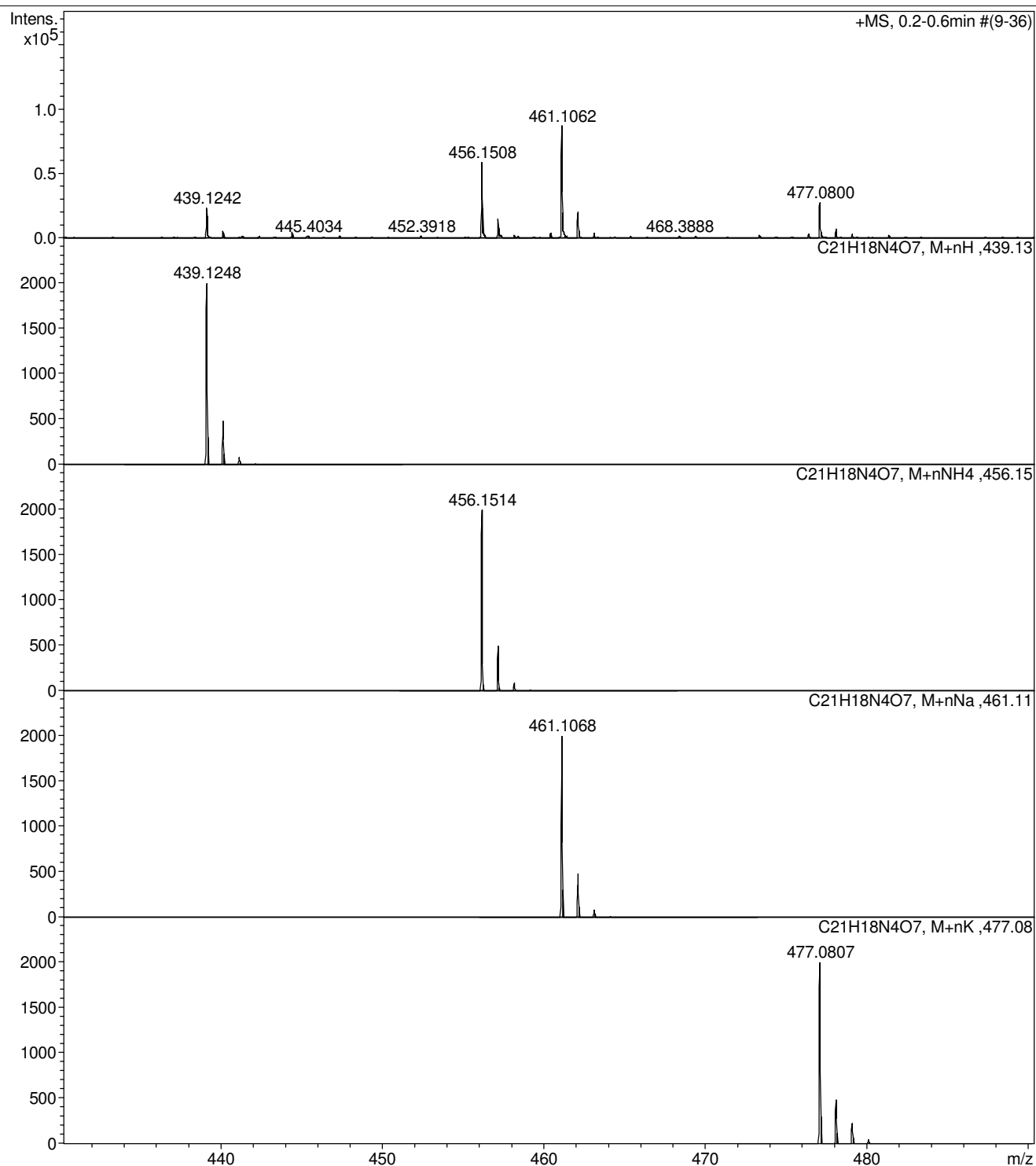
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0925008.d
Method tune_50-1600.m
Sample Name /LPIK AF-291
Comment C21H18N4O7 mH 439.1248 calibrant added

Acquisition Date 25.09.2019 12:53:52

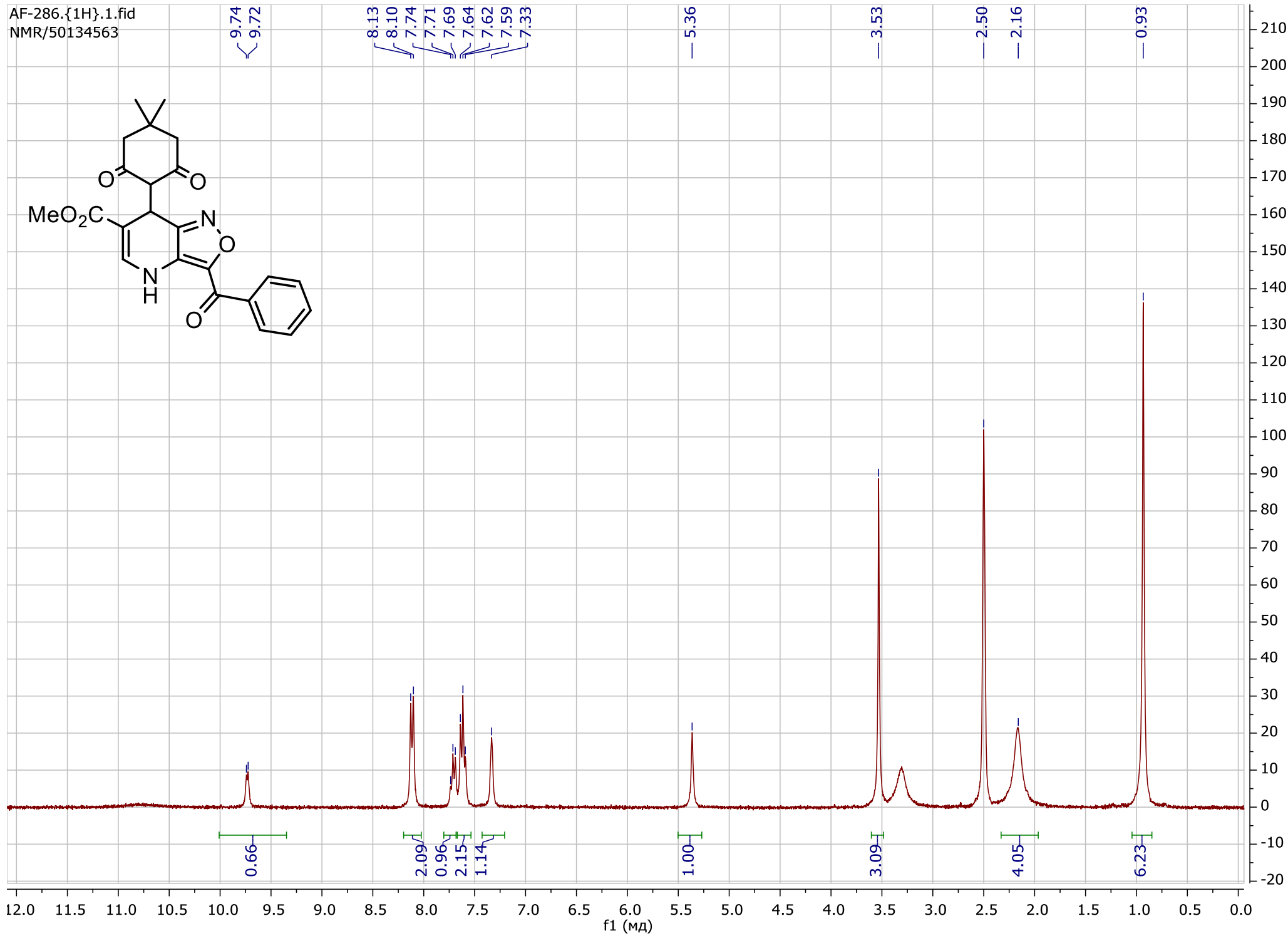
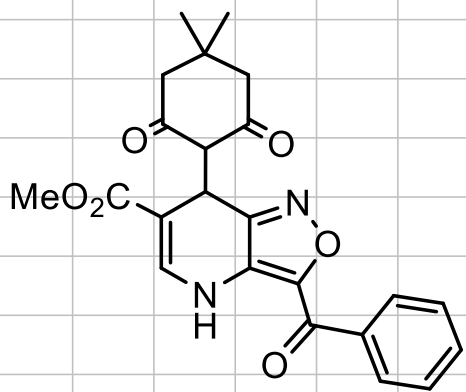
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

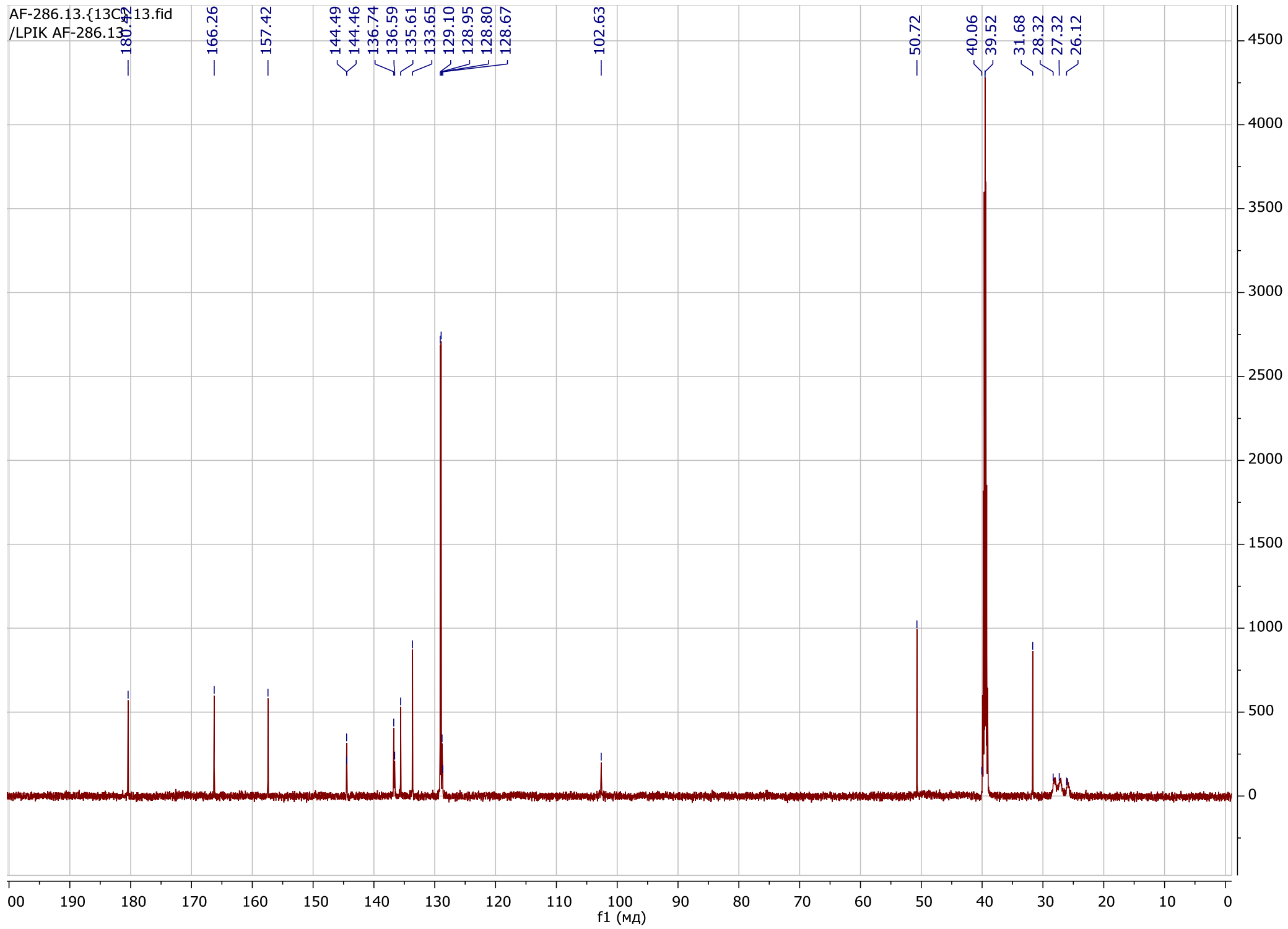
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-286.{1H}.1.fid
NMR/50134563



AF-286.13.{13C}.13.fid
/LPIK AF-286.13



Display Report

Analysis Info

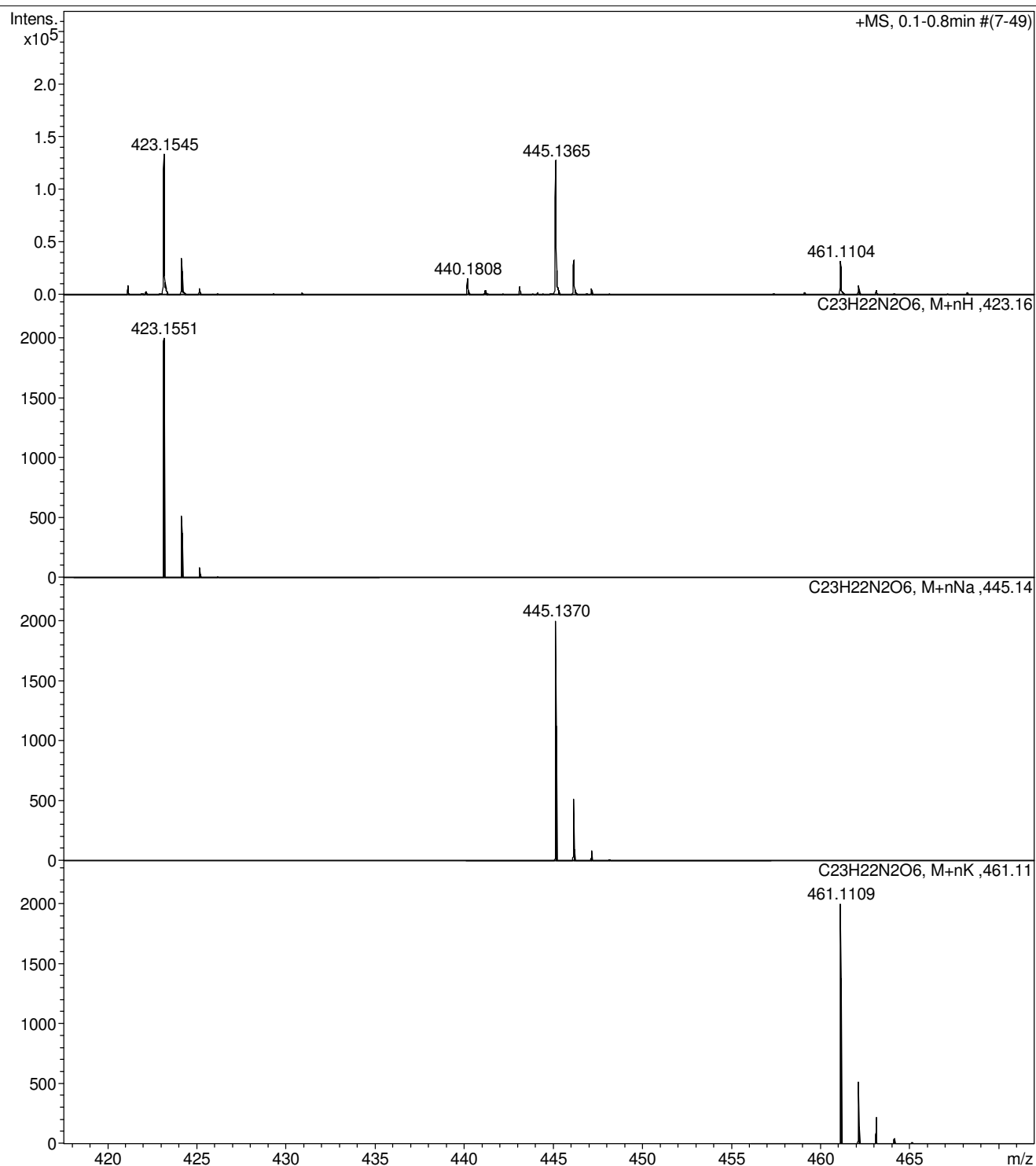
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0423026.d
Method tune_50-1600.m
Sample Name /LPIK AF-286
Comment C23H22N2O6 mH 423.1550 calibrant added

Acquisition Date 23.04.2019 12:54:40

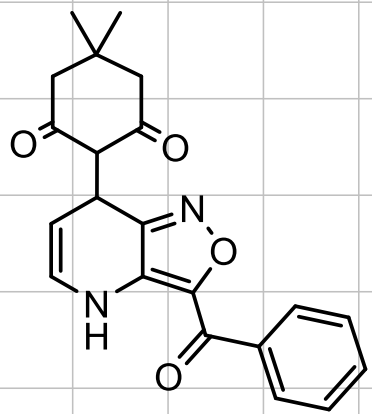
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-299.1.{1H}.1.fid
/LPIK AF-299.1



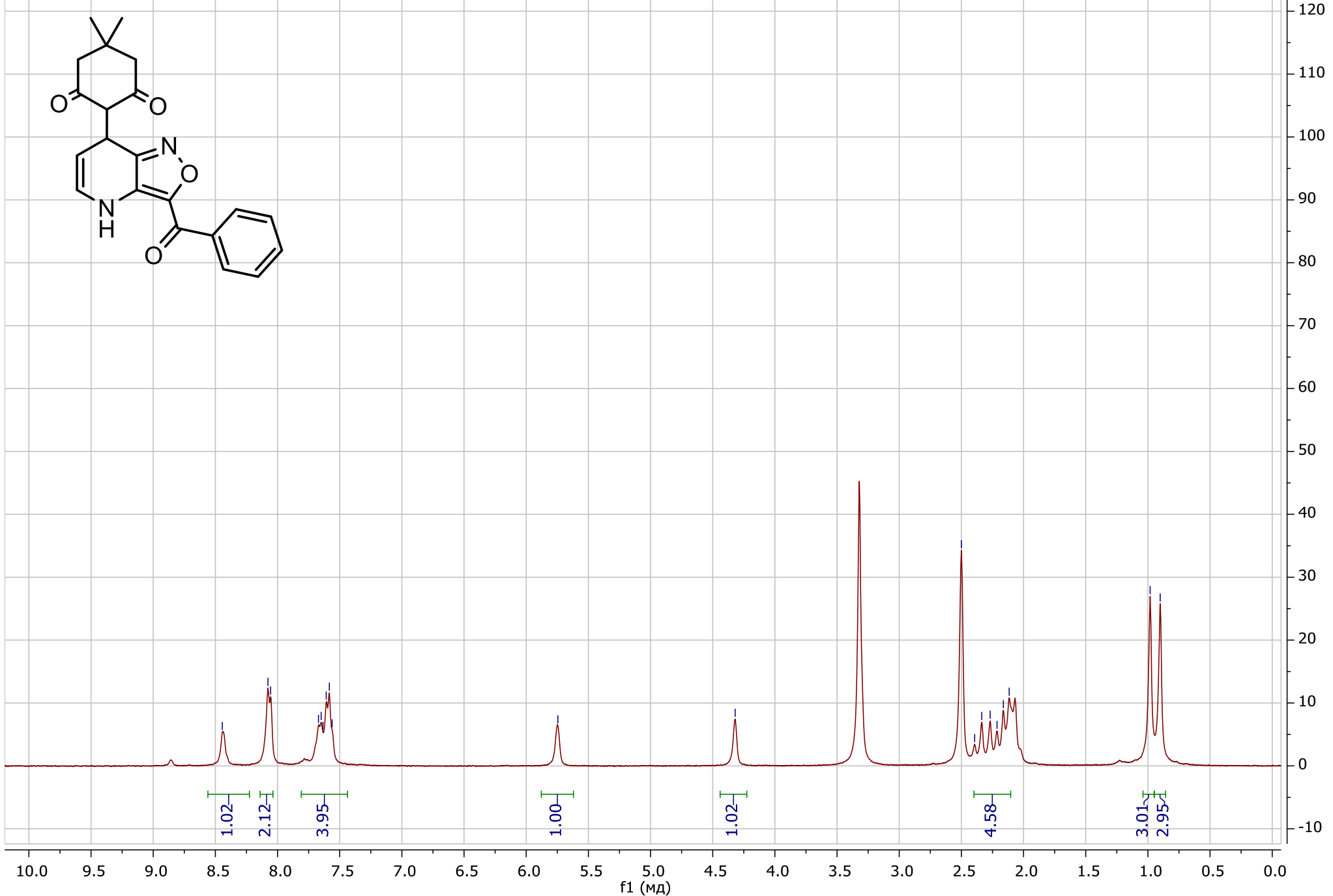
8.44
8.08
8.06
7.67
7.65
7.63
7.61
7.58
7.56

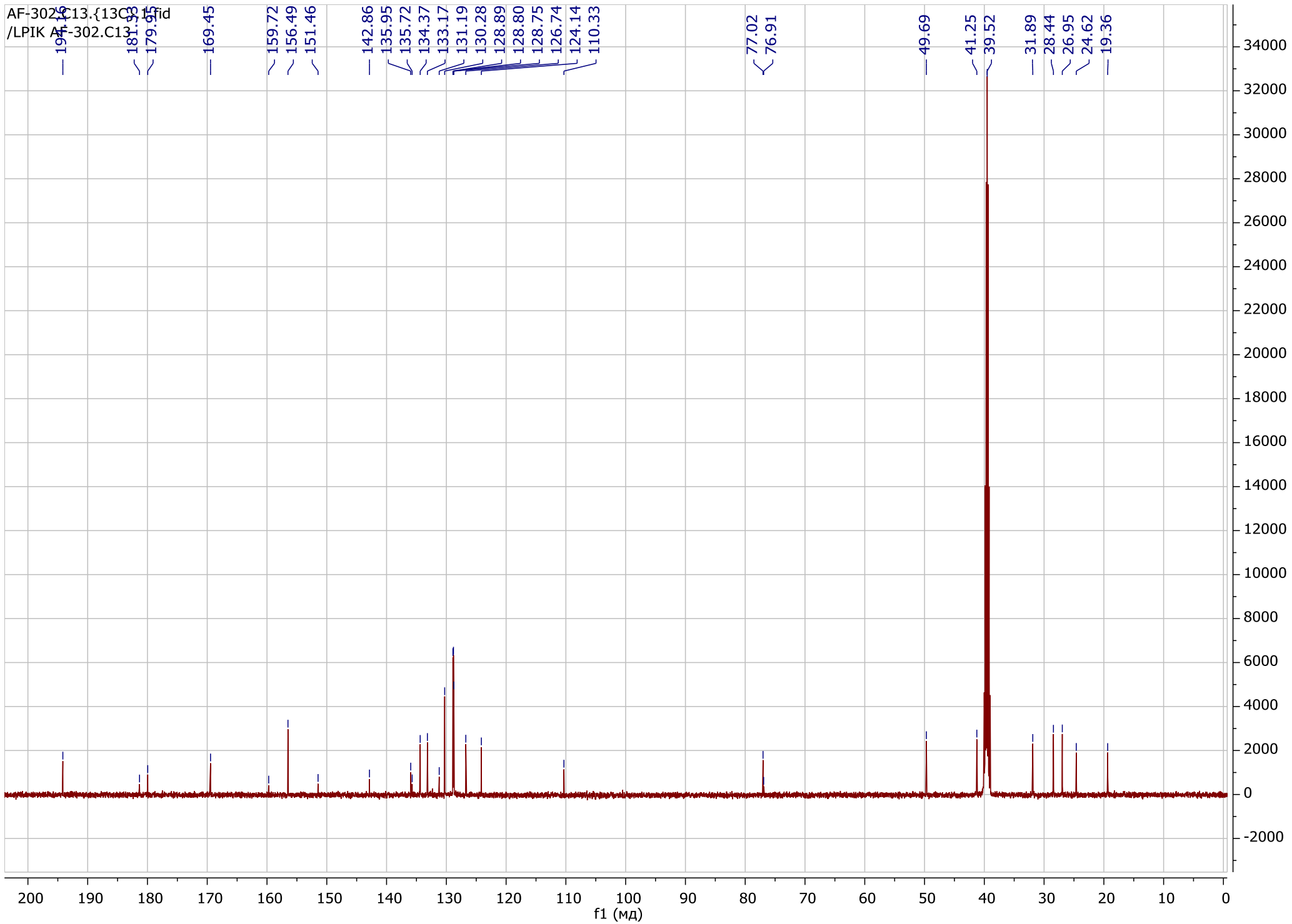
5.75

4.32

2.50
2.39
2.34
2.27
2.21
2.16
2.12

0.98
0.90





Display Report

Analysis Info

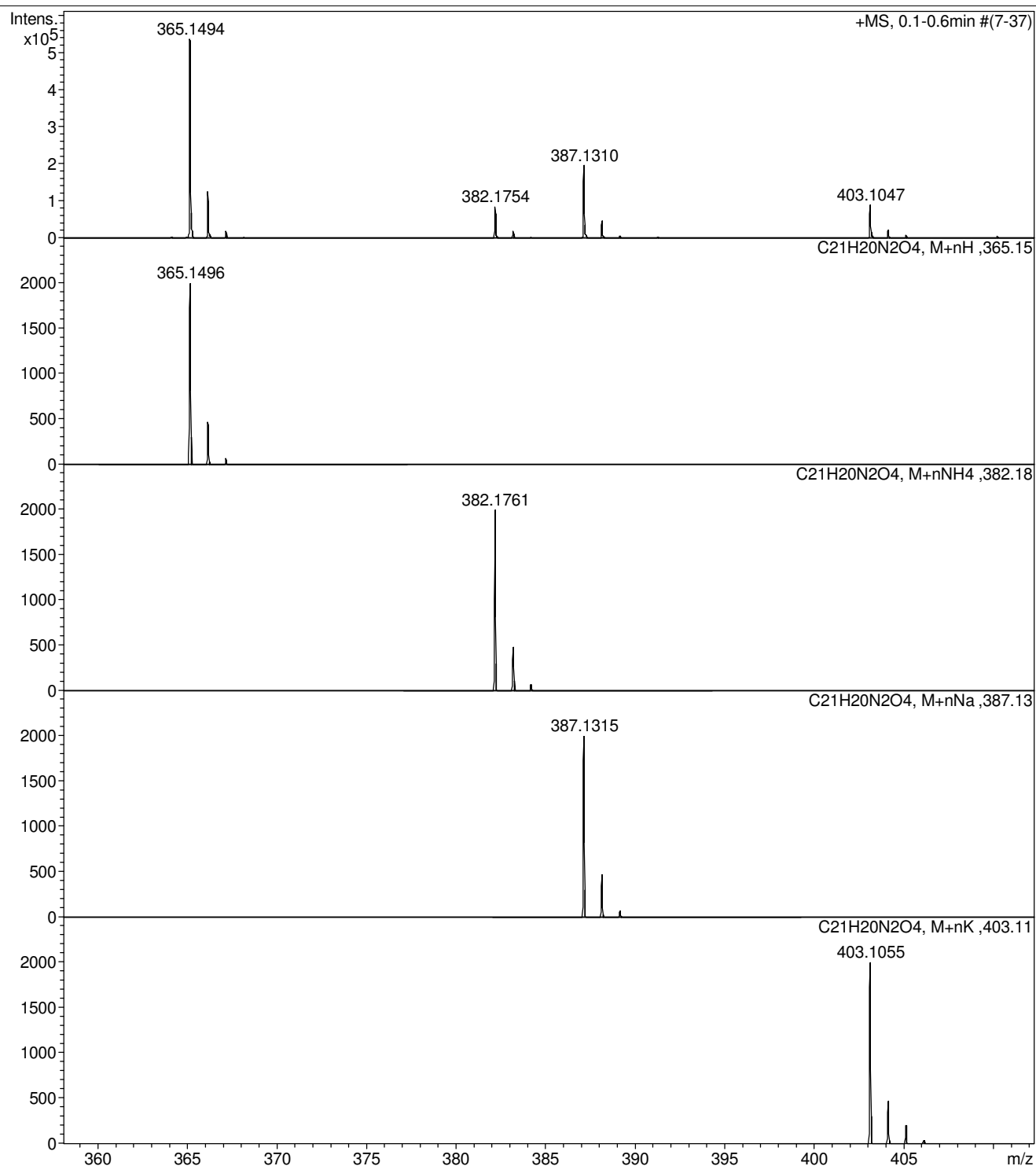
Analysis Name D:\Data\Kolotyrykina\2019\Bastrakov\0925007.d
Method tune_50-1600.m
Sample Name /LPIK AF-302
Comment C21H20N2O4 mH 365.1495 calibrant added

Acquisition Date 25.09.2019 12:48:55

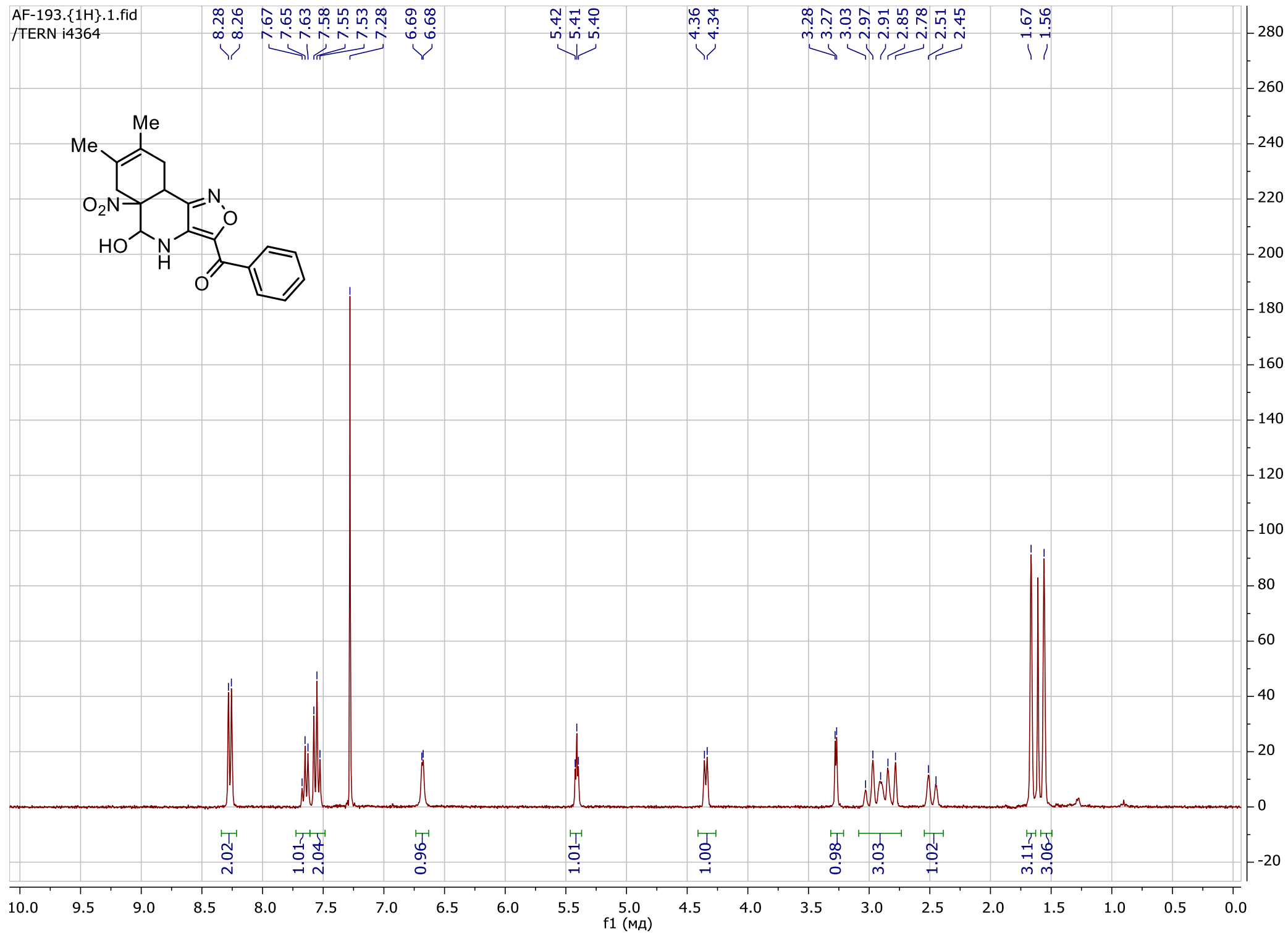
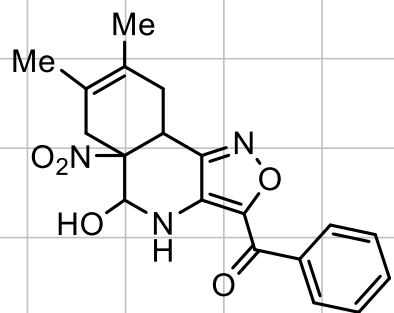
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

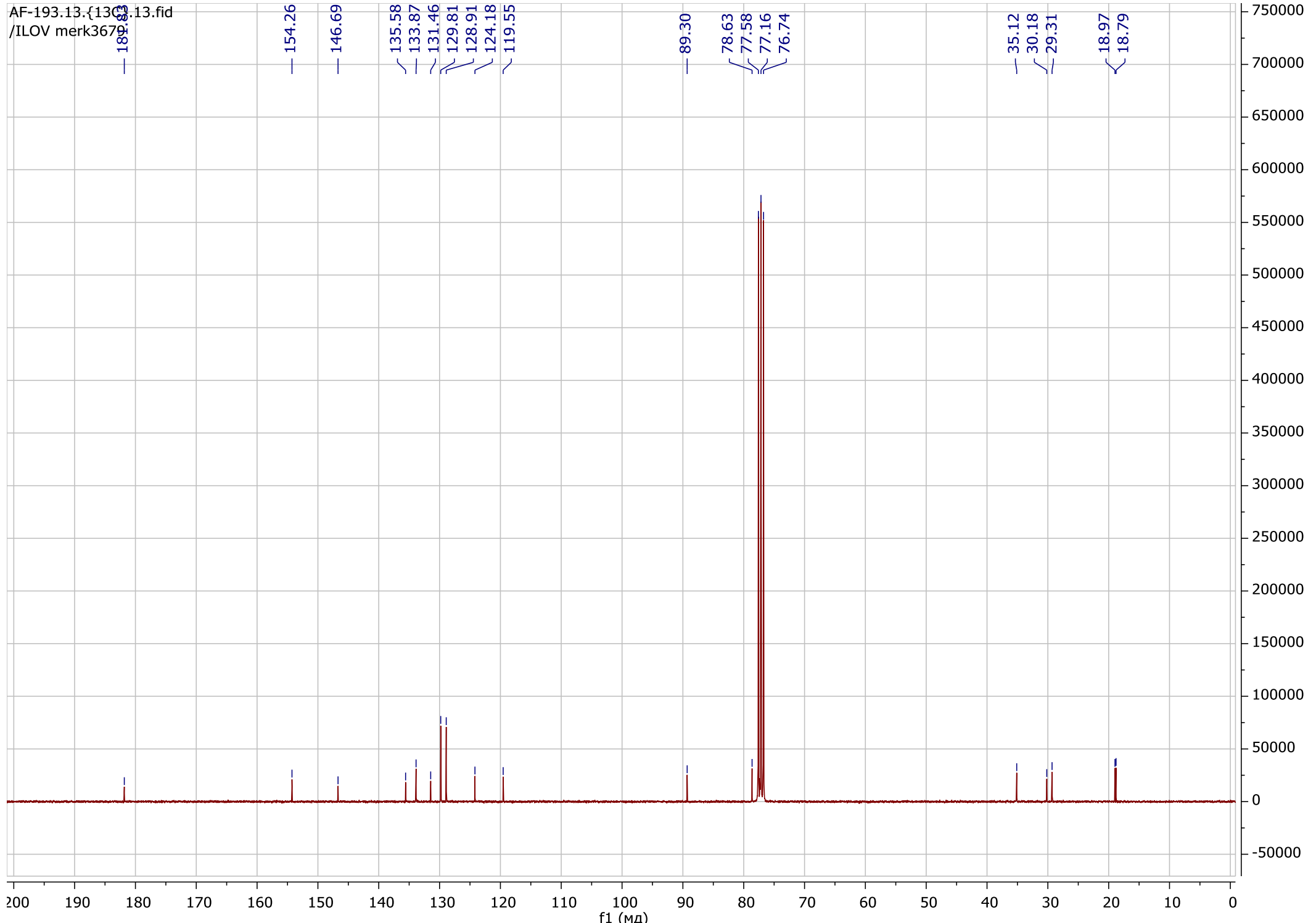
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-193-{1H}.1.fid
/TERN i4364



AF-193.13.{13C}.13.fid
/ILOV merk367



Display Report

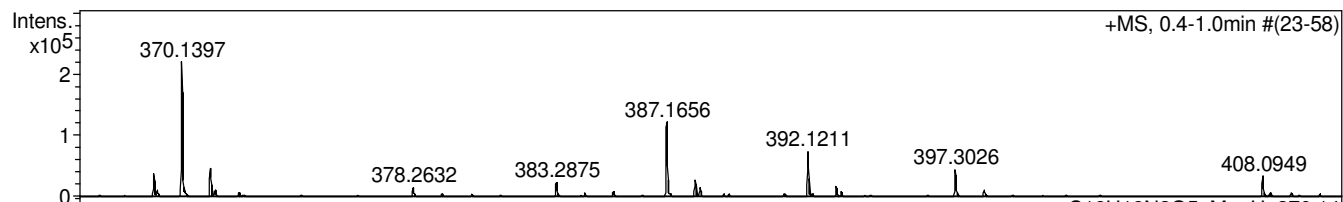
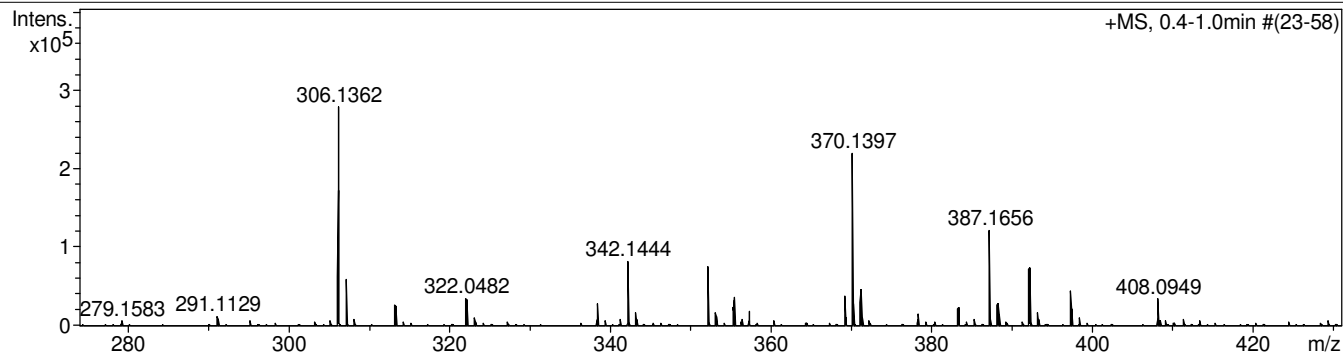
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2018\Bastrakov\1113020.d
Method tune_50-1600.m
Sample Name /LPIK AF-193
Comment C19H19N3O5 mH 370.1397 calibrant added

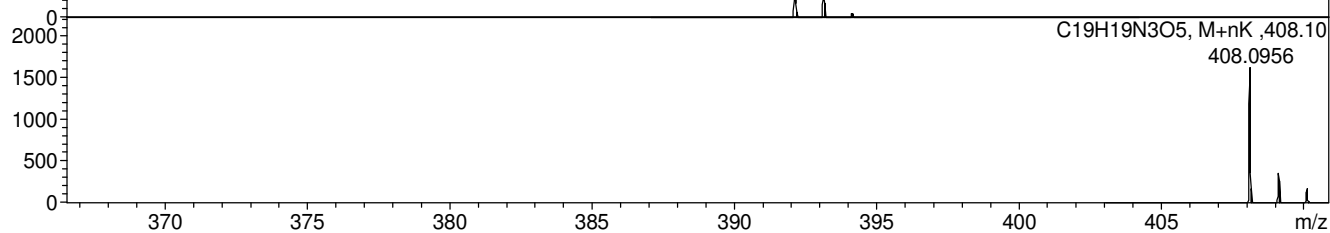
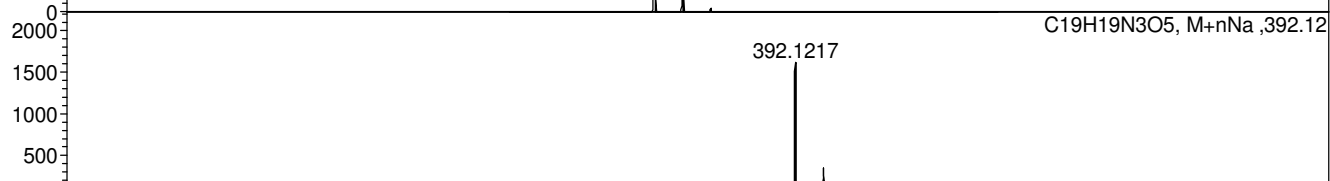
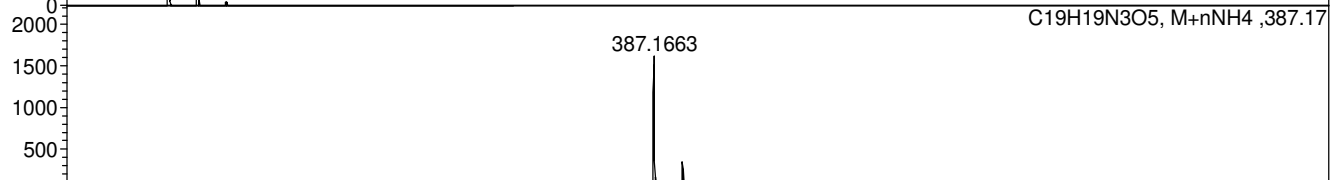
Acquisition Date 13.11.2018 12:05:43
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

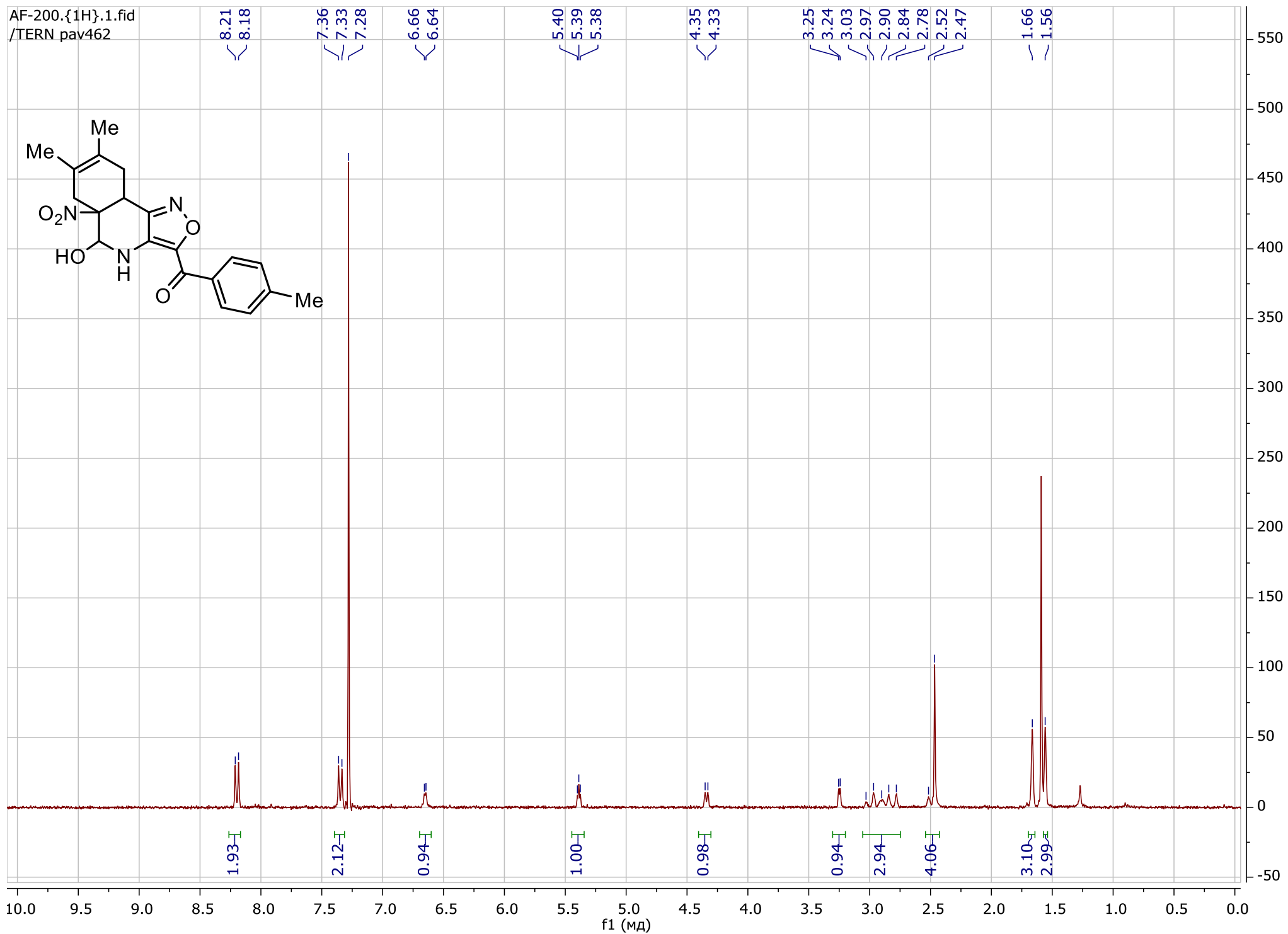
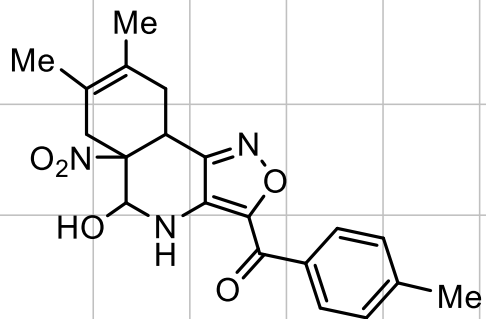
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



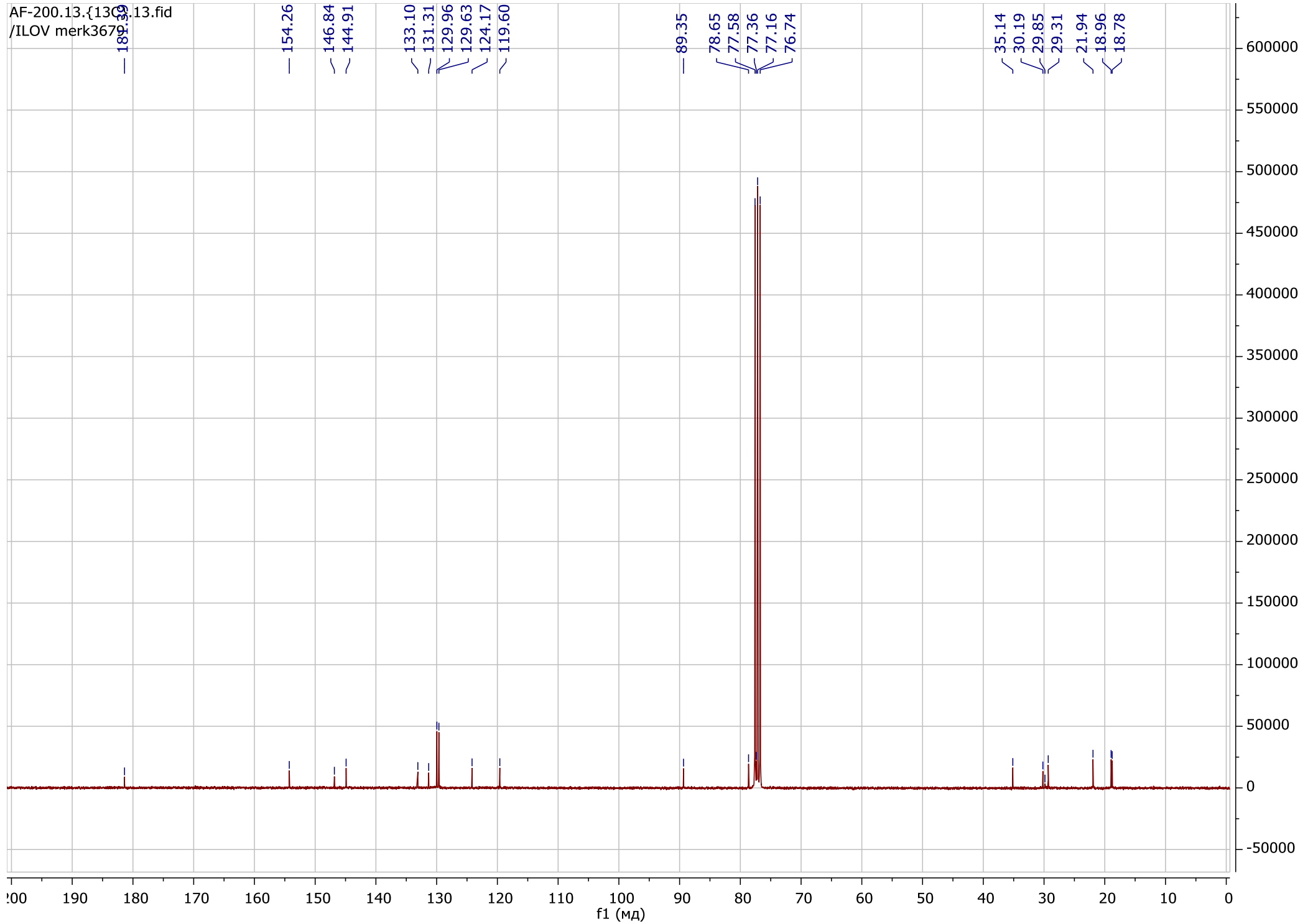
C19H19N3O5, M+nH ,370.14



AF-200.{1H}.1.fid
/TERN pav462



AF-200.13.{13C}.13.fid
/ILOV merk367



Display Report

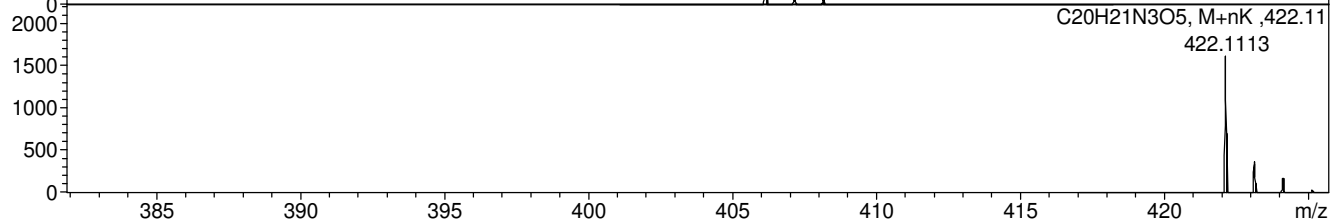
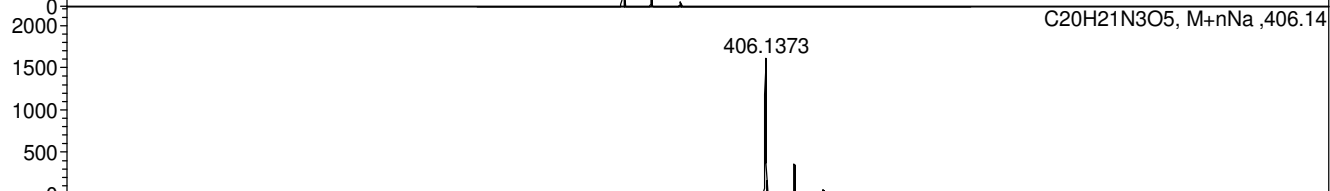
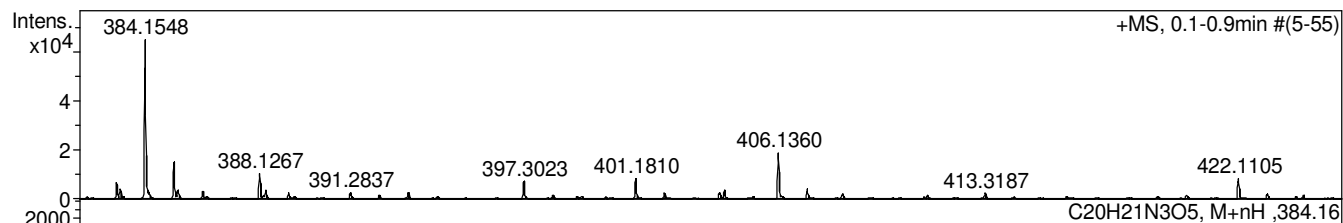
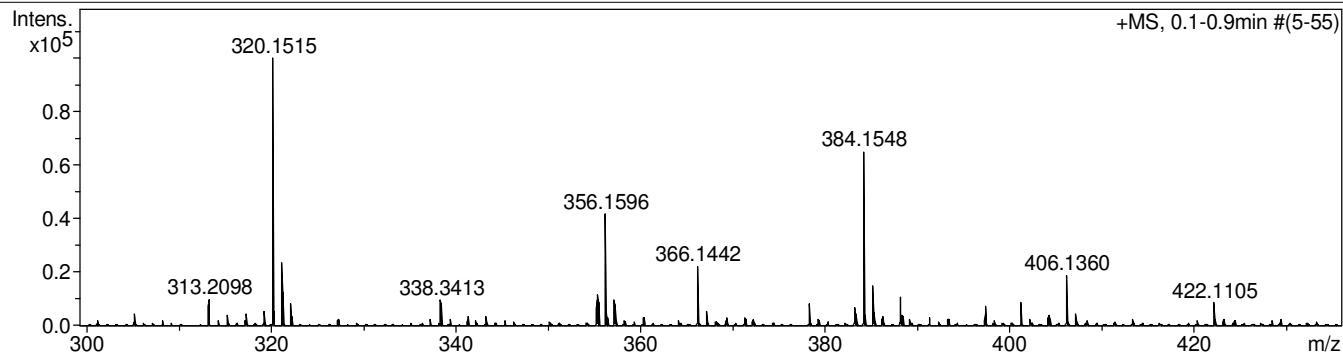
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2018\Bastrakov\1113019.d
Method tune_50-1600.m
Sample Name /LPIK AF-200
Comment C20H21N3O5 mH 384.1553 calibrant added

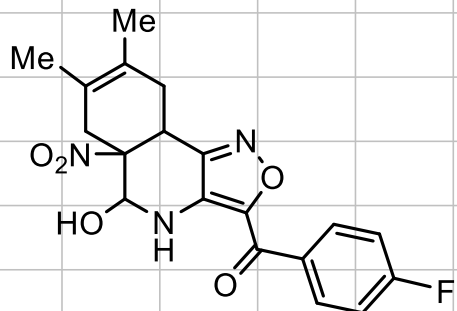
Acquisition Date 13.11.2018 11:57:14
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-227-{1H}.1.fid
NMR/50122684



8.36
8.34
8.33
8.32

7.28
7.26
7.23
7.20

6.66
6.65

5.42
5.41
5.40

4.35
4.33

3.19
3.18
3.02

2.96
2.91
2.85

2.79
2.51
2.45

1.67
1.56

2.18

2.13

0.99

1.00

1.04

0.98

3.19

1.07

3.27

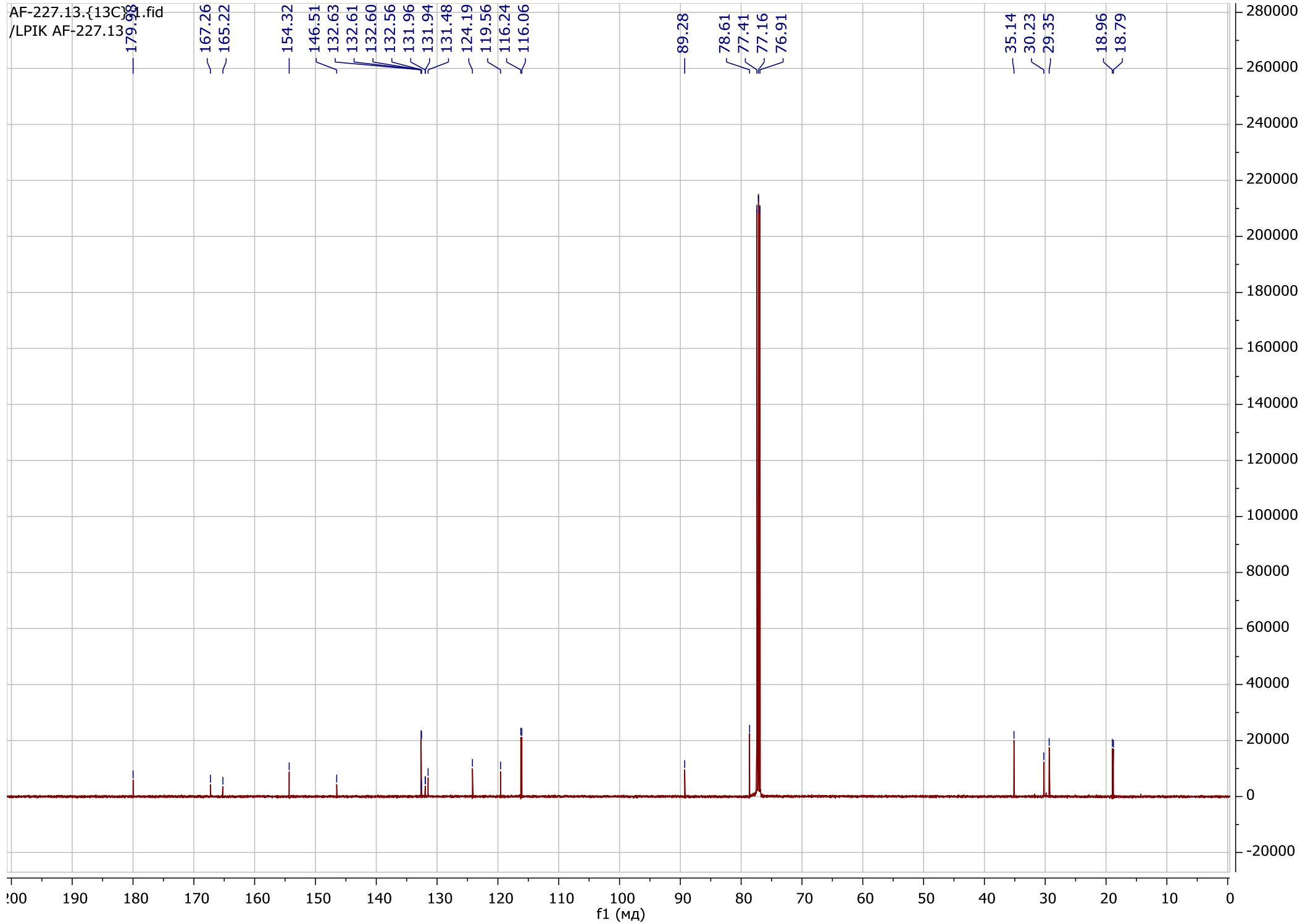
3.17

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (M μ)

400
380
360
340
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20

AF-227.13-¹³C.fid
/LPIK AF-227.13



Display Report

Analysis Info

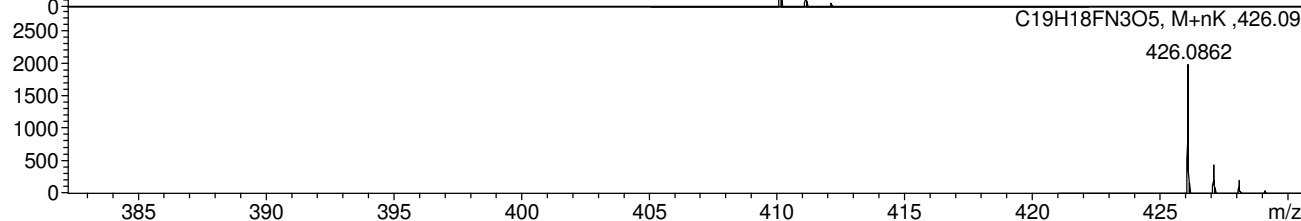
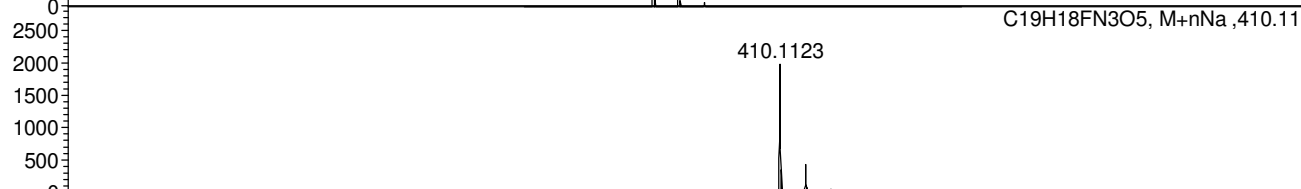
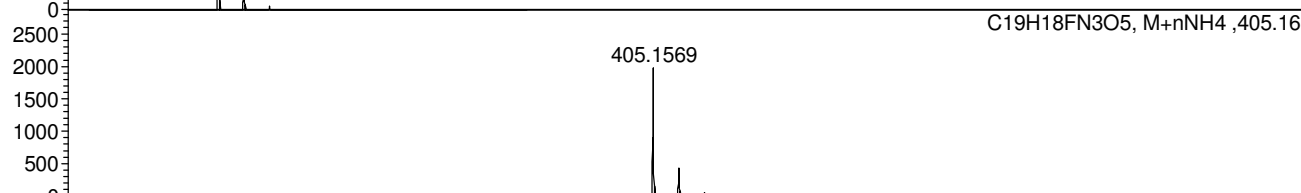
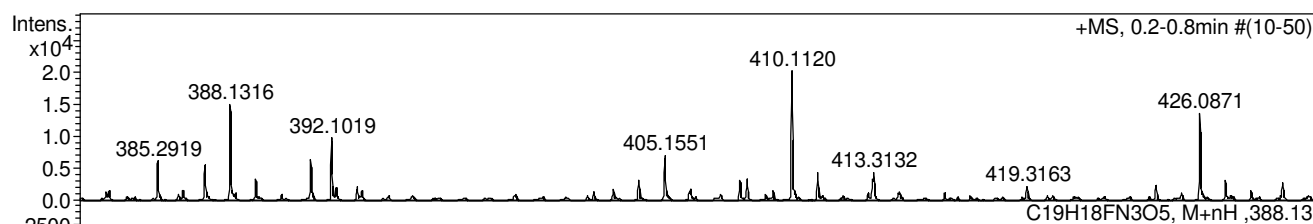
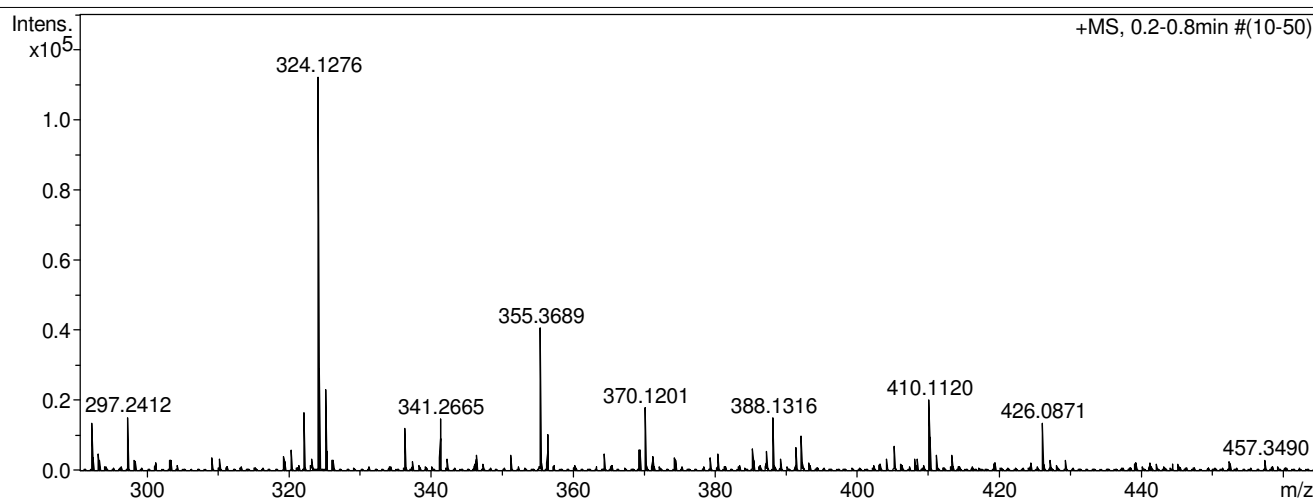
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\0326042.d
Method tune_50-1600.m
Sample Name /LPIK AF-227
Comment C19H18FN3O5 mH 388.1303 calibrant added CH3CN

Acquisition Date 26.03.2019 19:28:30

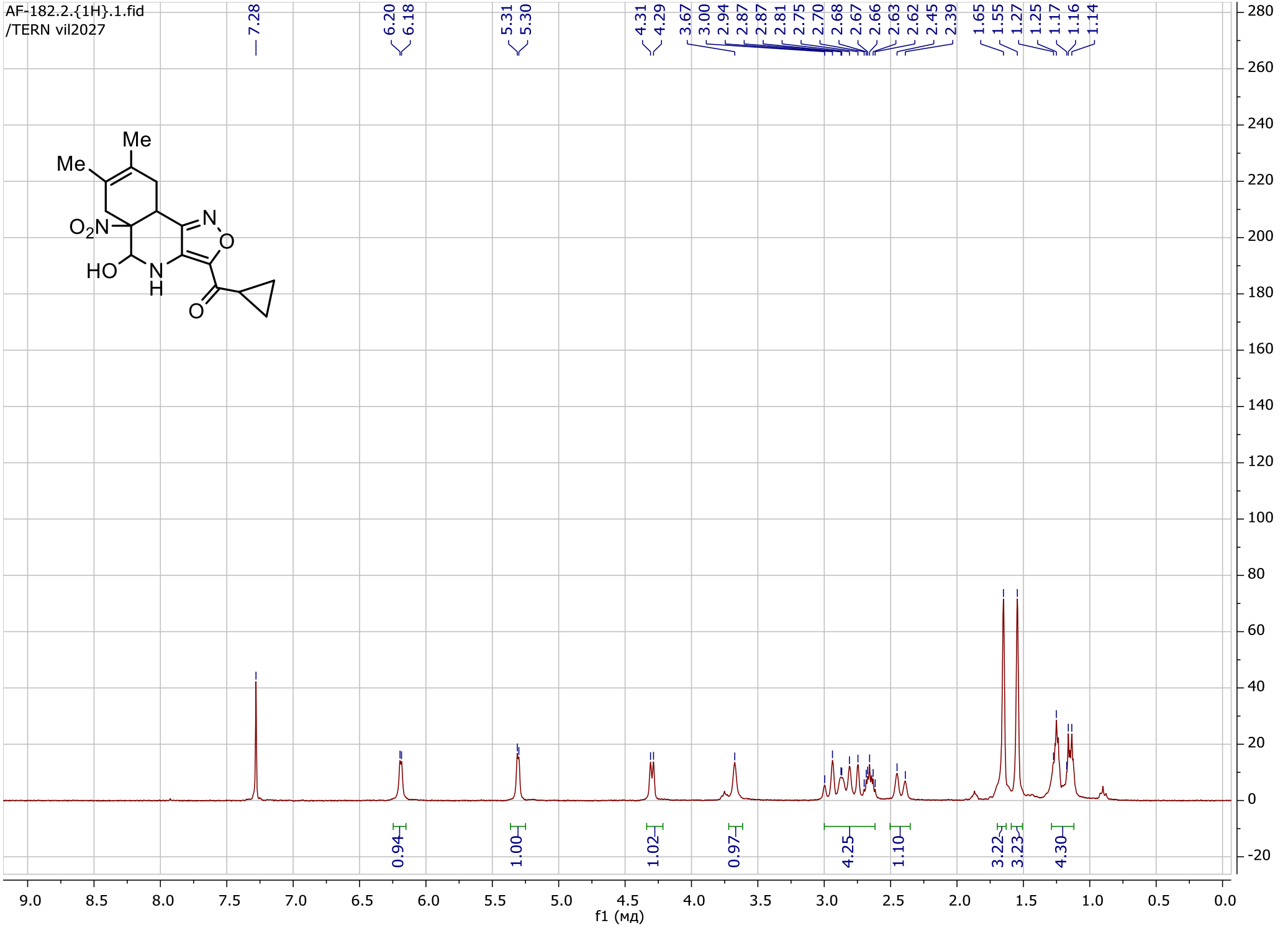
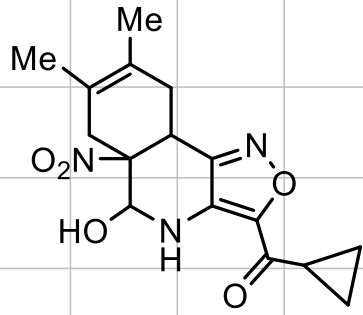
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

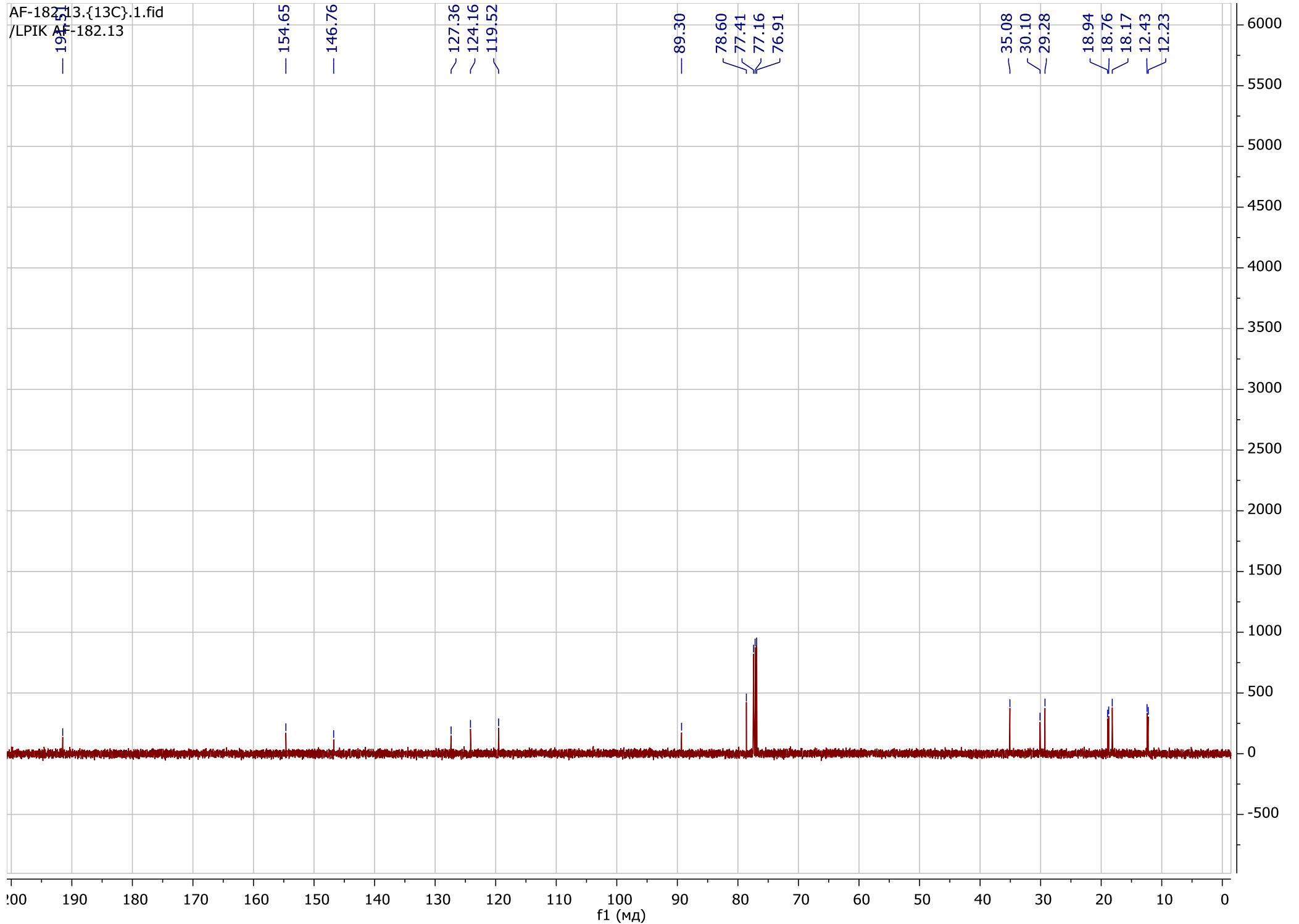
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-182.2.{1H}.1.fid
/TERN vil2027



AF-18213.{13C}.1.fid
/LPIK AF-182.13



Display Report

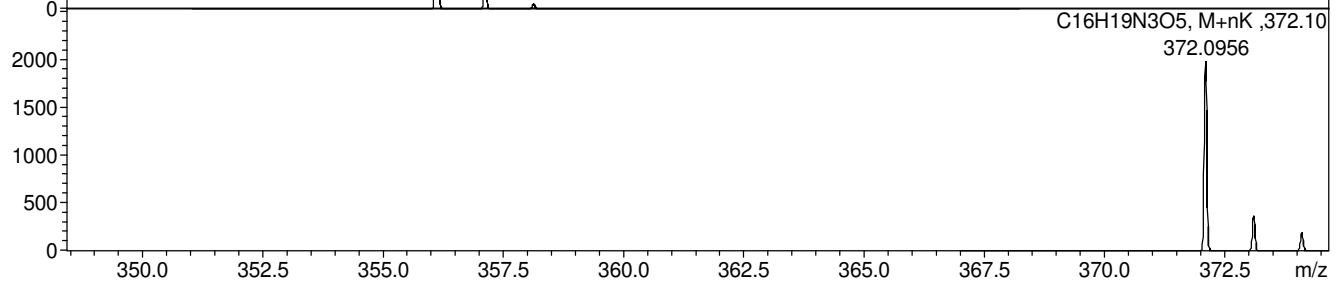
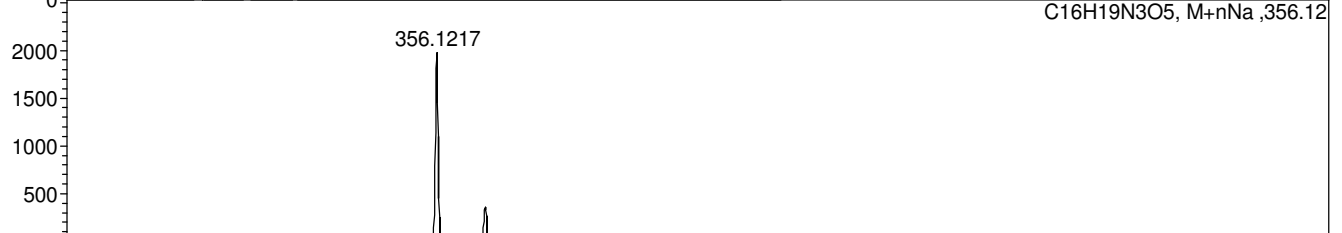
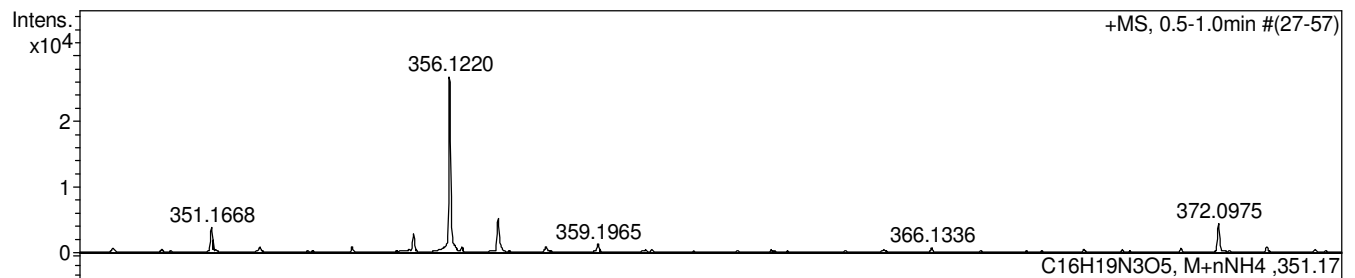
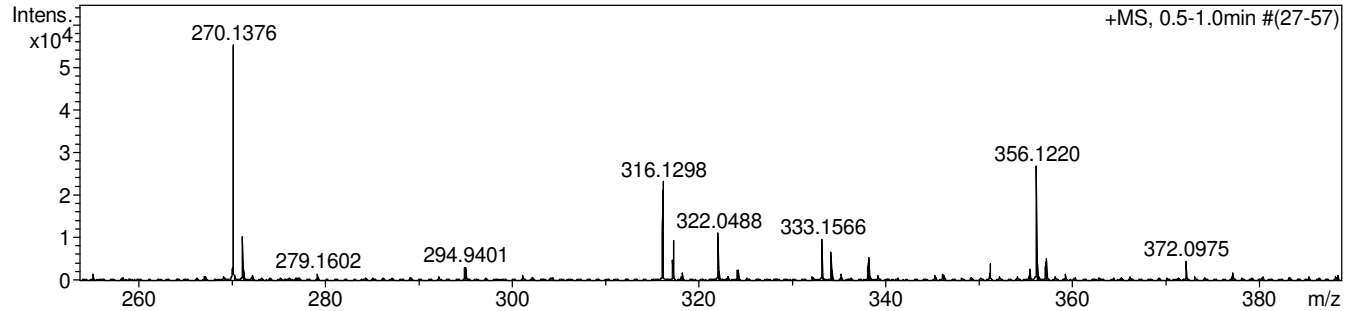
Analysis Info

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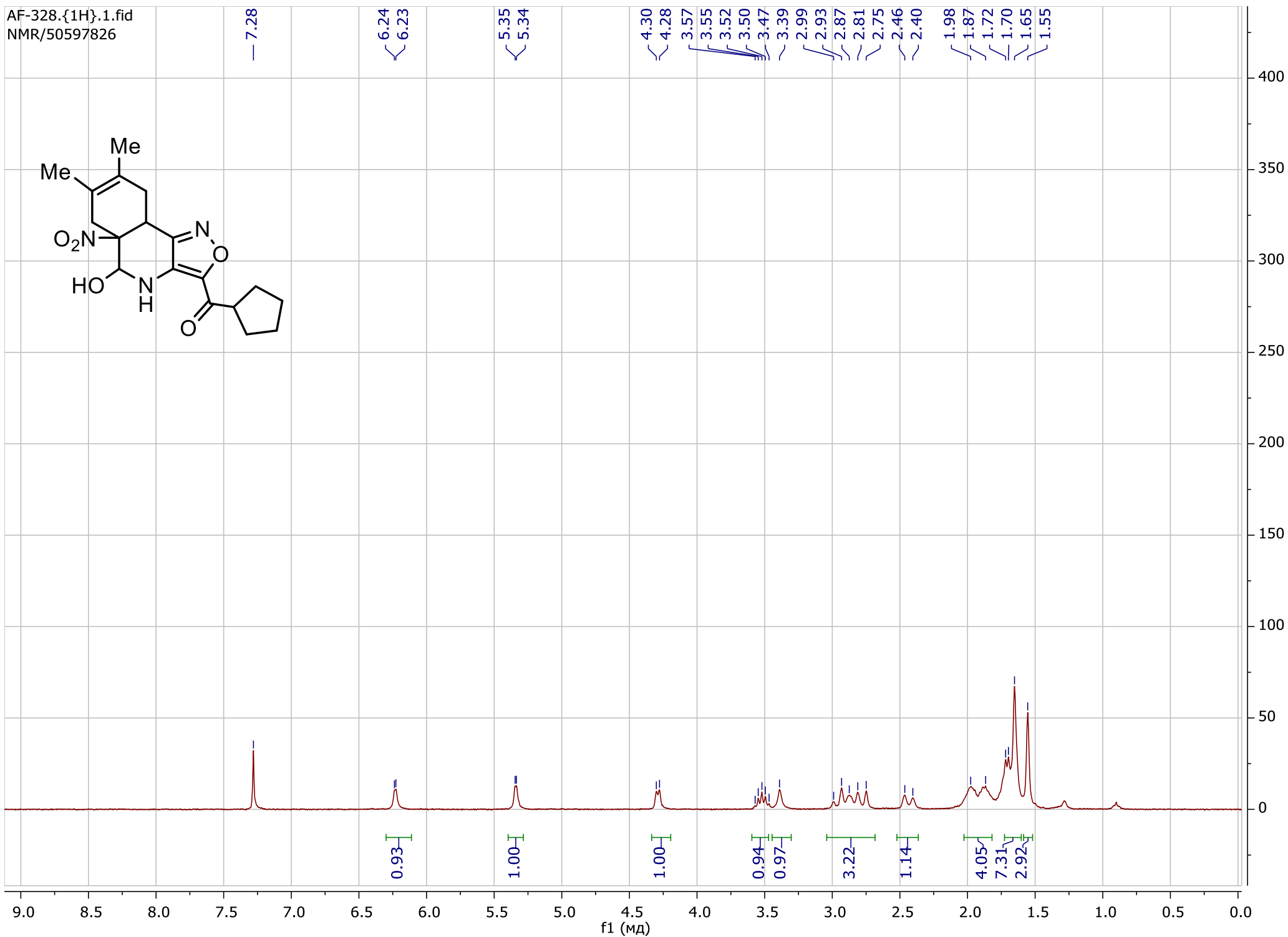
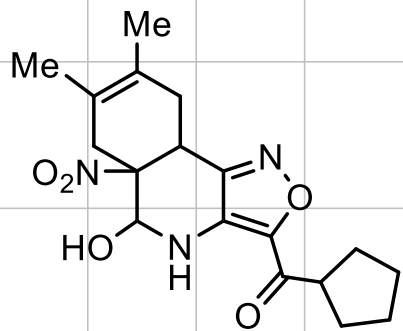
Acquisition Date 03.07.2018 11:09:21
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

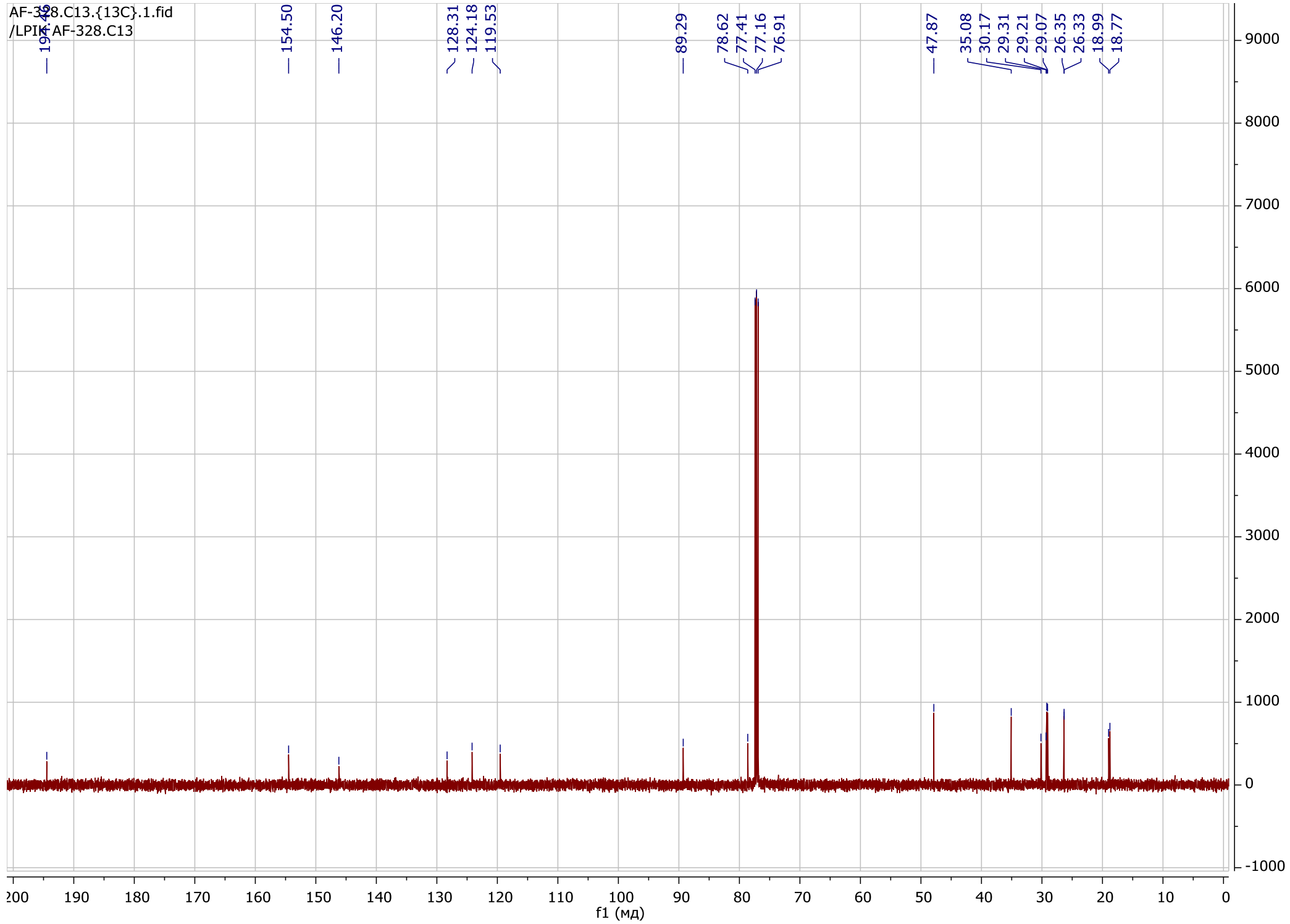
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Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-328.{1H}.1.fid
NMR/50597826



AF-328.C13.{13C}.1.fid
/LPIK AF-328.C13



Display Report

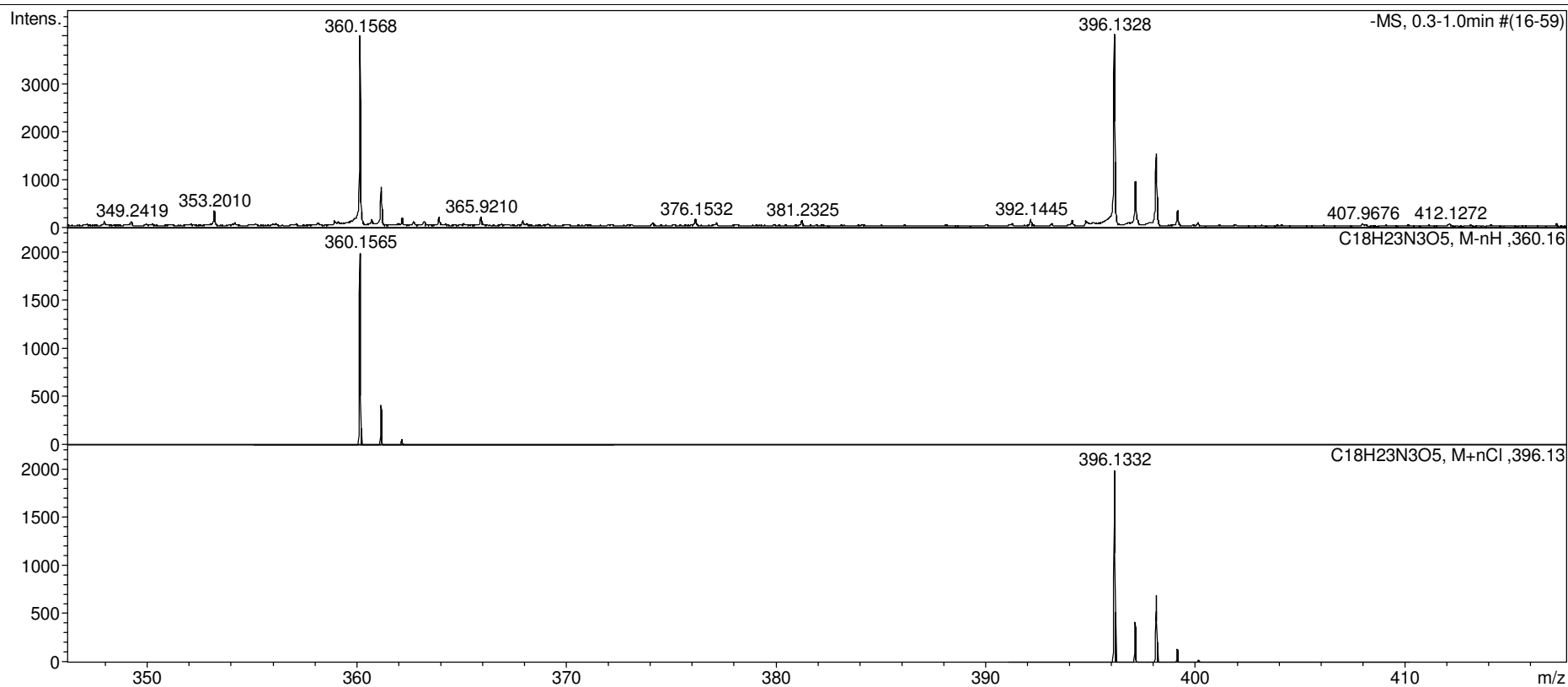
Analysis Info

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Method tune_50-1600_neg.m
Sample Name /LPIK AF-328
Comment C18H23N3O5 mH 362.1710 calibrant added CH3CN

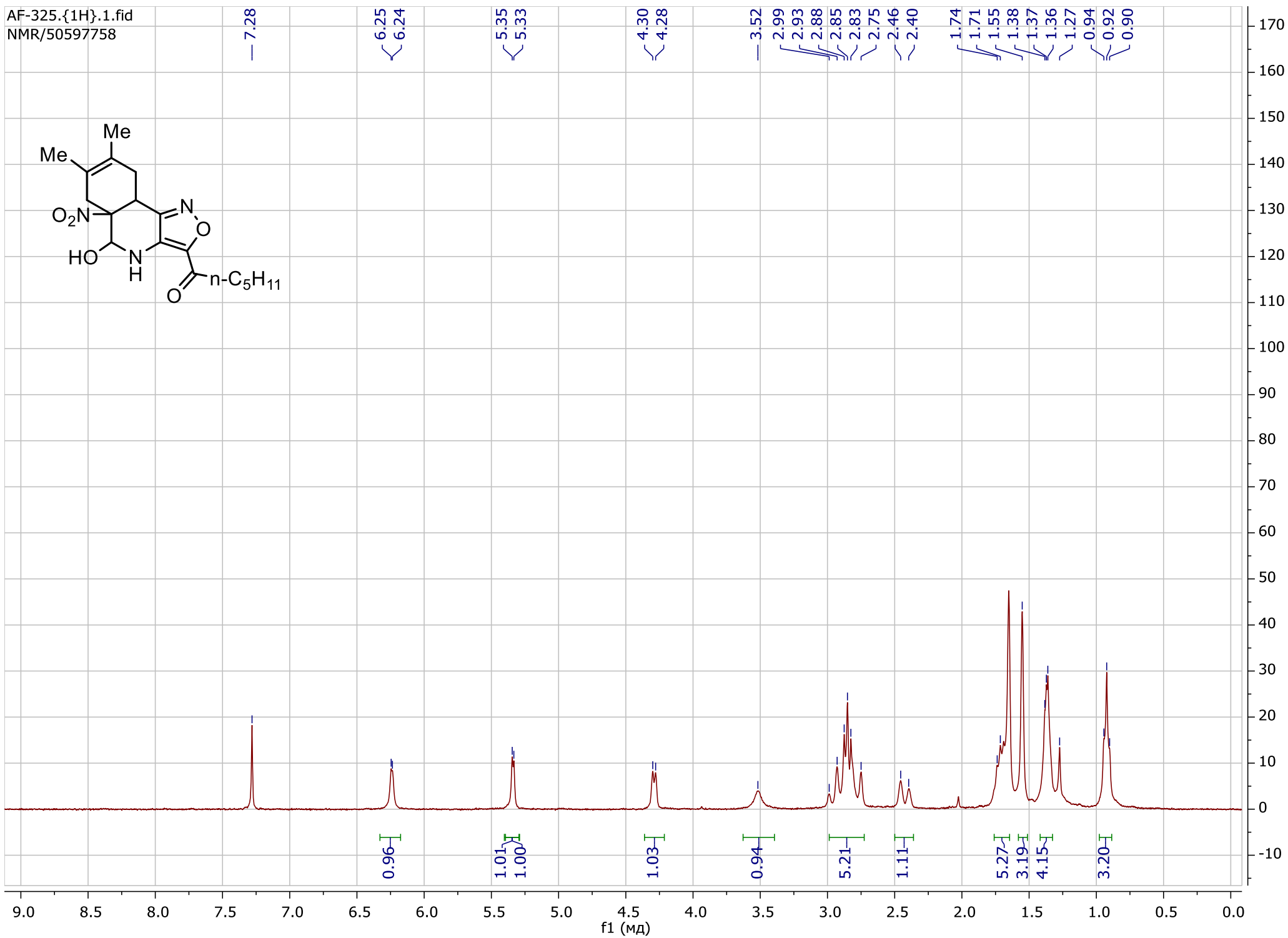
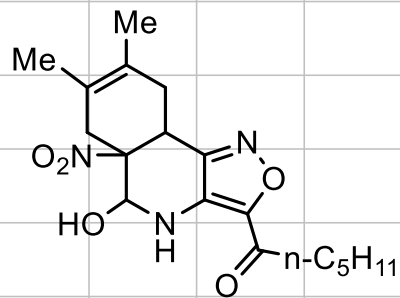
Acquisition Date 21.01.2020 16:47:06
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

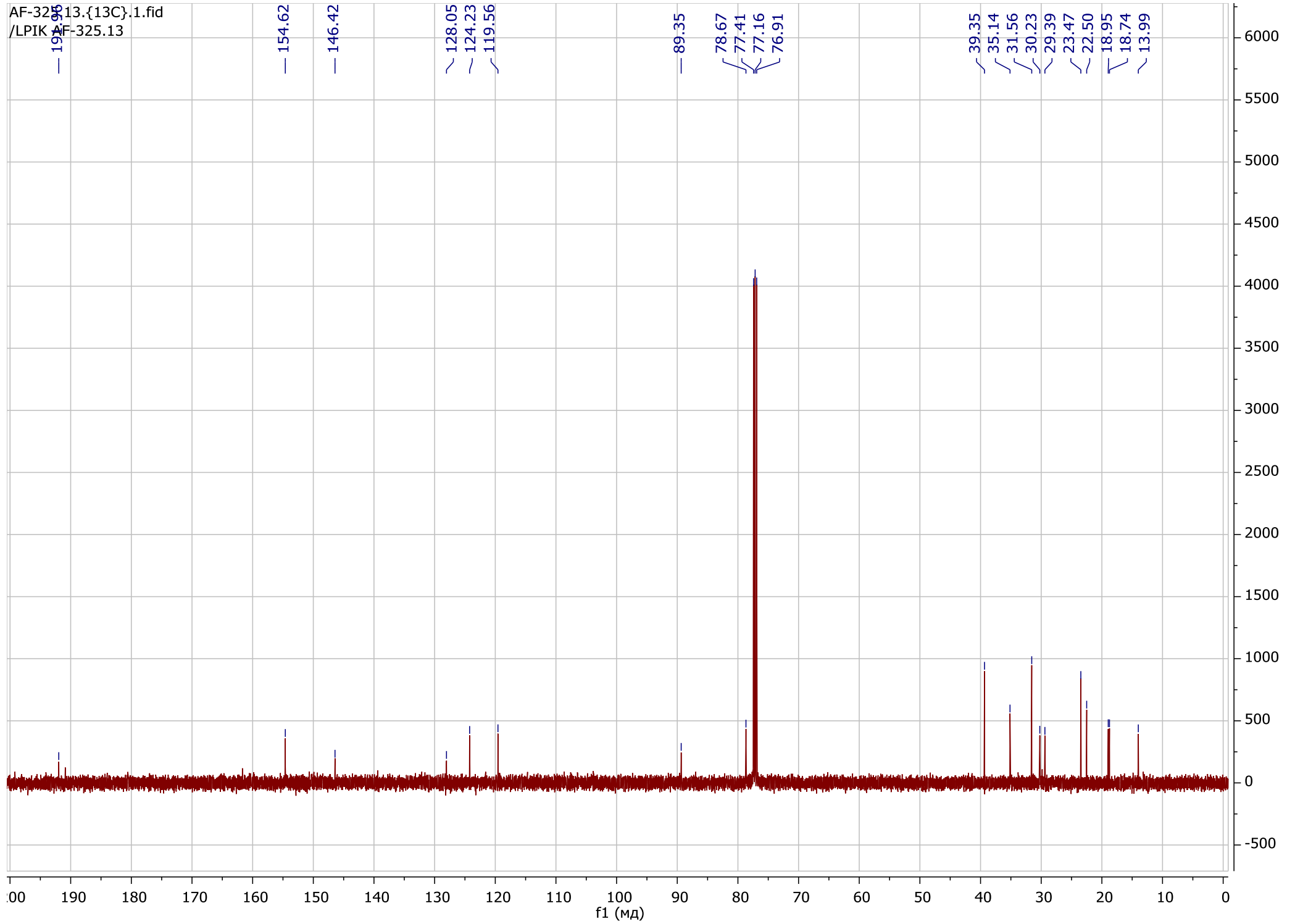
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Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	3200 V	Set Dry Gas	4.0 l/min
Scan End	1650 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-325.{1H}.1.fid
NMR/50597758



AF-325.13.{13C}.1.fid
/LPIK AF-325.13



Display Report

Analysis Info

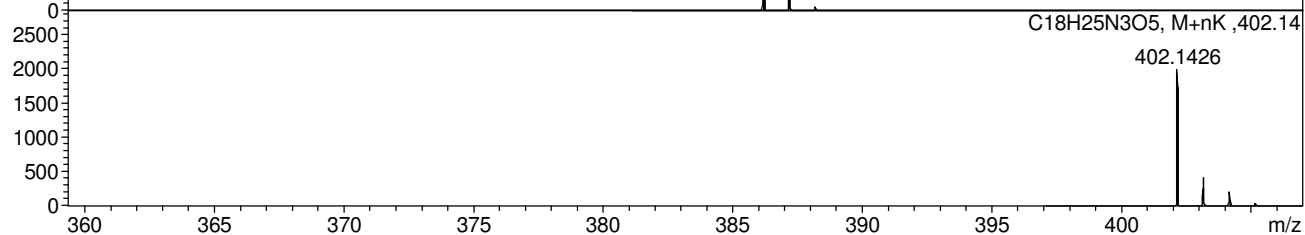
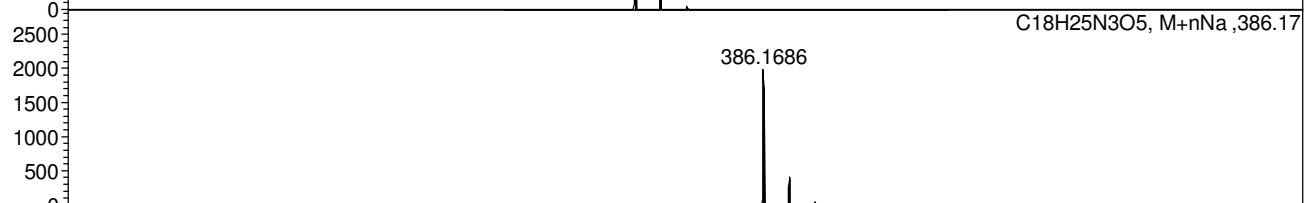
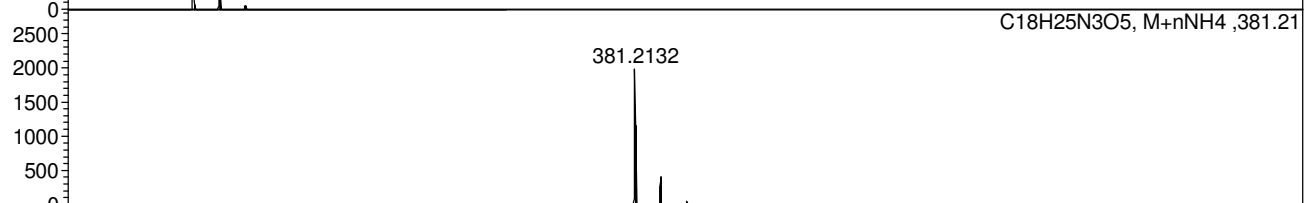
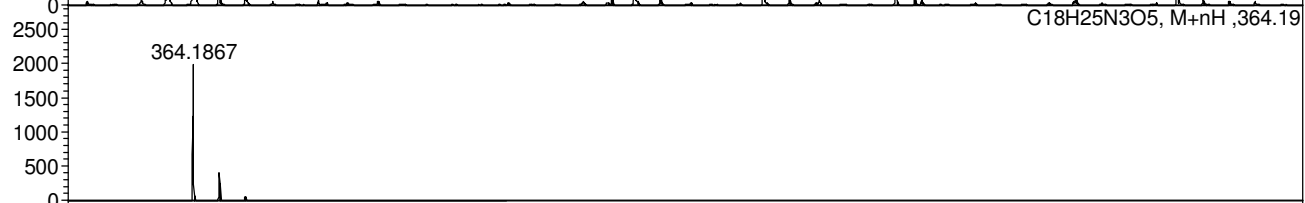
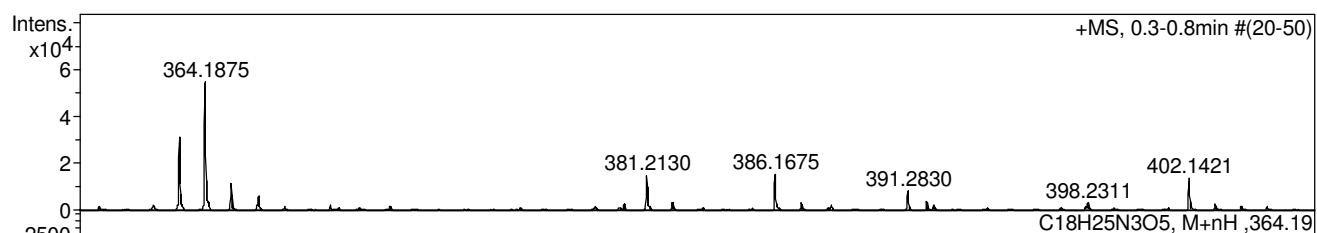
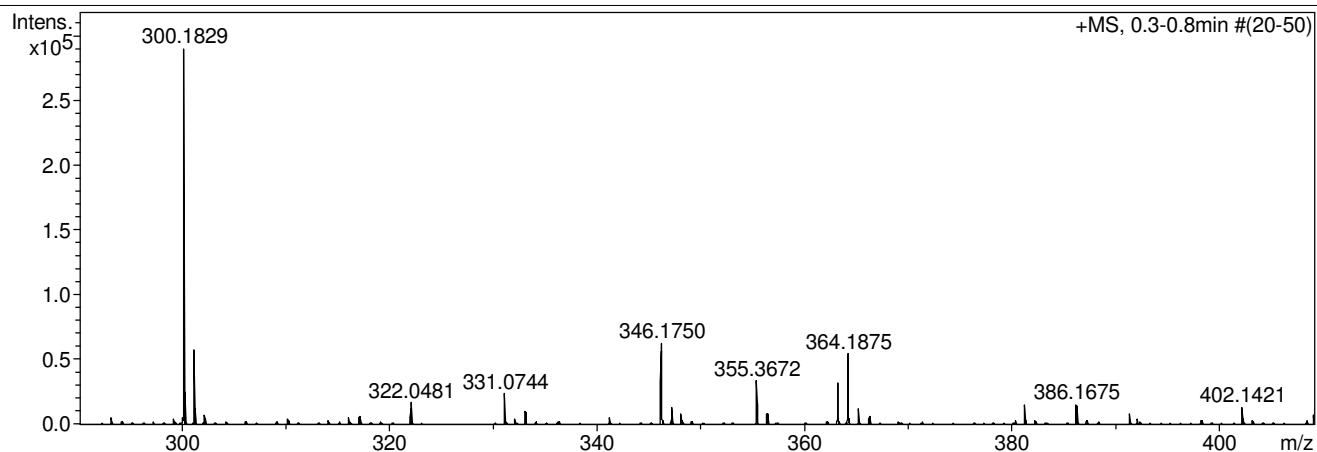
Analysis Name D:\Data\Kolotyrkina\2019\Bastrakov\1009018.d
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Sample Name /LPIK AF-325
Comment C18H25N3O5 mH 364.1866 calibrant added

Acquisition Date 09.10.2019 16:54:25

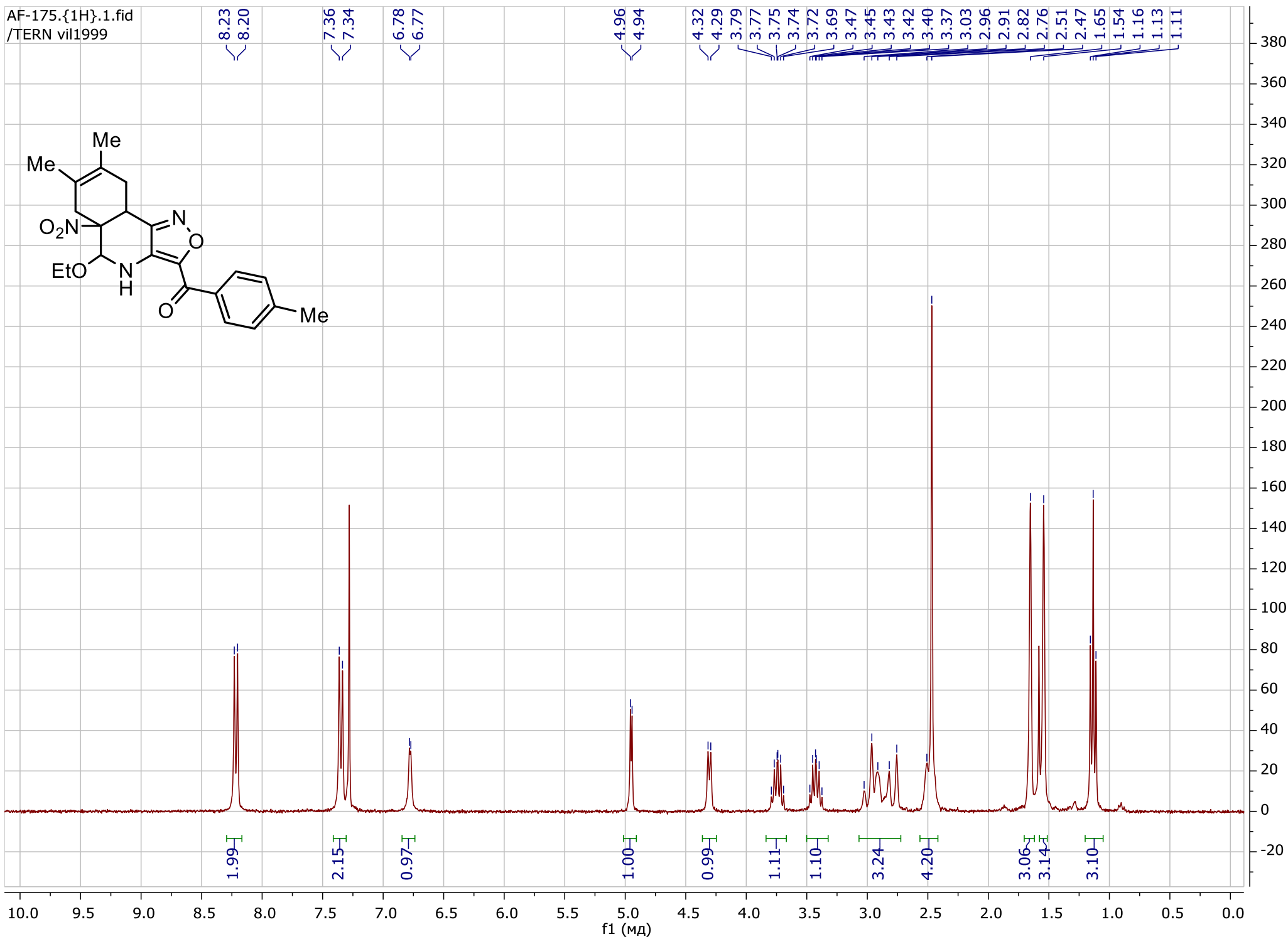
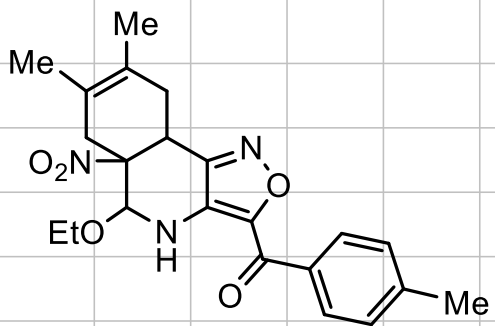
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

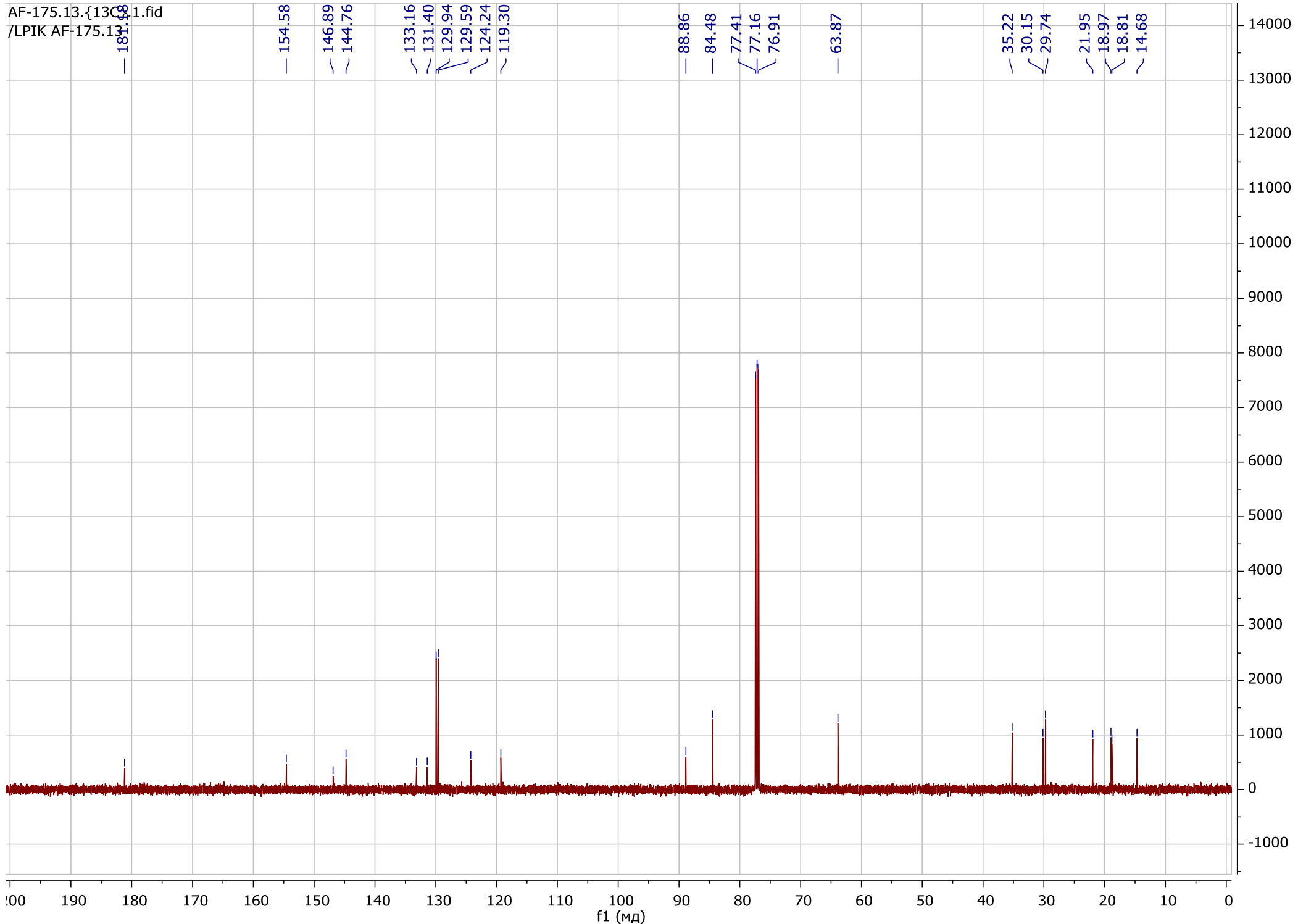
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



AF-175-¹H}.1.fid
/TERN vil1999



AF-175.13.{13C
/LPIK AF-175.13



Display Report

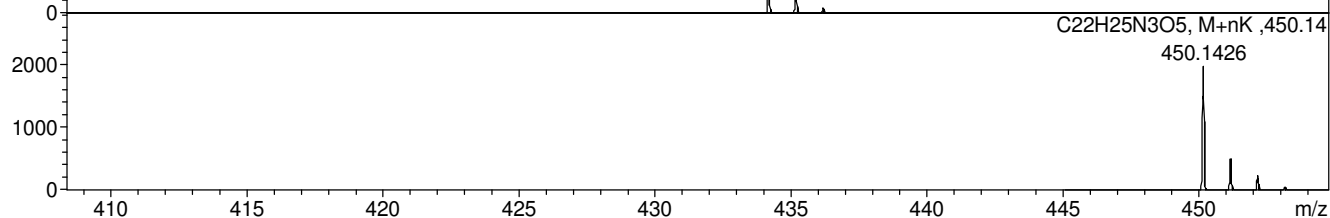
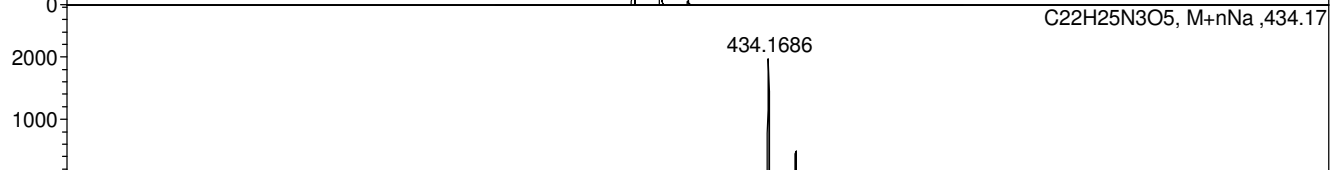
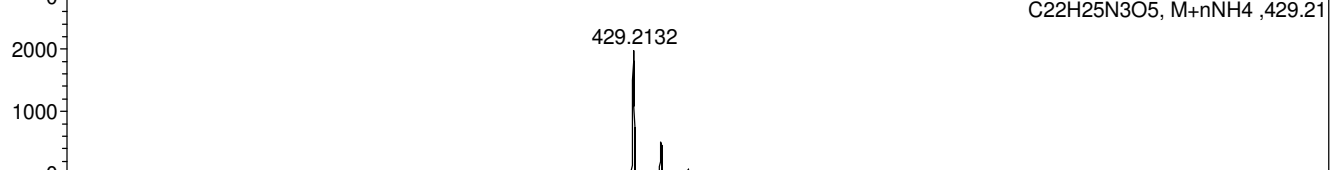
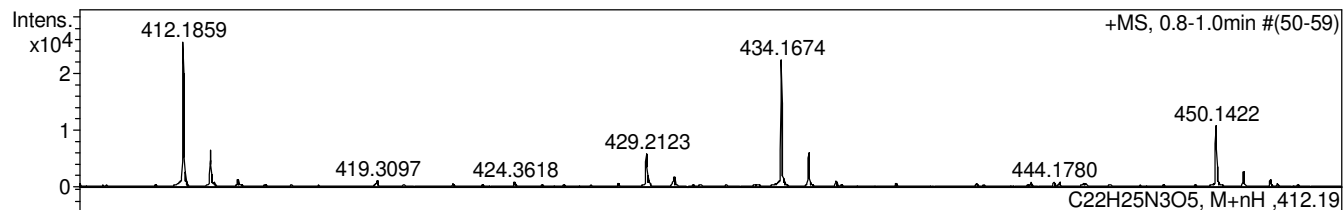
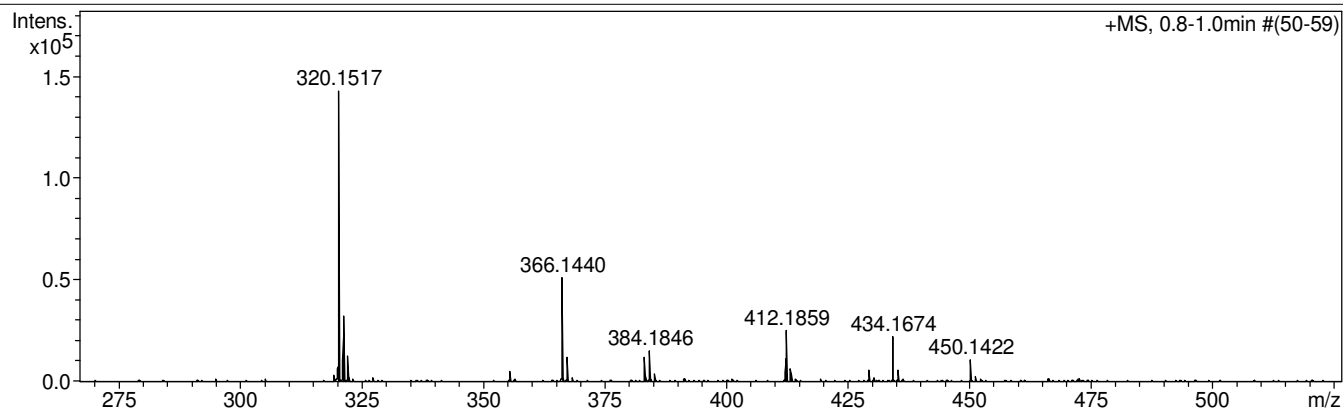
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2018\Bastrakov\0703002.d
Method tune_50-1600.m
Sample Name /LPIK AF-175
Comment C22H24N3O5 mH 412.1866 calibrant added

Acquisition Date 03.07.2018 10:33:01
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dnp-cc-ph

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: dnp-cc-ph

Bond precision: C-C = 0.0019 A Wavelength=0.71073

Cell: a=7.3210(4) b=7.1462(4) c=22.6111(13)
 alpha=90 beta=91.163(1) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	1182.71(11)	1182.71(11)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H7 N3 O4	C13 H7 N3 O4
Sum formula	C13 H7 N3 O4	C13 H7 N3 O4
Mr	269.22	269.22
Dx,g cm-3	1.512	1.512
Z	4	4
Mu (mm-1)	0.116	0.116
F000	552.0	552.0
F000'	552.30	
h,k,lmax	10,10,31	10,10,31
Nref	3448	3447
Tmin,Tmax	0.968,0.979	0.388,0.433
Tmin'	0.968	

Correction method= # Reported T Limits: Tmin=0.388 Tmax=0.433
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 29.995

R(reflections)= 0.0396(2321) wR2(reflections)= 0.0889(3447)

S = 1.006 Npar= 181

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● Alert level CPLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.568 Report

● Alert level G

PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C8	--C9	.	6.0	s.u.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond	C2	- C7	.	1.43	Ang.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond	C8	- C9	.	1.44	Ang.
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				1	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...				6	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				14	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by				1	Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-

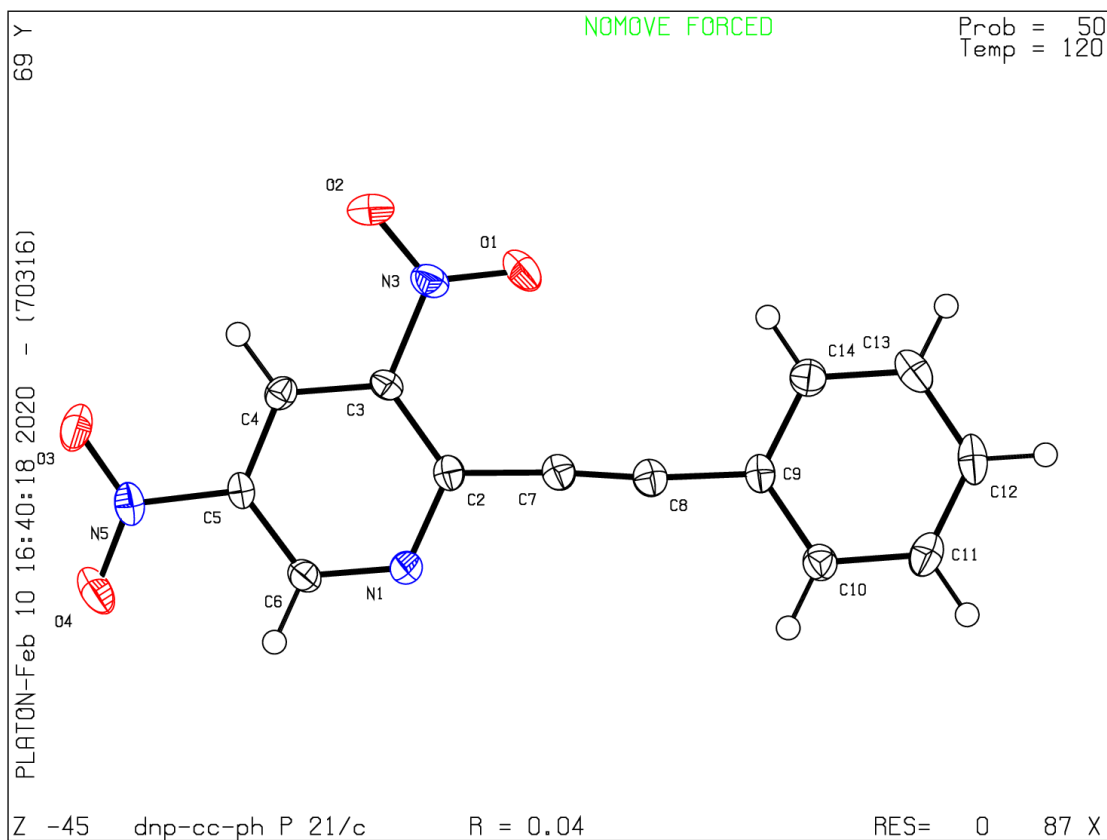
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dnp-cc-phf

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: dnp-cc-phf

Bond precision: C-C = 0.0019 A Wavelength=0.71073

Cell: a=7.2818(5) b=7.1802(4) c=22.6490(14)
 alpha=90 beta=90.592(1) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	1184.14(13)	1184.13(13)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H6 F N3 O4	C13 H6 F N3 O4
Sum formula	C13 H6 F N3 O4	C13 H6 F N3 O4
Mr	287.21	287.21
Dx,g cm-3	1.611	1.611
Z	4	4
Mu (mm-1)	0.133	0.133
F000	584.0	584.0
F000'	584.36	
h,k,lmax	10,10,31	10,10,31
Nref	3454	3454
Tmin,Tmax	0.947,0.961	0.810,0.862
Tmin'	0.946	

Correction method= # Reported T Limits: Tmin=0.810 Tmax=0.862
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 29.997

R(reflections)= 0.0438(2424) wR2(reflections)= 0.0992(3454)

S = 1.033 Npar= 190

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● **Alert level C**

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.595 Check

● **Alert level G**

PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C2 - C7 . 1.43 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C8 - C9 . 1.43 Ang.
PLAT960_ALERT_3_G Number of Intensities with $I < - 2*\text{sig}(I)$... 5 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 12 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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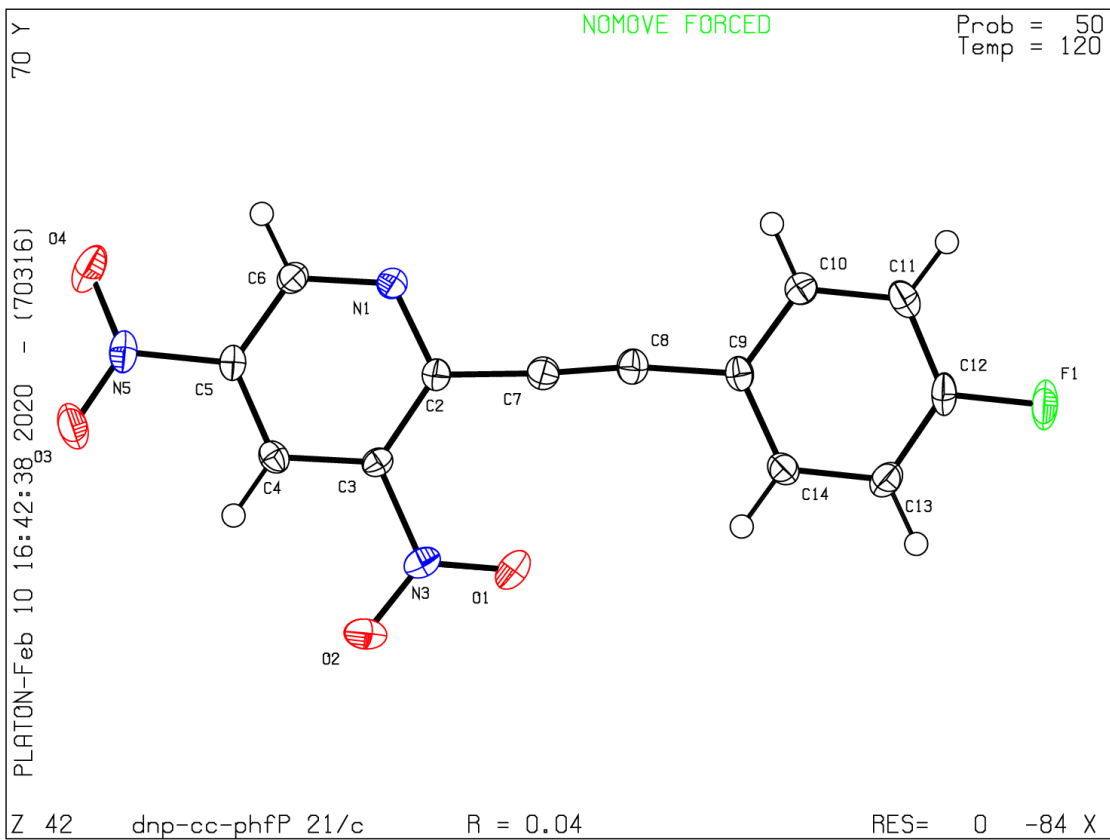
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

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PLATON version of 22/12/2019; check.def file version of 13/12/2019



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ka-14

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: ka-14

Bond precision: C-C = 0.0023 A Wavelength=0.71073

Cell: a=6.6772(4) b=7.2749(4) c=25.0344(14)
 alpha=90 beta=90 gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	1216.07(12)	1216.07(12)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C14 H9 N3 O4	C14 H9 N3 O4
Sum formula	C14 H9 N3 O4	C14 H9 N3 O4
Mr	283.24	283.24
Dx,g cm-3	1.547	1.547
Z	4	4
Mu (mm-1)	0.117	0.117
F000	584.0	584.0
F000'	584.31	
h,k,lmax	9,10,35	9,10,35
Nref	3546[2069]	3548
Tmin,Tmax	0.970,0.979	0.832,0.862
Tmin'	0.969	

Correction method= # Reported T Limits: Tmin=0.832 Tmax=0.862
AbsCorr = MULTI-SCAN

Data completeness= 1.71/1.00 Theta(max)= 29.996

R(reflections)= 0.0357(3328) wR2(reflections)= 0.0920(3548)

S = 1.028 Npar= 191

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● Alert level G

PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	14 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

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1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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Publication of your CIF in other journals

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PLATON version of 22/12/2019; check.def file version of 13/12/2019

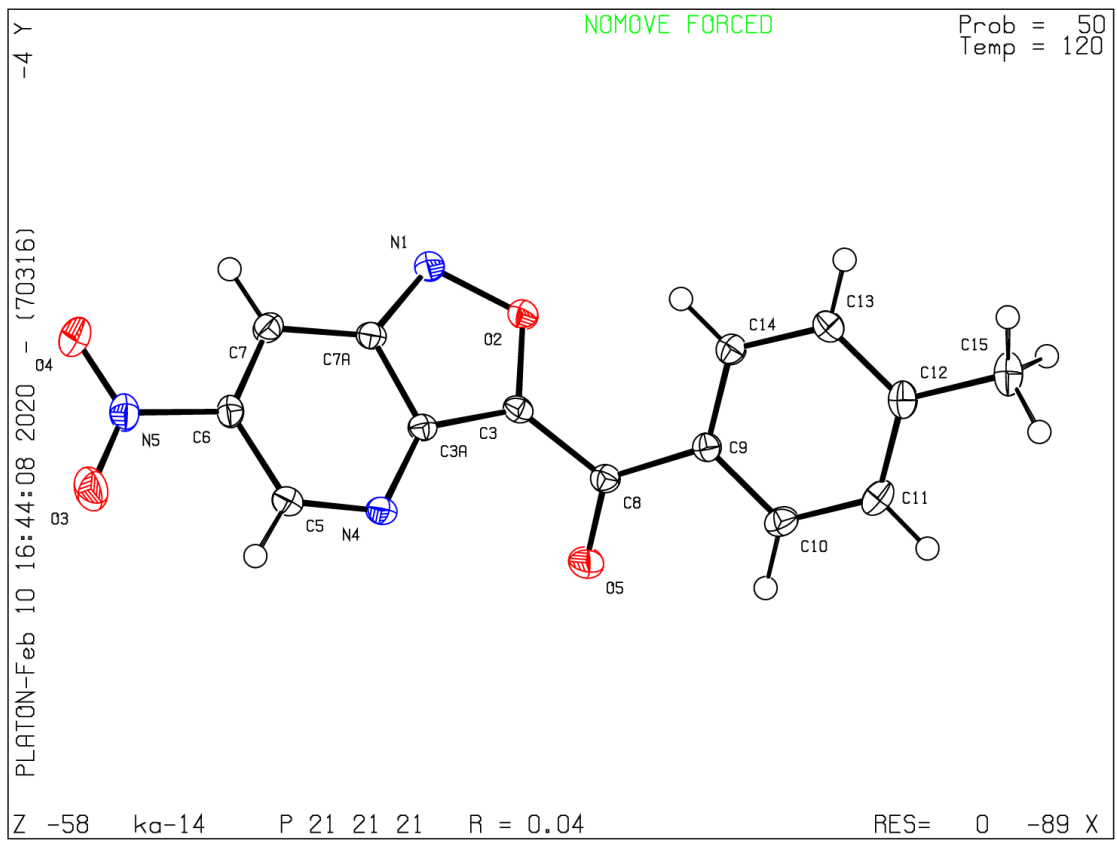


Table 3. Crystallographic data for **2a**, **2c** and **3b**.

	2a	2c	3b
CCDC	1983532	1983530	1983531
Formula	C ₁₃ H ₇ N ₃ O ₄	C ₁₃ H ₆ FN ₃ O ₄	C ₁₄ H ₉ N ₃ O ₄
Formula weight	269.22	287.21	283.24
<i>T</i> , K	120	120	120
Crystal system	monoclinic	monoclinic	orthorhombic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>Z</i> / <i>Z'</i>	4 / 1	4 / 1	4 / 1
<i>a</i> , Å	7.3210(4)	7.2818(5)	6.6772(4)
<i>b</i> , Å	7.1462(4)	7.1802(4)	7.2749(4)
<i>c</i> , Å	22.6111(13)	22.6490(14)	25.0344(14)
β , °	91.1630(10)	90.5920(10)	
<i>V</i> , Å ³	1182.71(11)	1184.13(13)	1216.07(12)
<i>d</i> _{calc} , g cm ⁻³	1.512	1.611	1.547
μ , cm ⁻¹	1.16	1.33	1.17
2 θ _{max} , °	60	60	60
Reflns. collected / independent	19354 / 3447	14535 / 3454	16184 / 3548
Observed reflections [<i>I</i> >2 σ (<i>I</i>)]	2321	2424	3328
<i>R</i> ₁	0.0396	0.0438	0.0357
<i>wR</i> ₂	0.0889	0.0992	0.0920
GOF	1.006	1.033	1.028
Residual density, e Å ⁻³ (<i>d</i> _{max} / <i>d</i> _{min})	0.303/-0.234	0.395/-0.238	0.396/-0.238