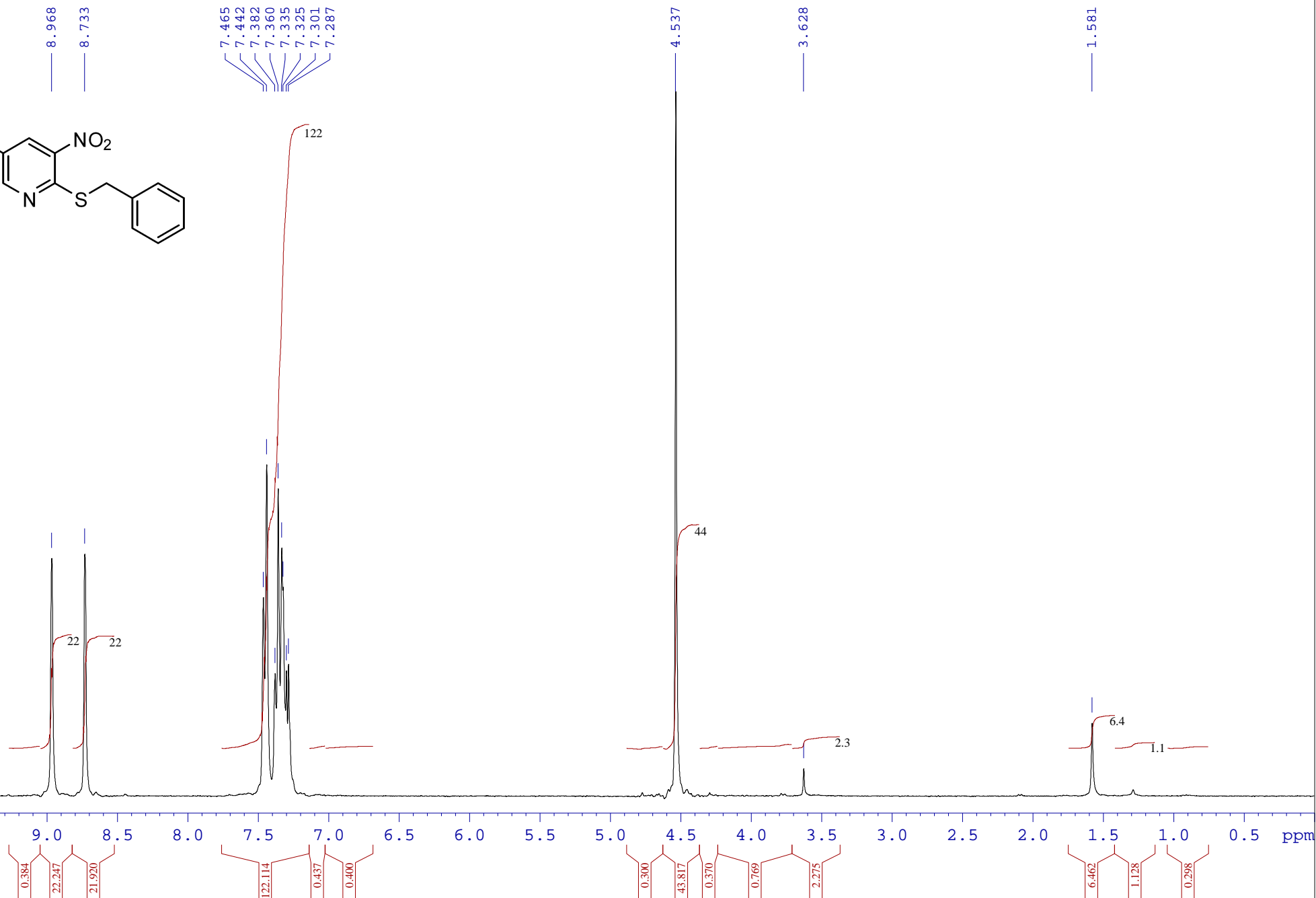
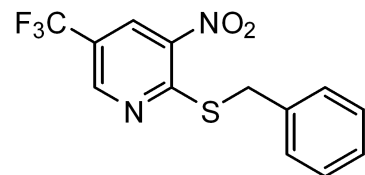


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NMR and HRMS spectra for 4h	S77-S79
NMR and HRMS spectra for 4i	S80-S82
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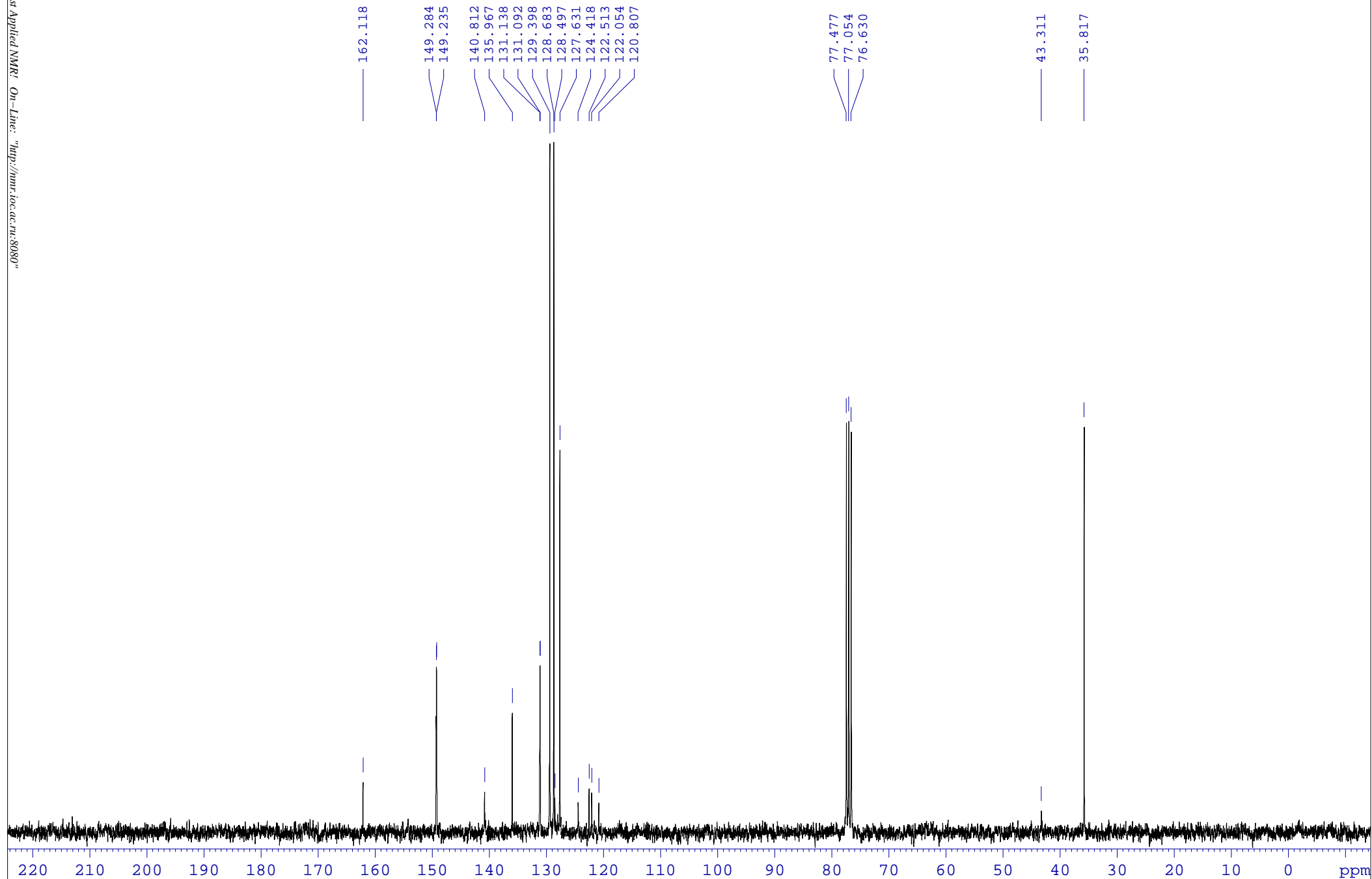


/LPIK AF-363





/LPIK AF-363.13 Kokorekin-20259



Display Report

Analysis Info

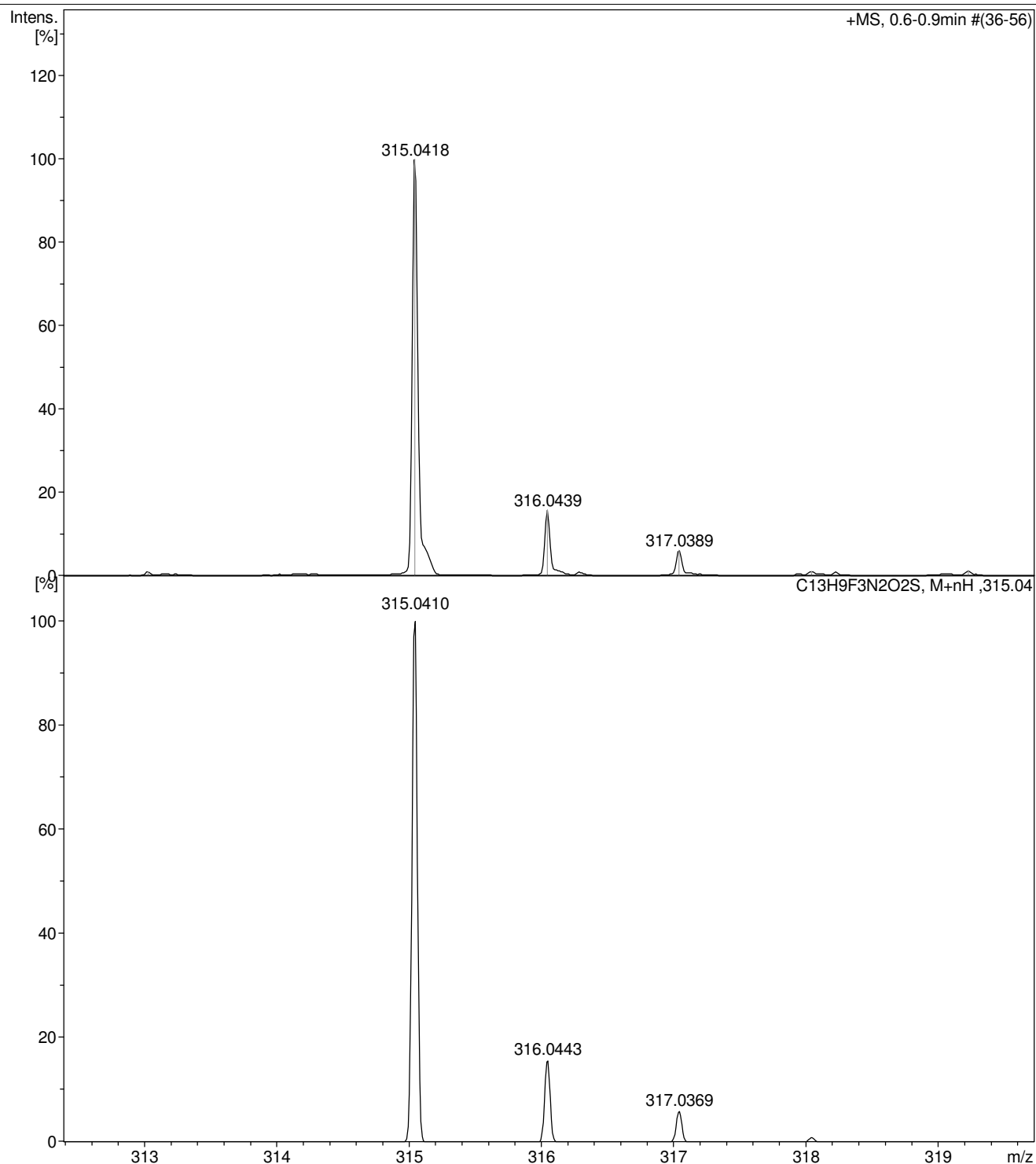
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0210024.d
Method tune_50-1600.m
Sample Name /LPIK AF-363
Comment C13H9F3N2O2S mH 315.0409 calibrant added CH3OH

Acquisition Date 10.02.2021 20:12:35

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

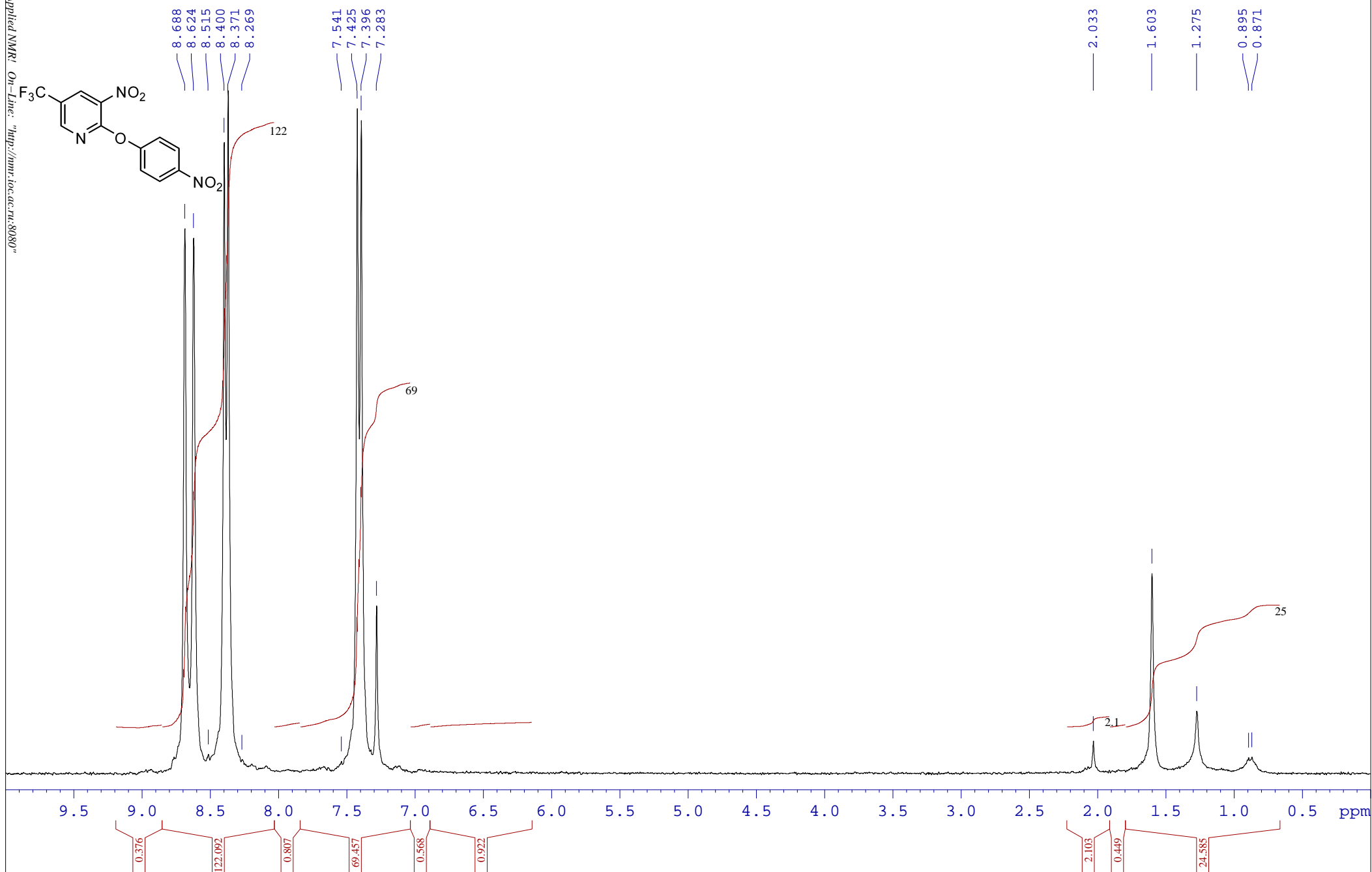
Acquisition Parameter

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



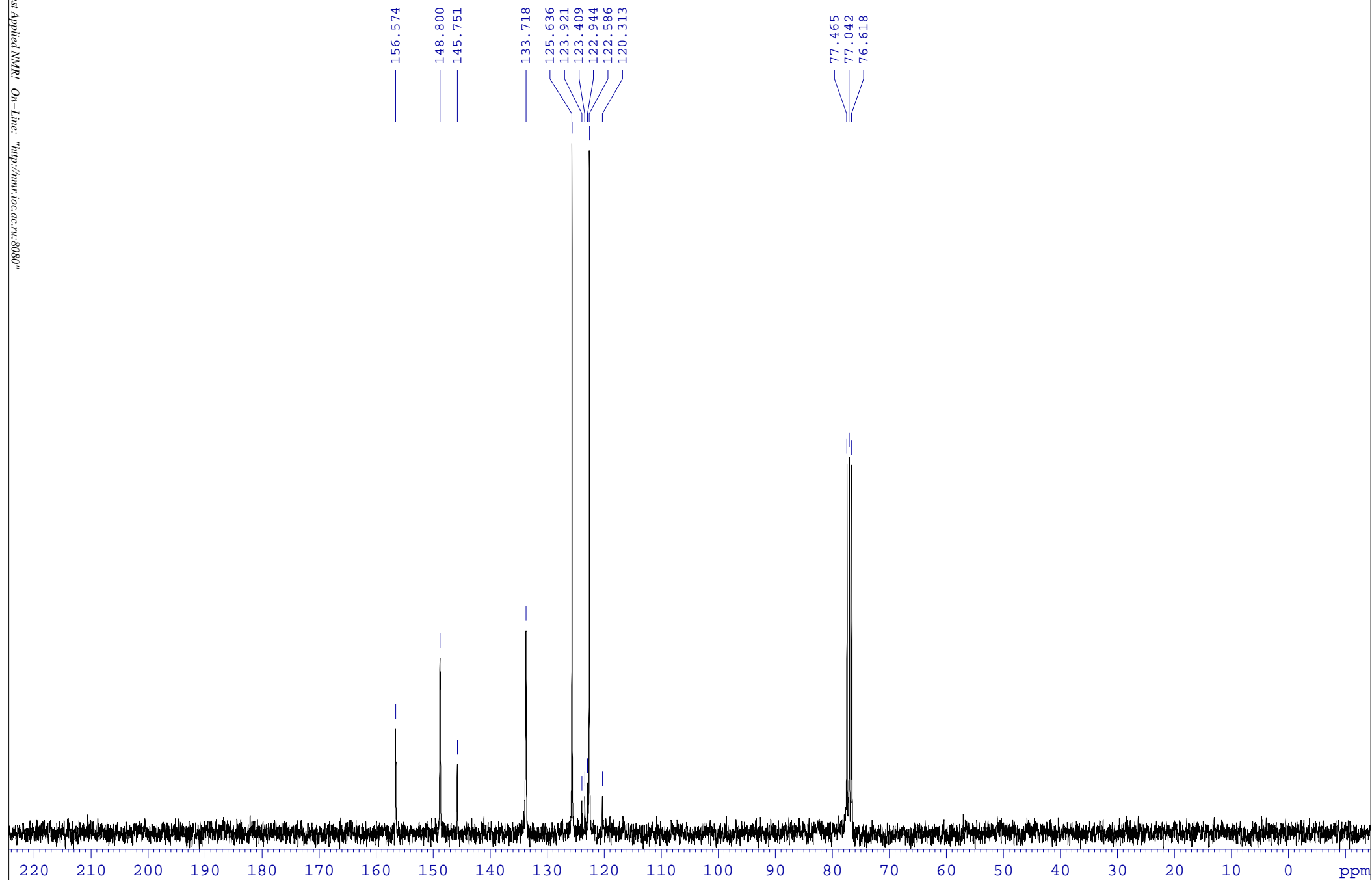


/LPIK AF-364





/LPIK AF-364.13 Kokorekin-20259



Display Report

Analysis Info

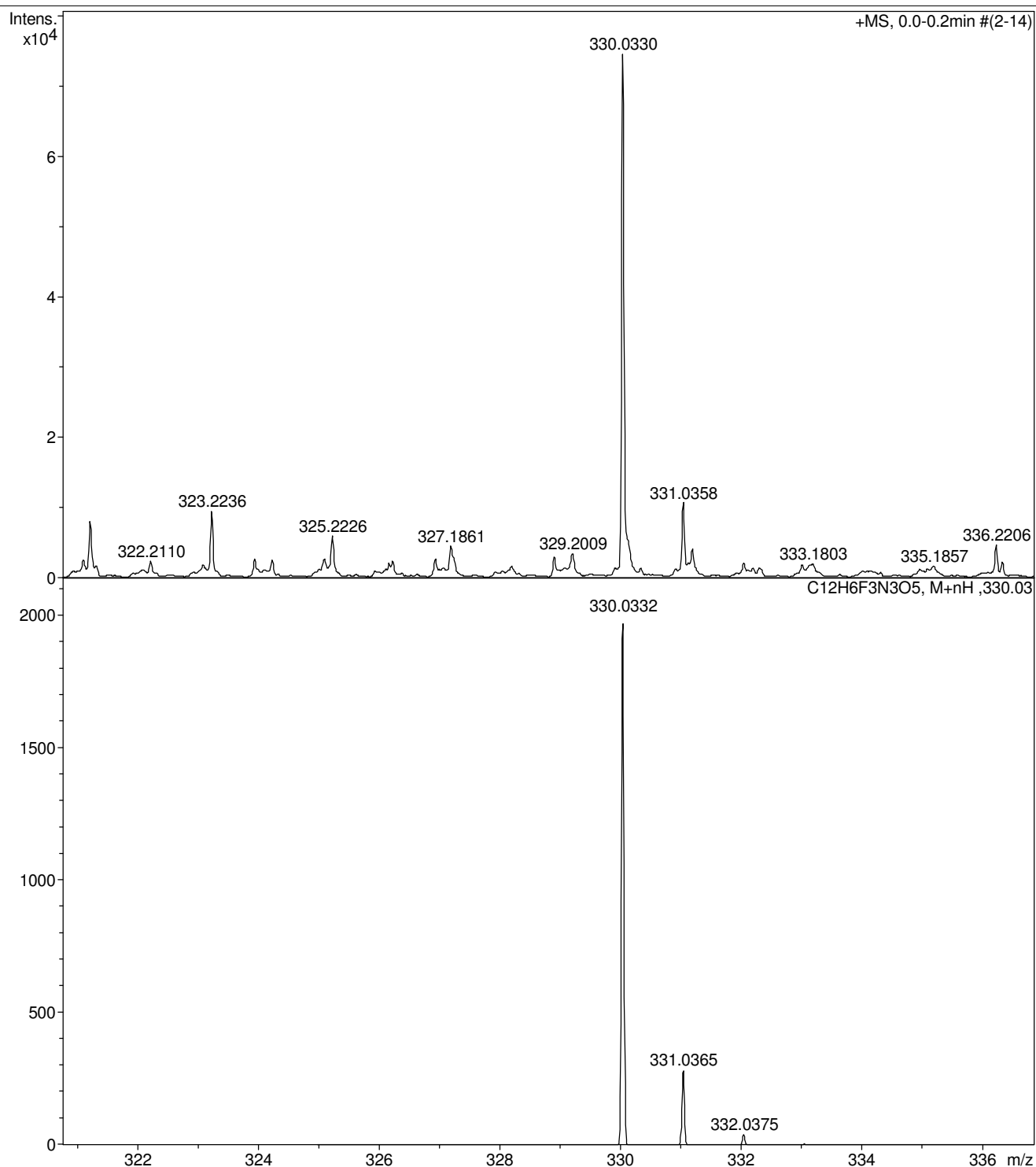
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0211019.d
Method tune_50-1600.m
Sample Name /LPIK AF-364
Comment C12H6F3N3O5 mH 330.0332 alibrant added CH3OH

Acquisition Date 11.02.2021 12:34:23

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



Display Report

Analysis Info

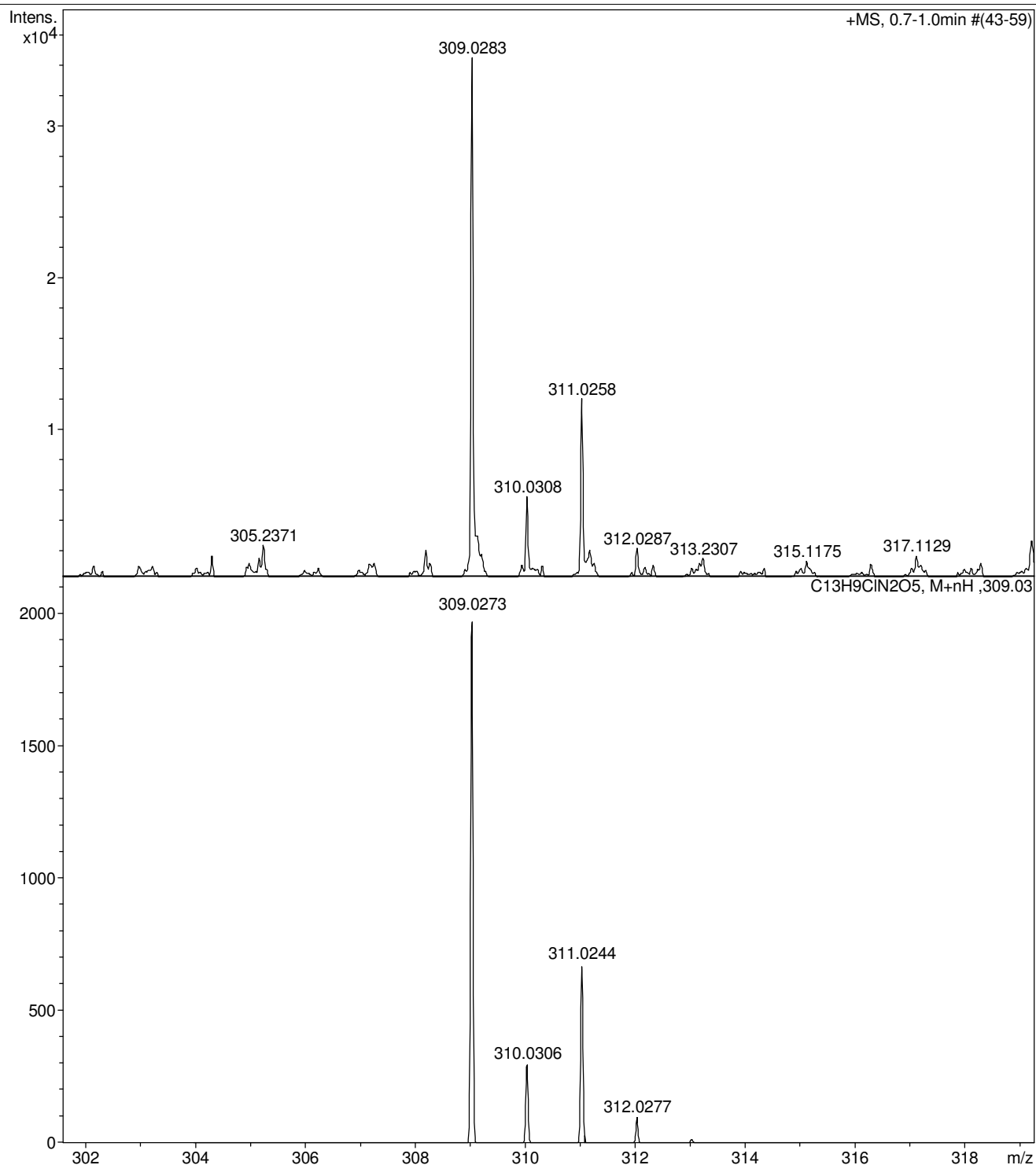
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Method tune_50-1600.m
Sample Name /LPIK AF-364
Comment C13H9CIN2O5 mH 309.0272 alibrant added CH3OH

Acquisition Date 11.02.2021 12:40:15

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

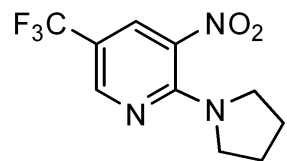
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Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





/LPIK AF-369



8.545

8.306

7.287

3.473

2.079

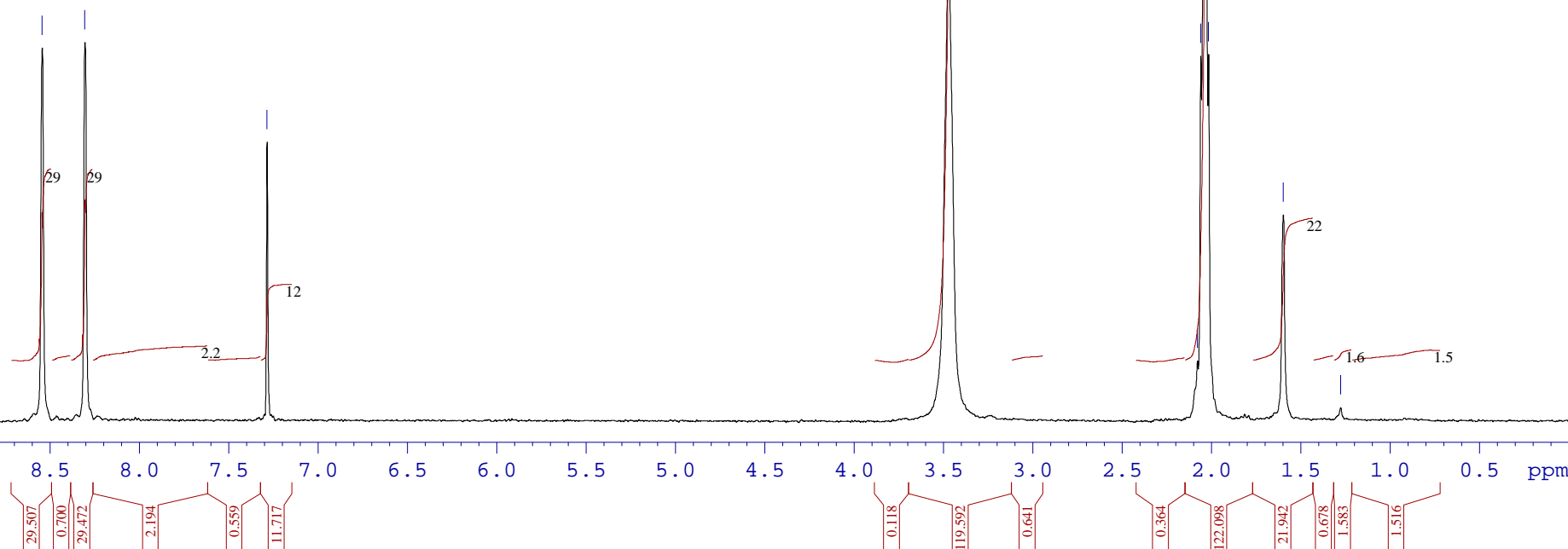
2.061

2.039

2.017

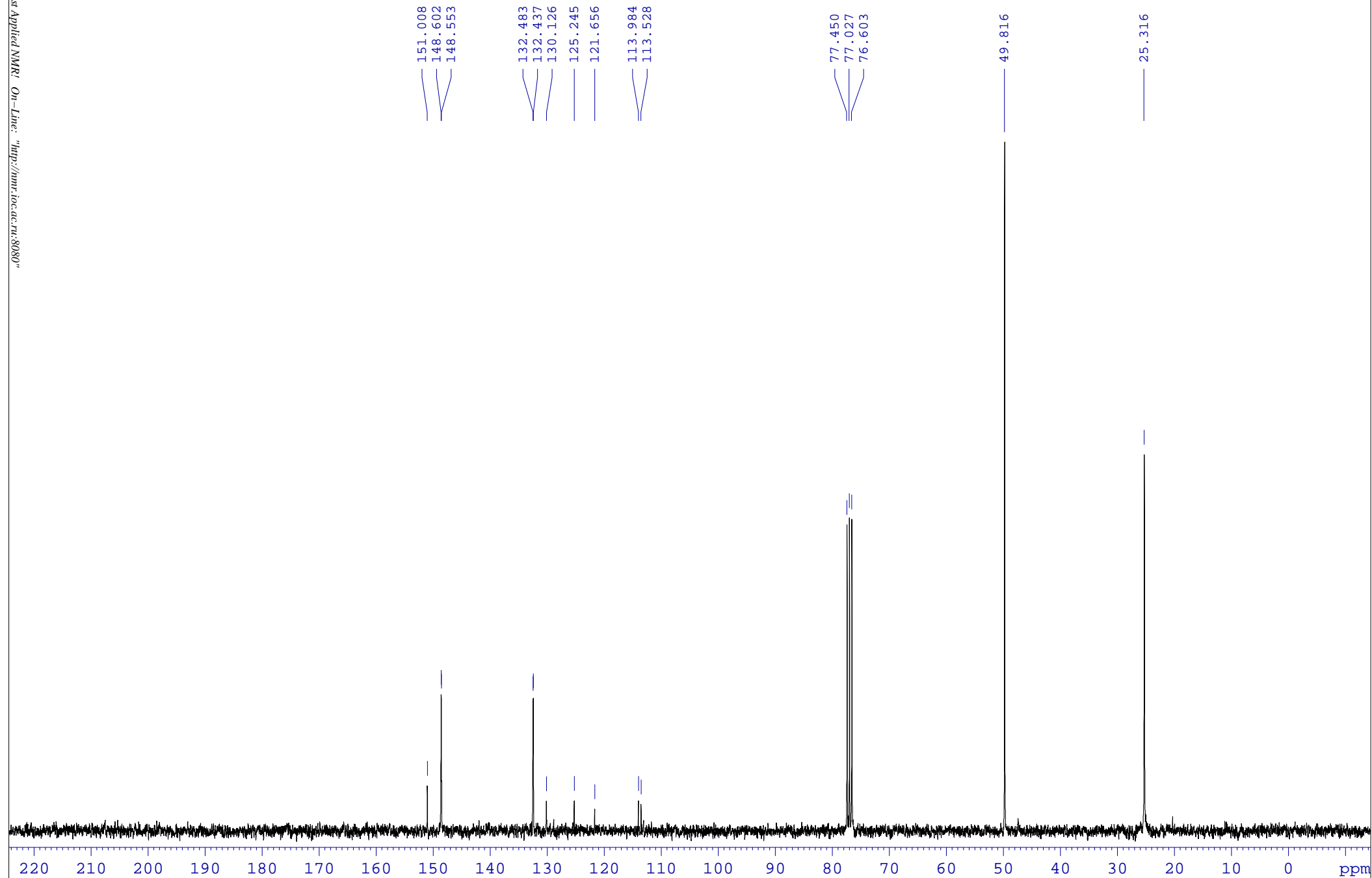
1.599

1.277





/LPIK AF-369.13 Kokorekin-20259



Display Report

Analysis Info

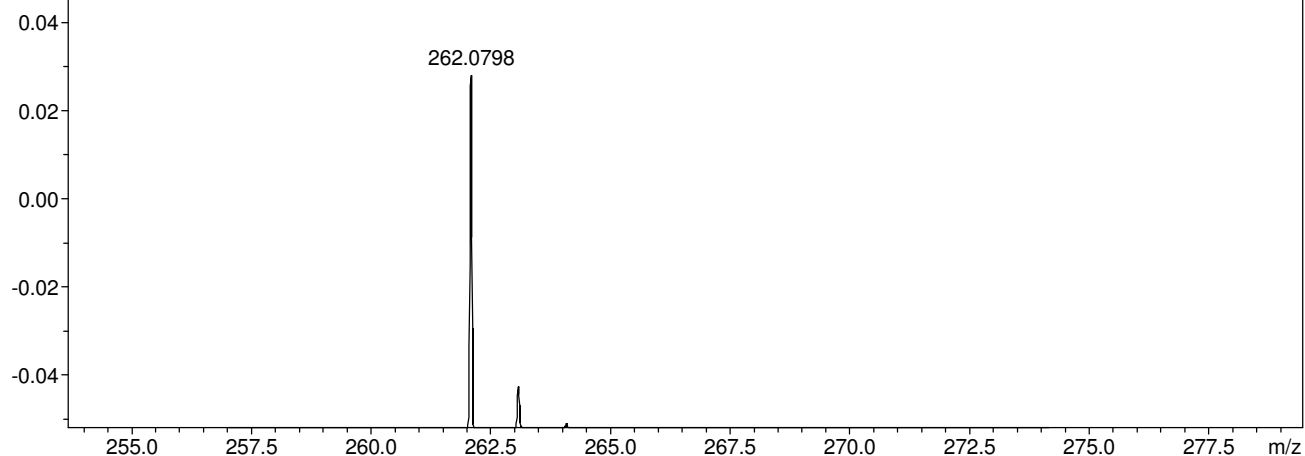
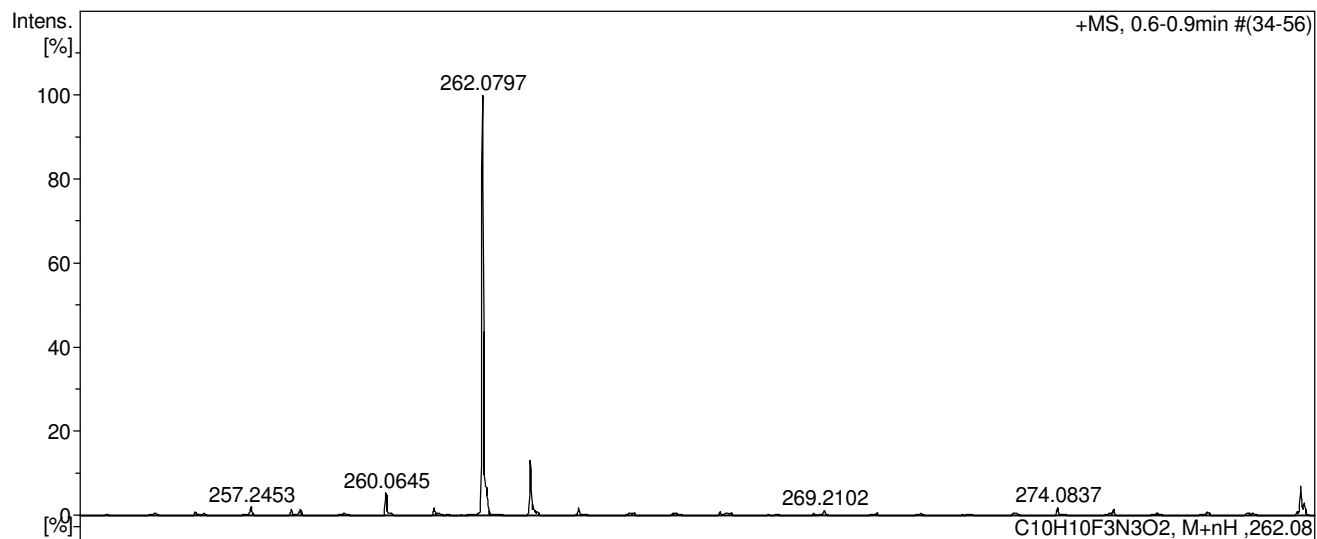
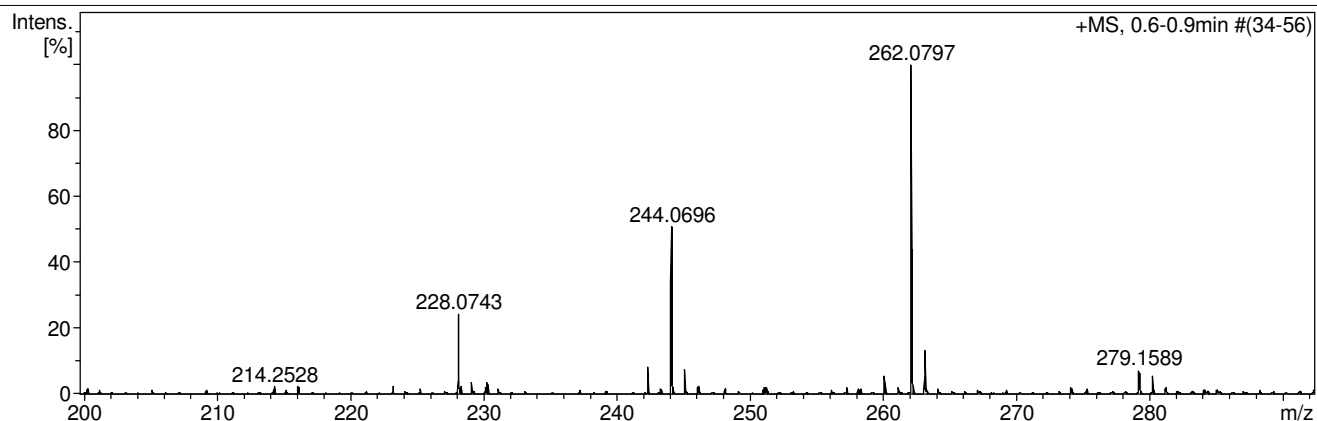
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Method tune_50-1600.m
Sample Name /LPIK AF-369
Comment C10H10F3N3O2 mH 262.0797 calibrant added CH3CN

Acquisition Date 10.02.2021 20:24:40

Operator BDAL@DE
Instrument / Ser# microTOF 10248

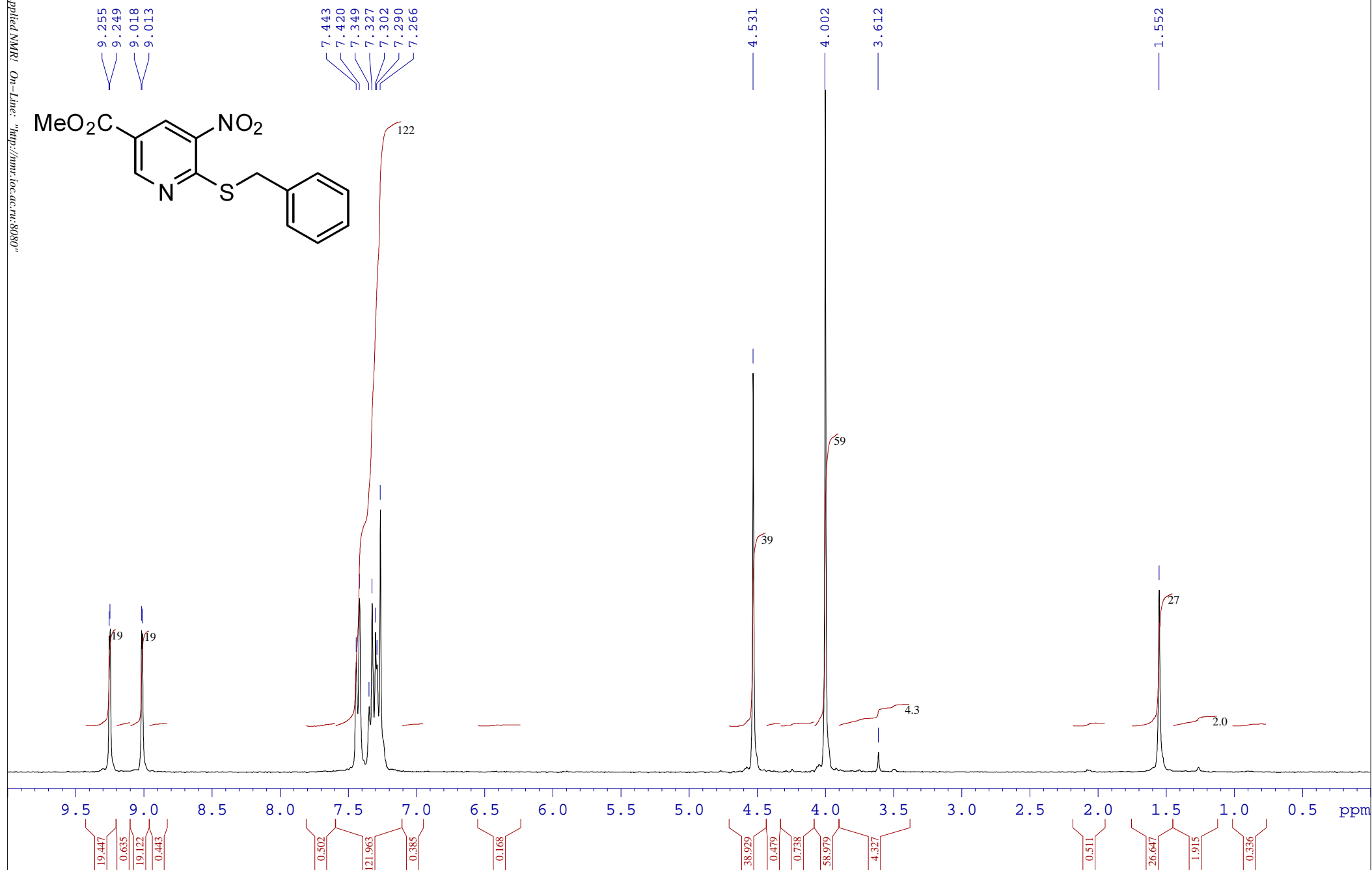
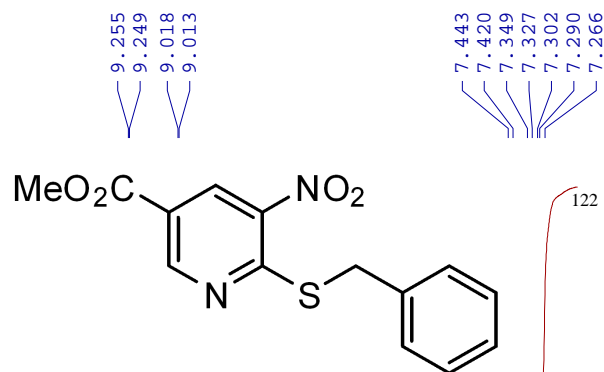
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Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





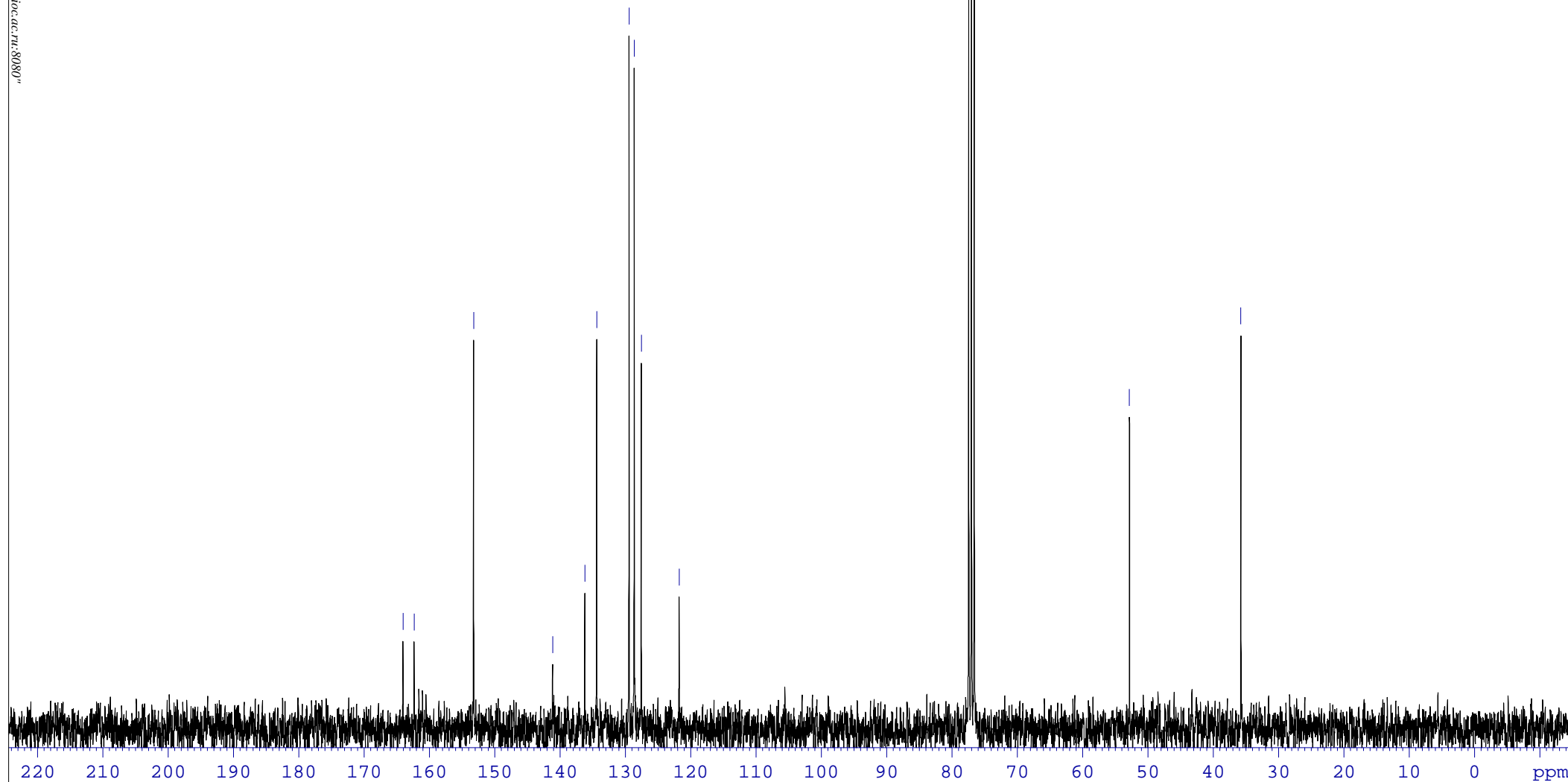
/LPIK AF-386





/LPIK AF-386.13 Kokorekin-20259

164.031
162.331
153.218
141.124
136.197
134.378
129.423
128.638
127.544
121.757
77.477
77.053
76.630
52.861
35.800



Display Report

Analysis Info

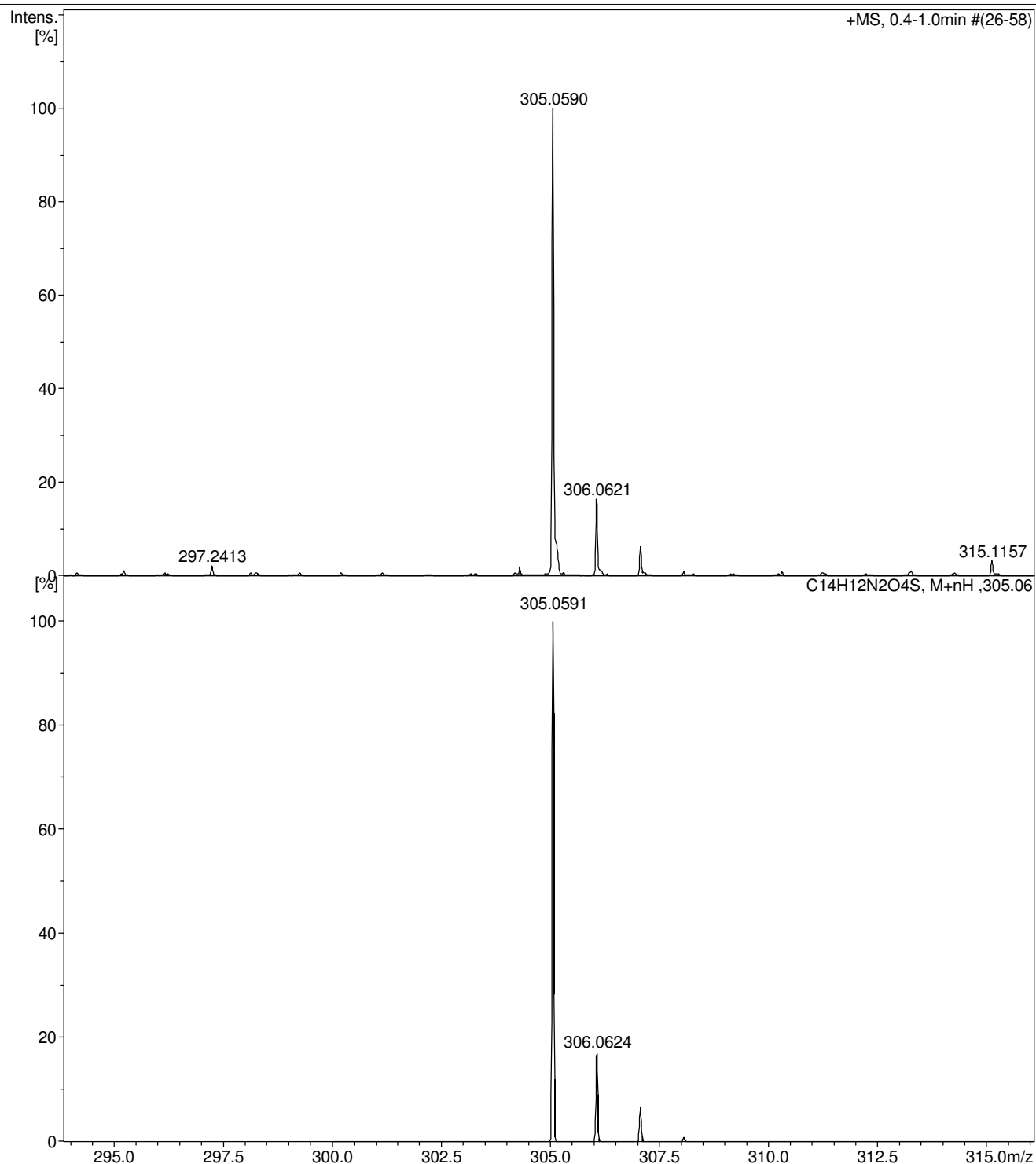
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Method tune_50-1600.m
Sample Name /LPIK AF-386
Comment C14H12N2O4S mH 305.050 calibrant added CH3CN

Acquisition Date 10.02.2021 20:41:38

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

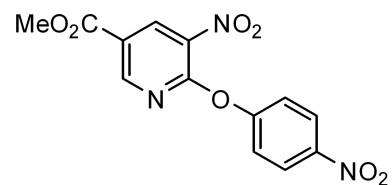
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Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





/LPIK AF-389



8.966
8.926
8.921

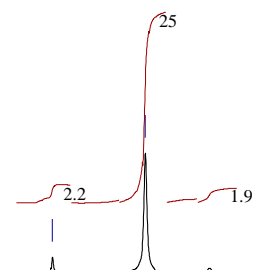
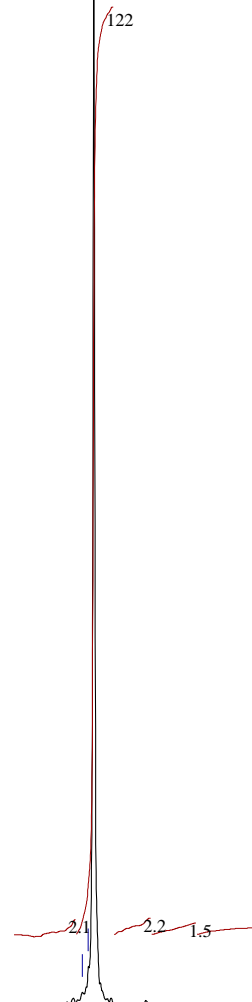
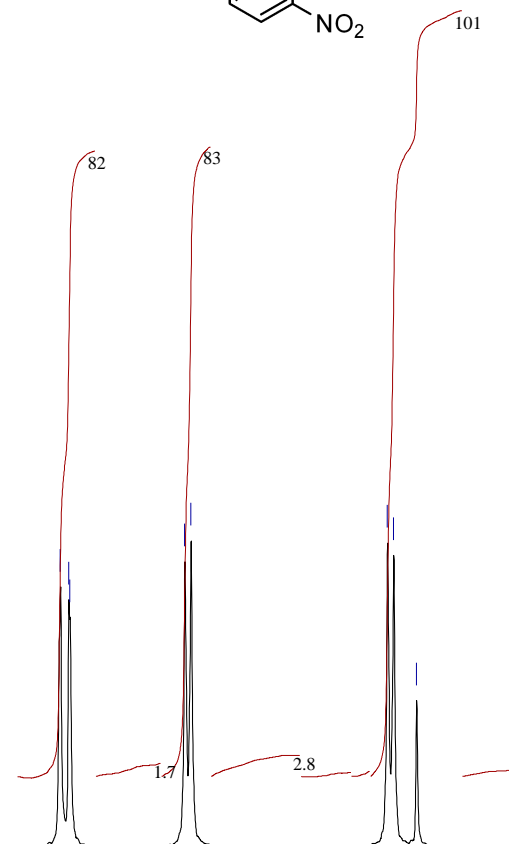
8.373
8.343

7.405
7.375
7.265

4.052
4.025
3.999

2.009

1.565



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 ppm

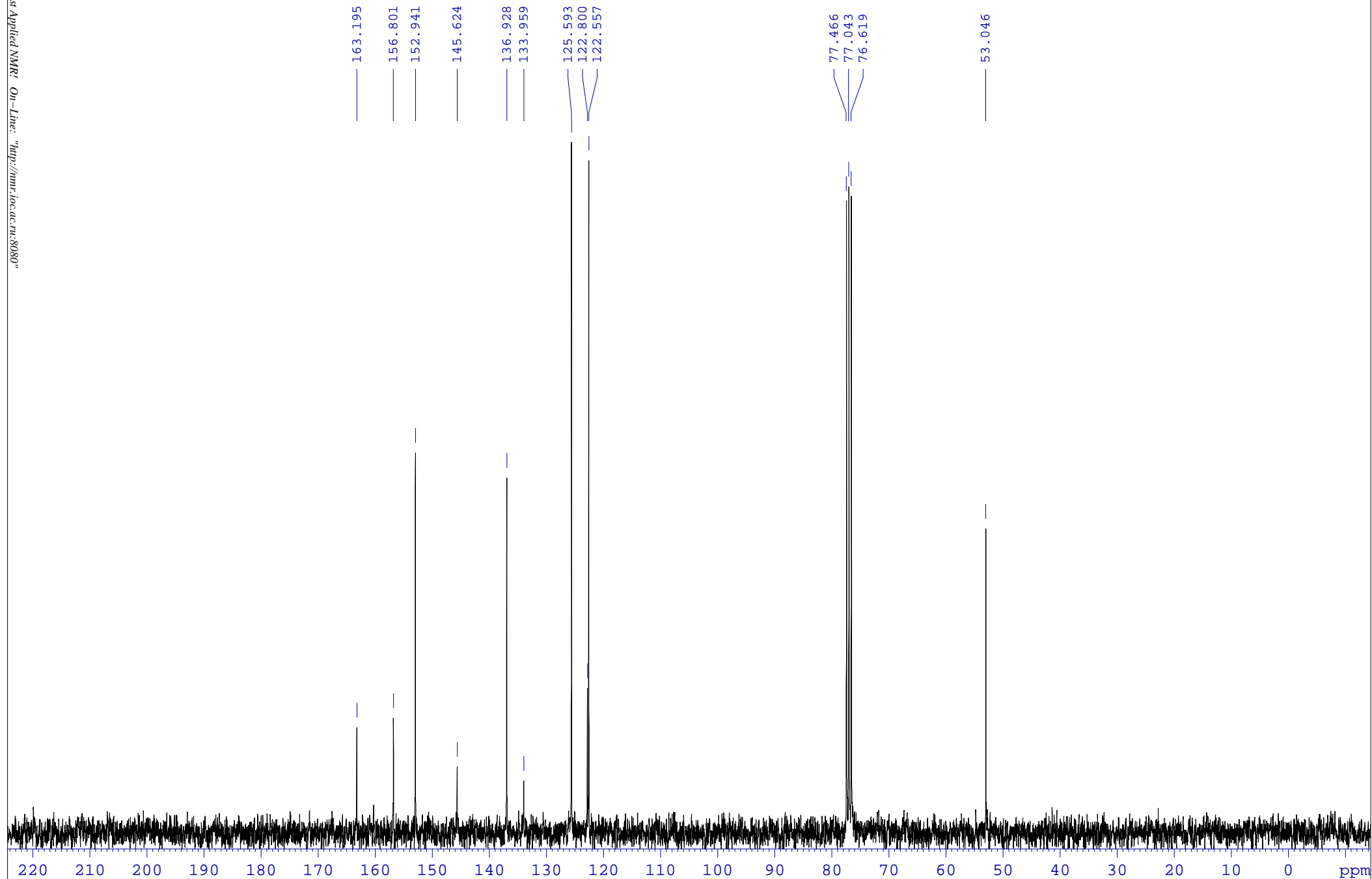
82.266
1.728
82.813
2.773
0.525
0.672
100.758
0.806

1.983
122.007
2.162
1.523
0.910

2.310
0.315
25.032
0.504
1.827



/LPIK AF-389.13 Kokorekin-20259



Display Report

Analysis Info

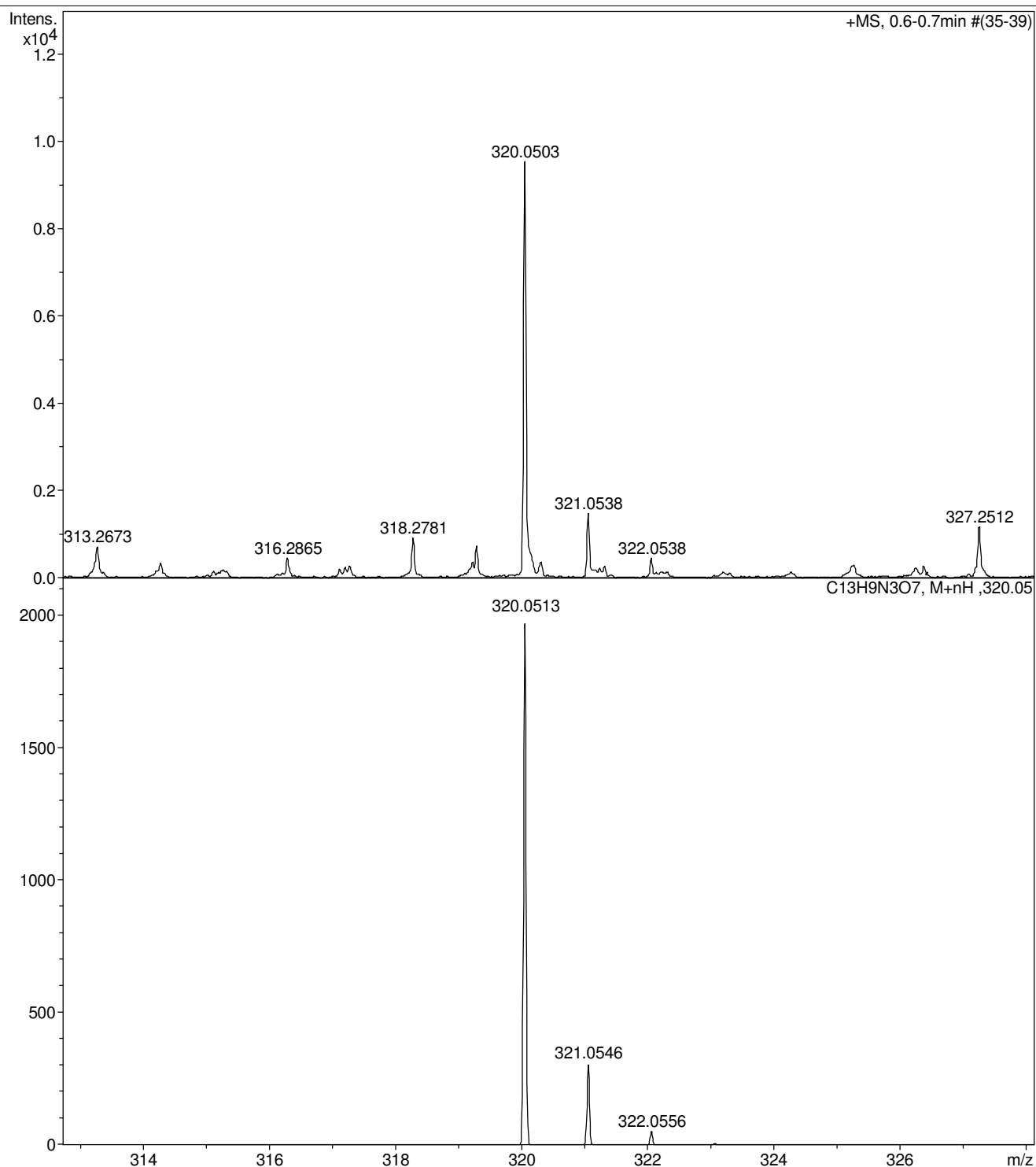
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Method tune_50-1600.m
Sample Name /LPIK AF-389
Comment C13H9N3O7 mH 320.0543calibrant added CH3CN

Acquisition Date 10.02.2021 20:47:05

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

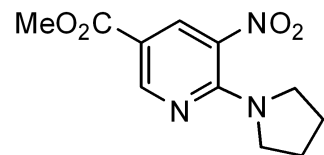
Acquisition Parameter

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





/LPIK AF-391



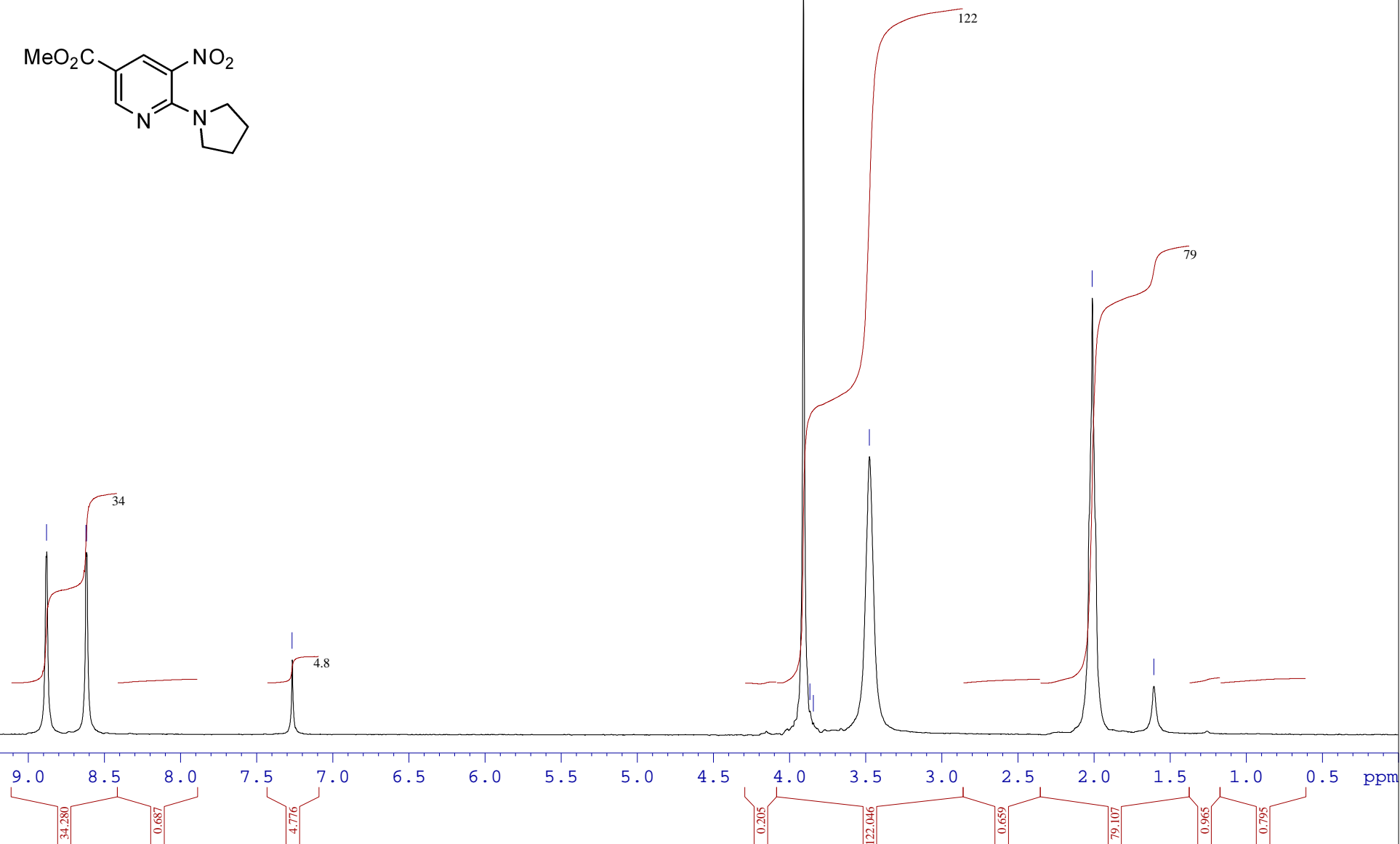
8.880
8.622
8.617

7.268

3.910
3.866
3.844
3.476

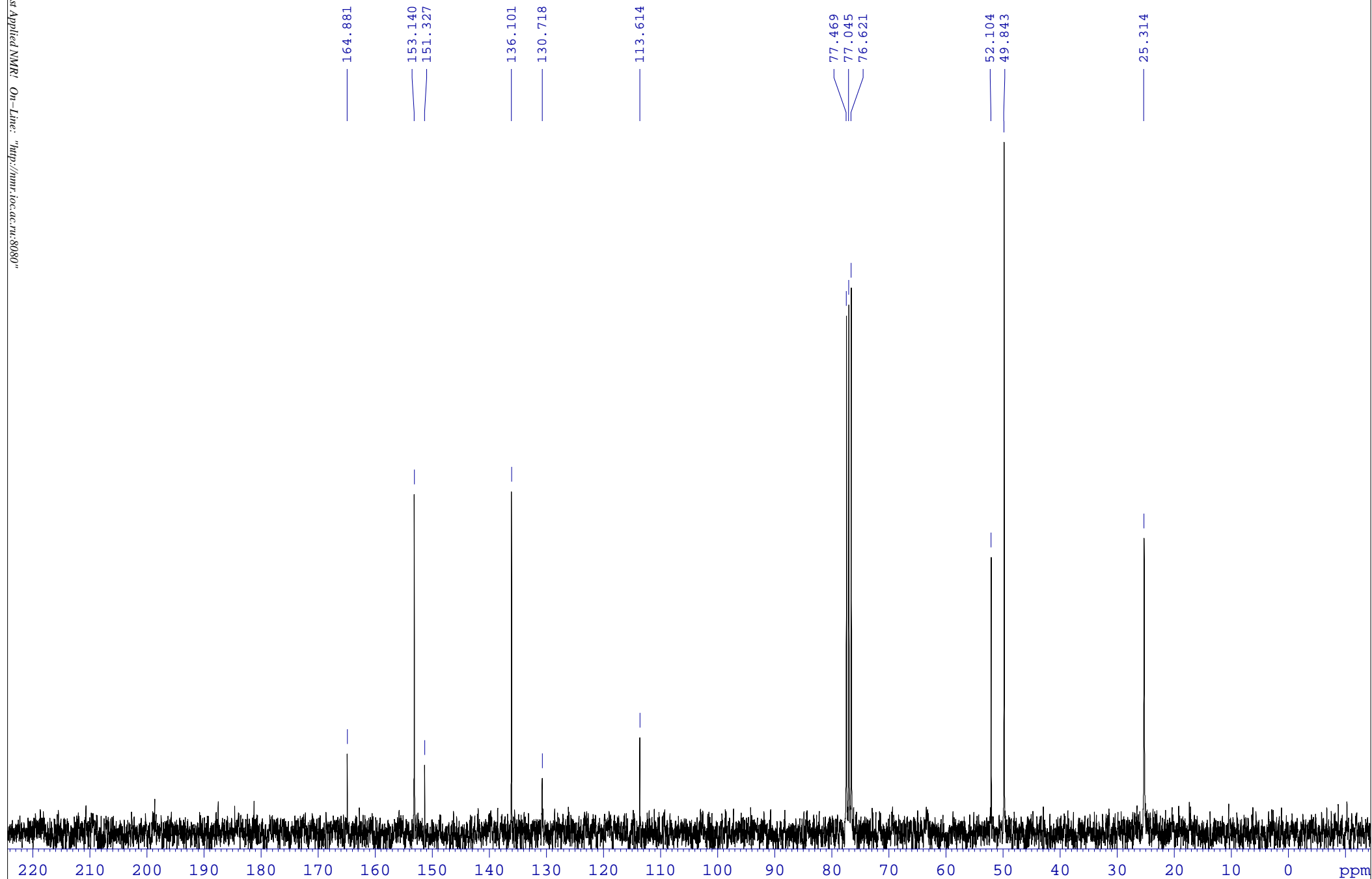
2.013

1.607





/LPIK AF-391.13 Kokorekin-20259



Display Report

Analysis Info

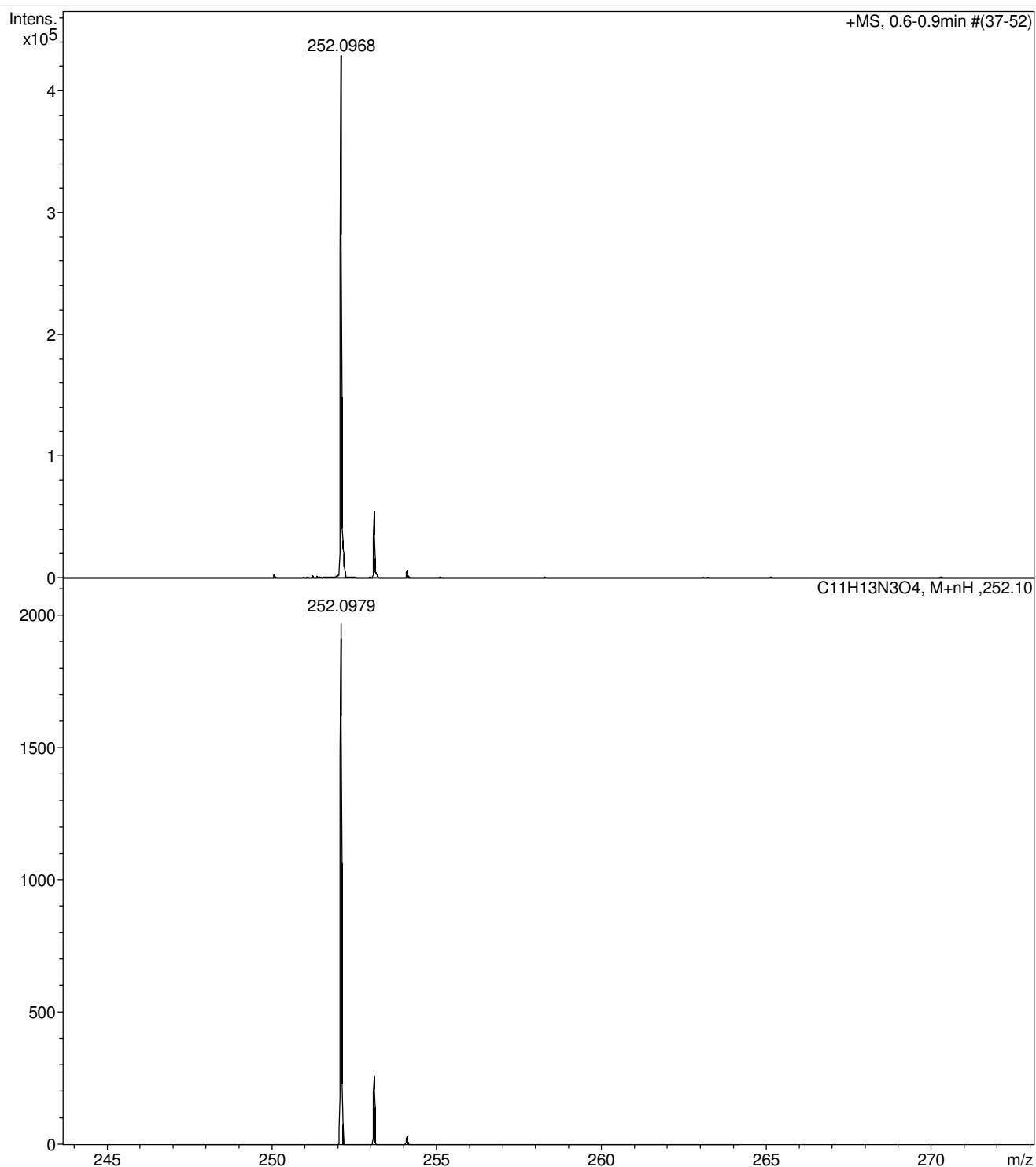
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Method tune_50-1600.m
Sample Name /LPIK AF-391
Comment C11H13N3O4 mH 252.0979 calibrant added CH3CN

Acquisition Date 10.02.2021 20:56:14

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

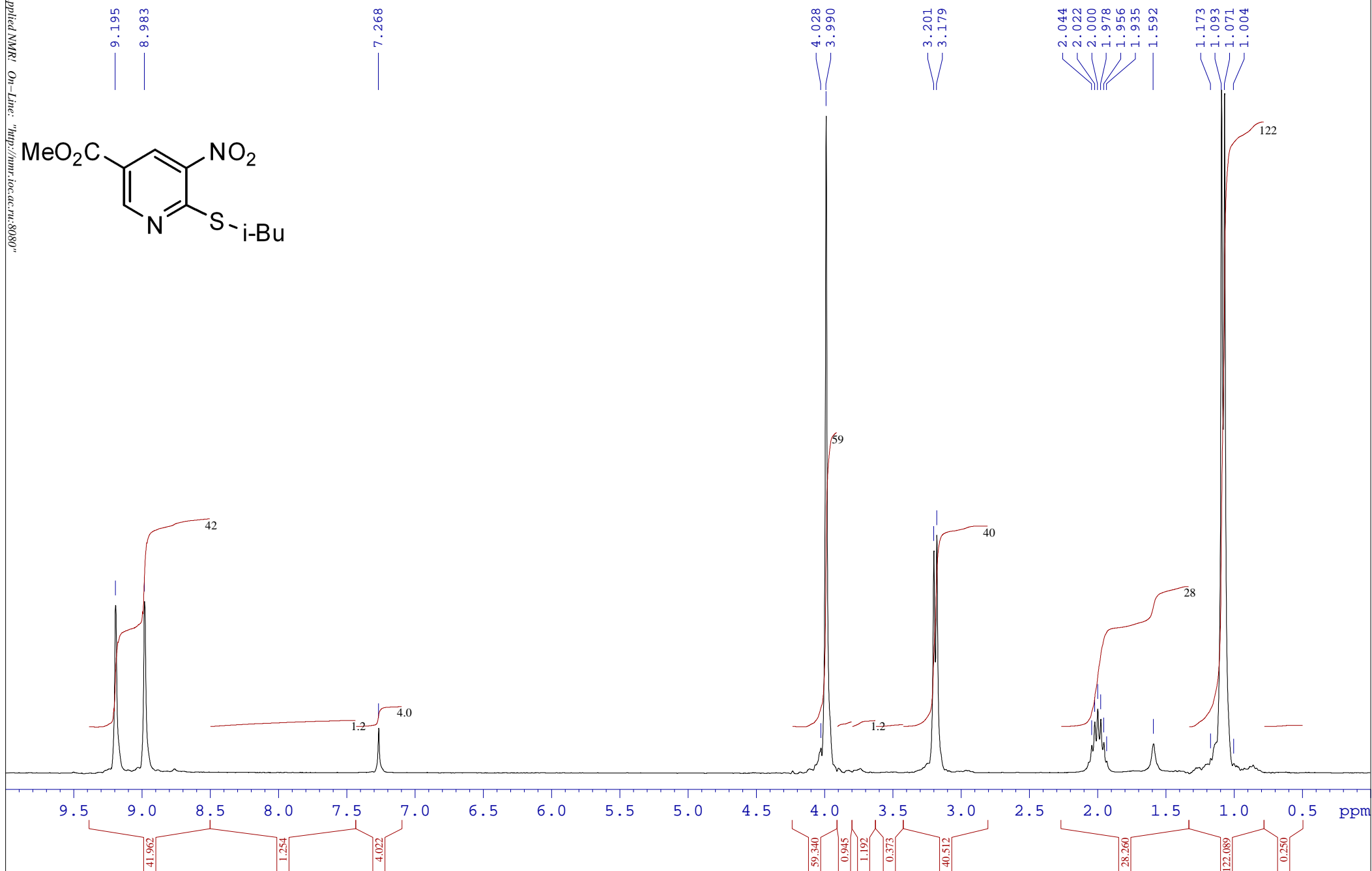
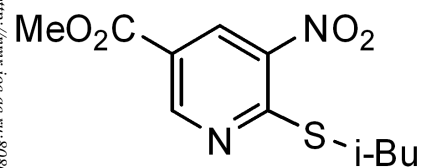
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Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



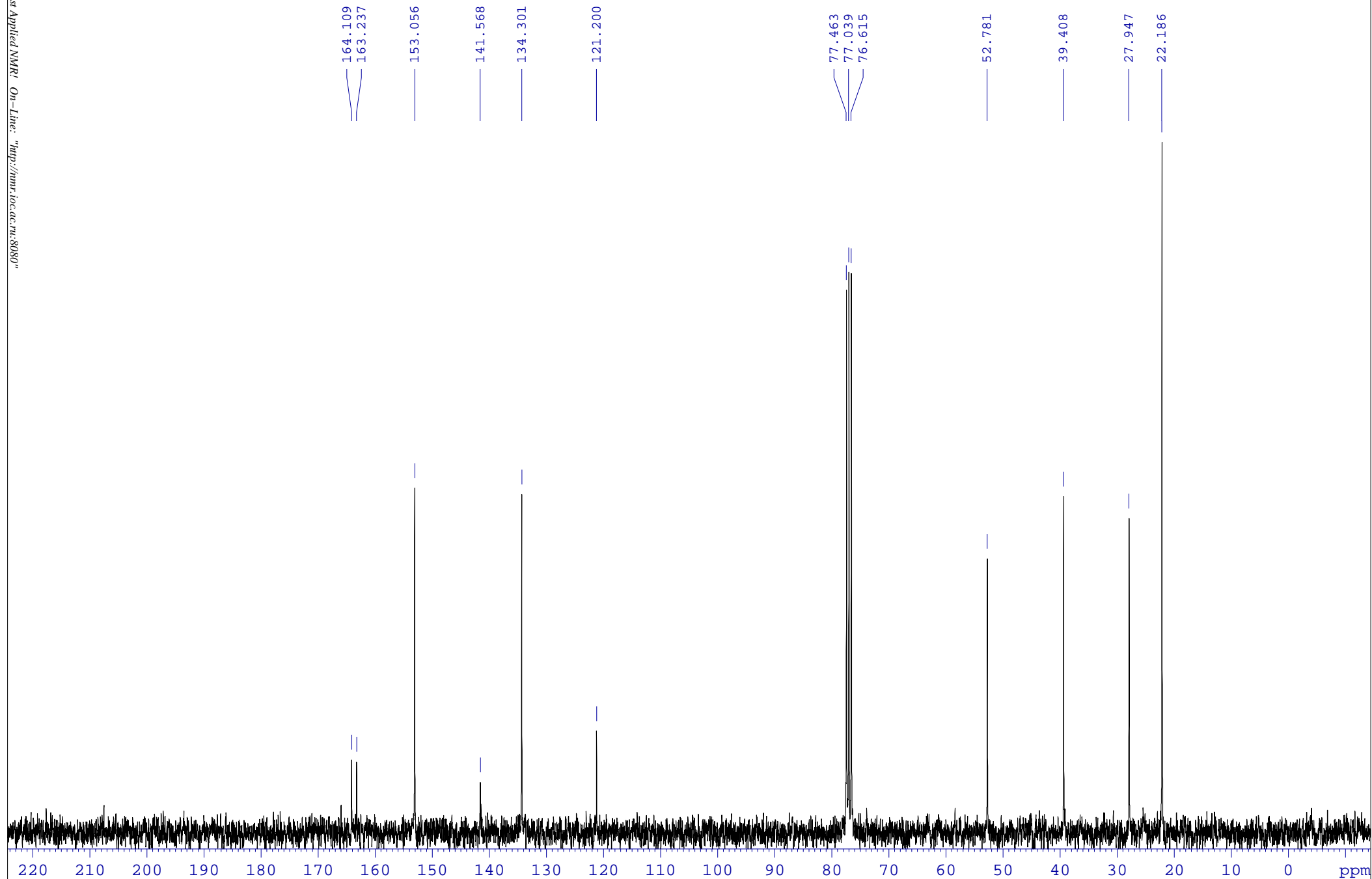


/LPIK AF-399





/LPIK AF-399.13 Kokorekin-20259



Display Report

Analysis Info

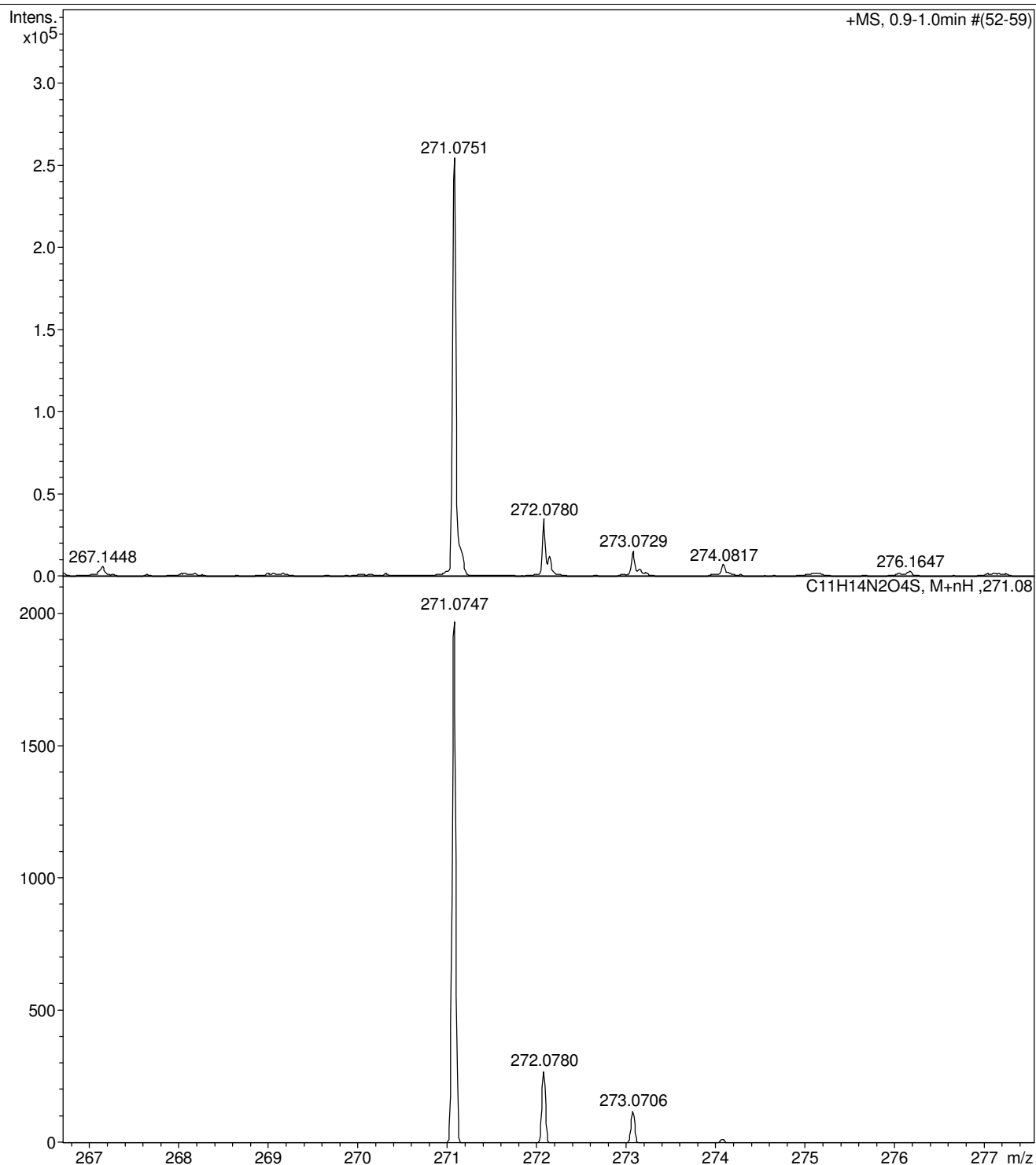
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Method tune_50-1600.m
Sample Name /LPIK AF-399
Comment C11H14N2O4S mH 271.0747 calibrant added CH3OH

Acquisition Date 11.02.2021 12:57:08

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

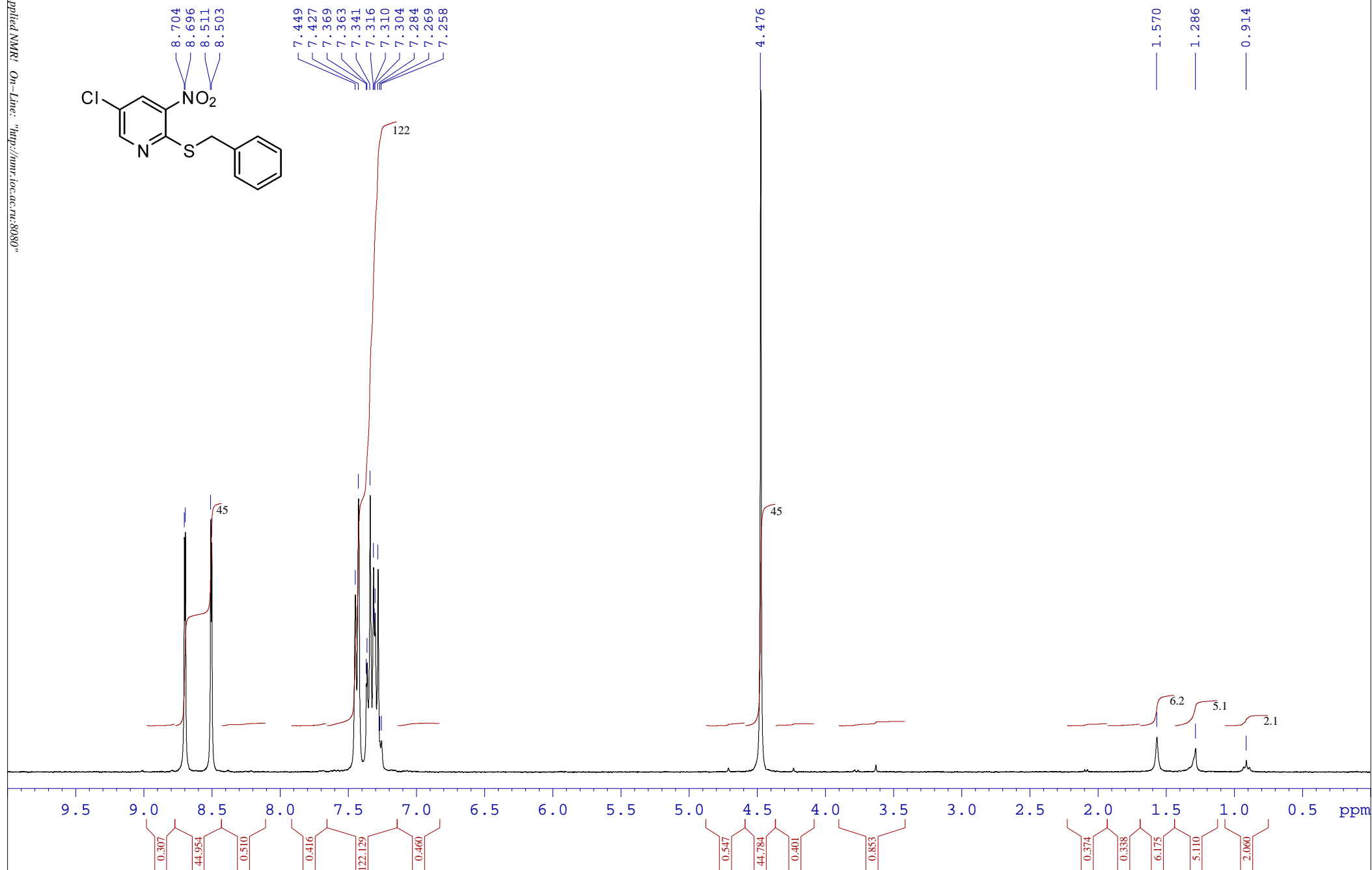
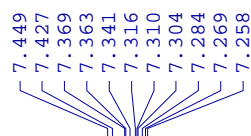
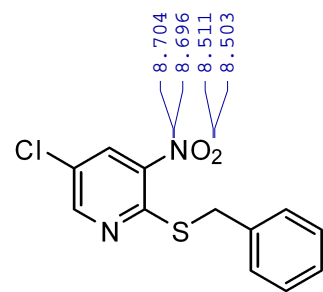
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Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



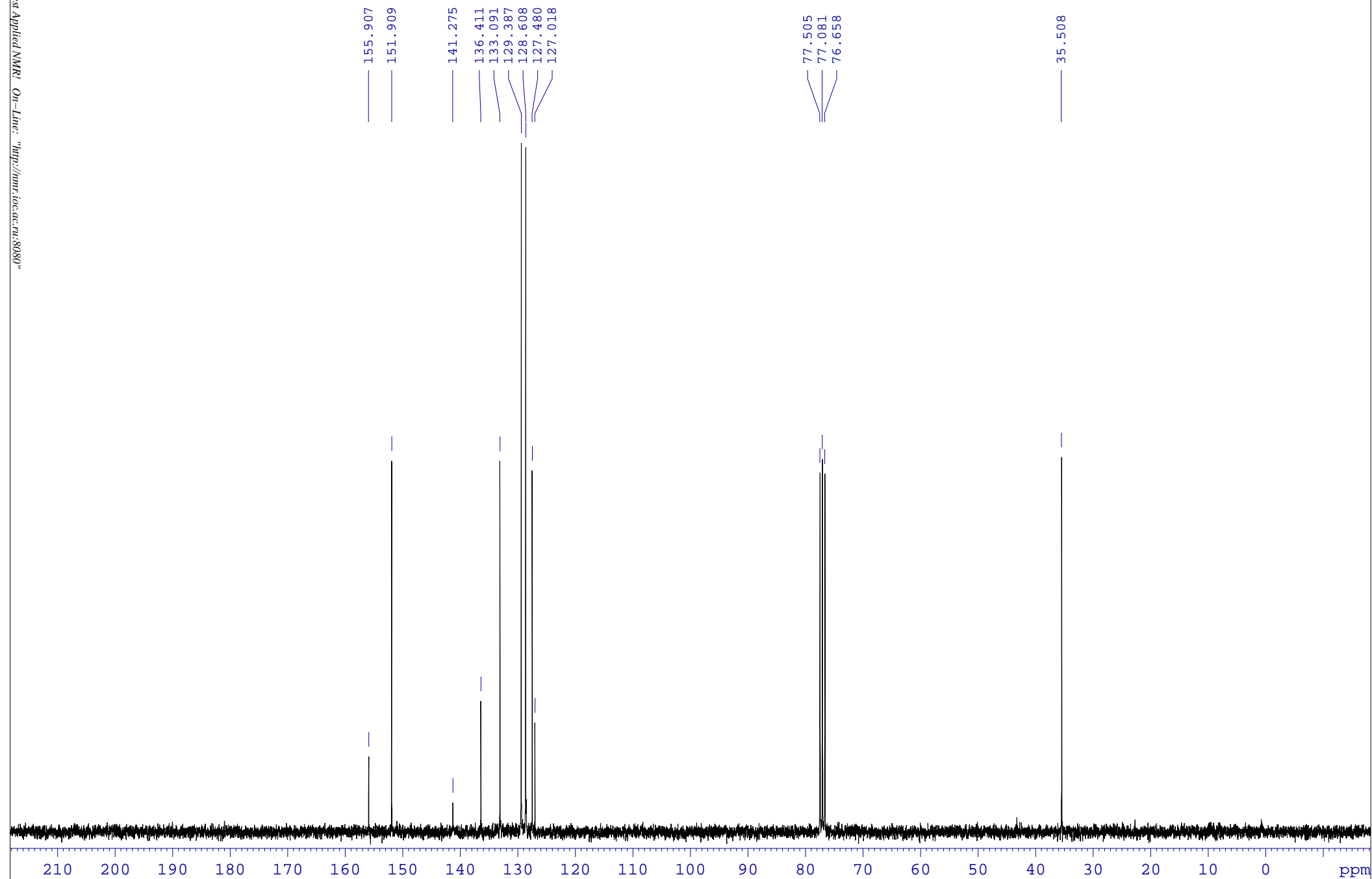


/LPIK AF-406 Kokorekin-20259





/LPIK AF-406.C15



Display Report

Analysis Info

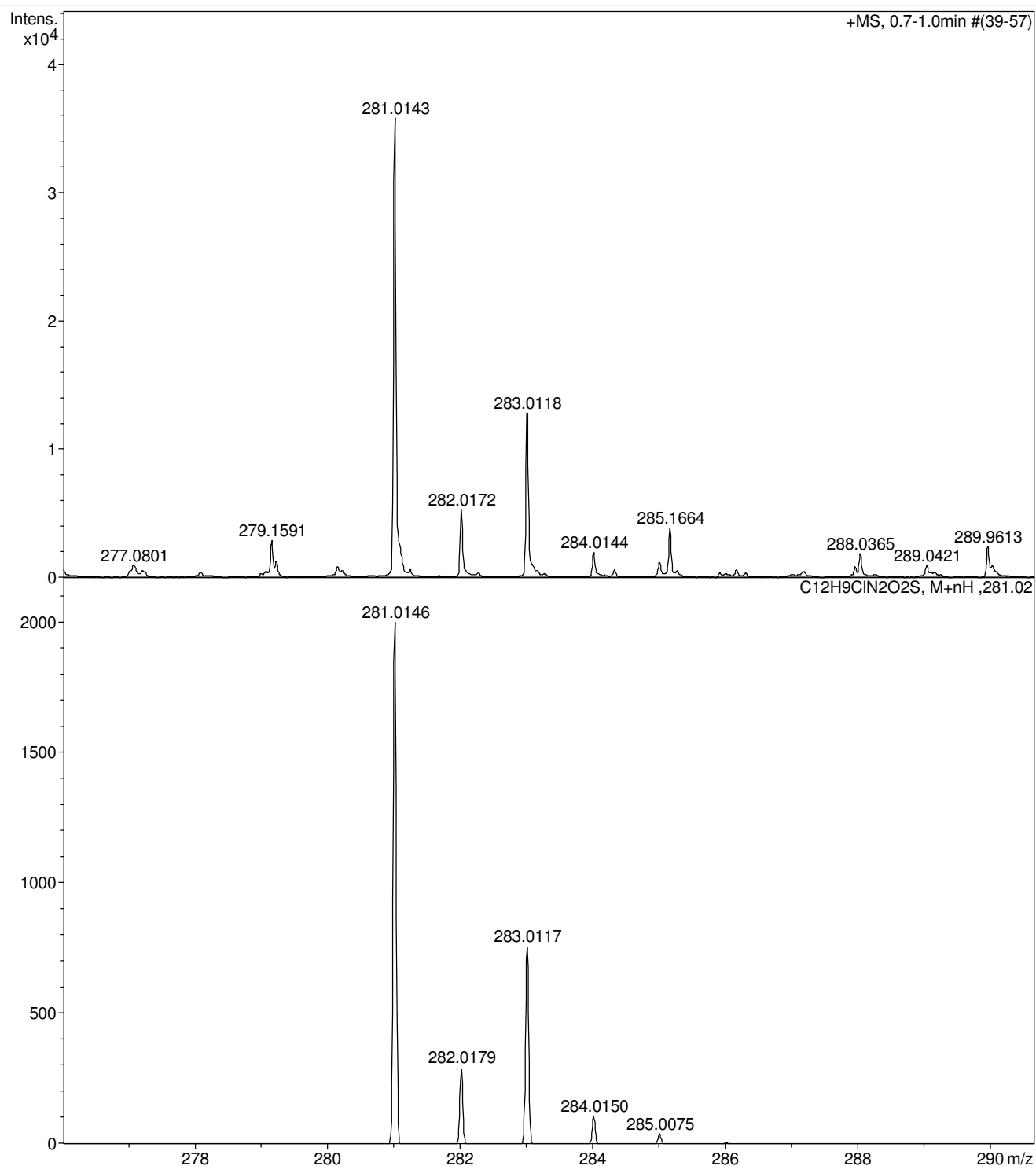
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428019.d
Method tune_50-1600.m
Sample Name /LPIK AF-406
Comment C12H9CIN2O2S mH 281.0146 clb added CH3OH

Acquisition Date 28.04.2021 12:10:25

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

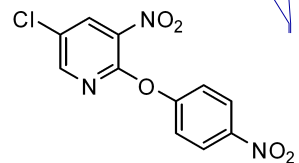
Acquisition Parameter

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





/LPIK AF-407R



8.445
8.438
8.368
8.339

7.380
7.350
7.281

2.027

1.582

1.274

122

61

9.6

12

2.8

1.2

1.1

1.1

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 ppm

1.072
122.125

0.152
0.387

0.829
61.032
9.656

1.142
0.411

0.229
0.292
1.267

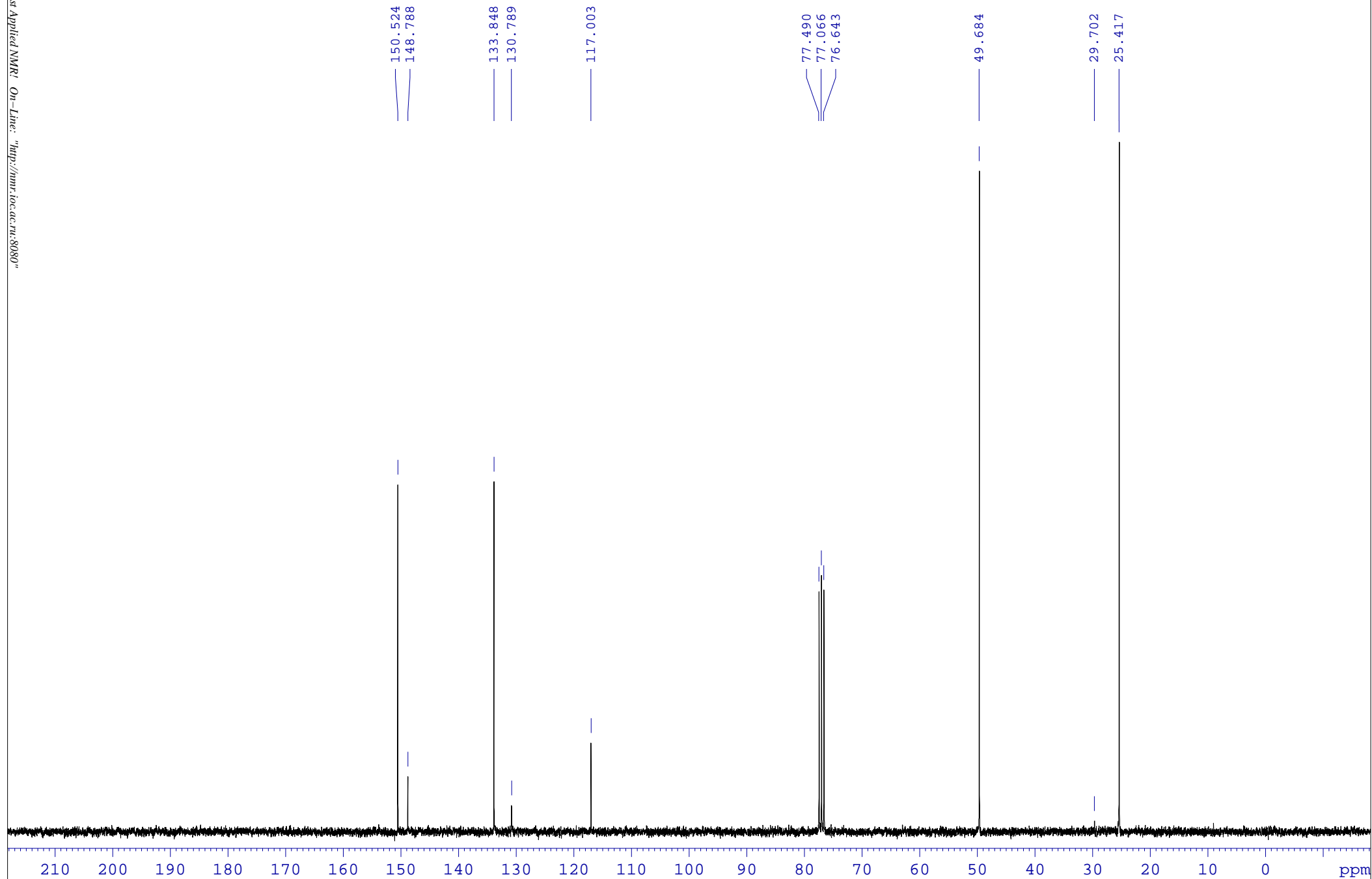
12.318
0.385
2.797

0.498
0.925

0.059



/LPIK AF-407.C13



Display Report

Analysis Info

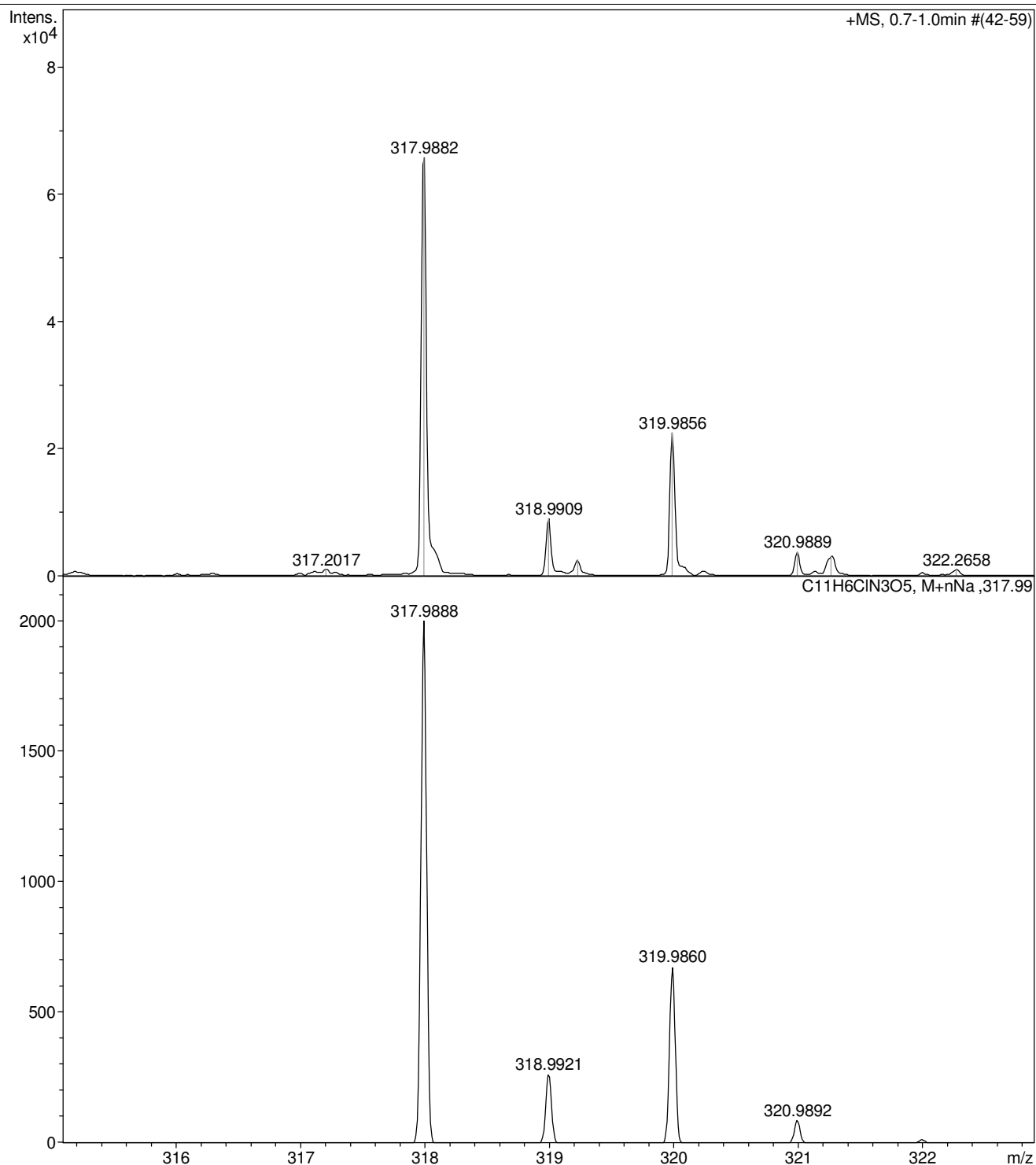
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Method tune_50-1600.m
Sample Name /LPIK AF-407
Comment C11H6ClN3O5 mH 296.0068 clb added CH3OH

Acquisition Date 28.04.2021 12:16:29

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

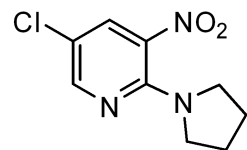
Acquisition Parameter

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





/LPIK AF-408 Kokorekin-20259



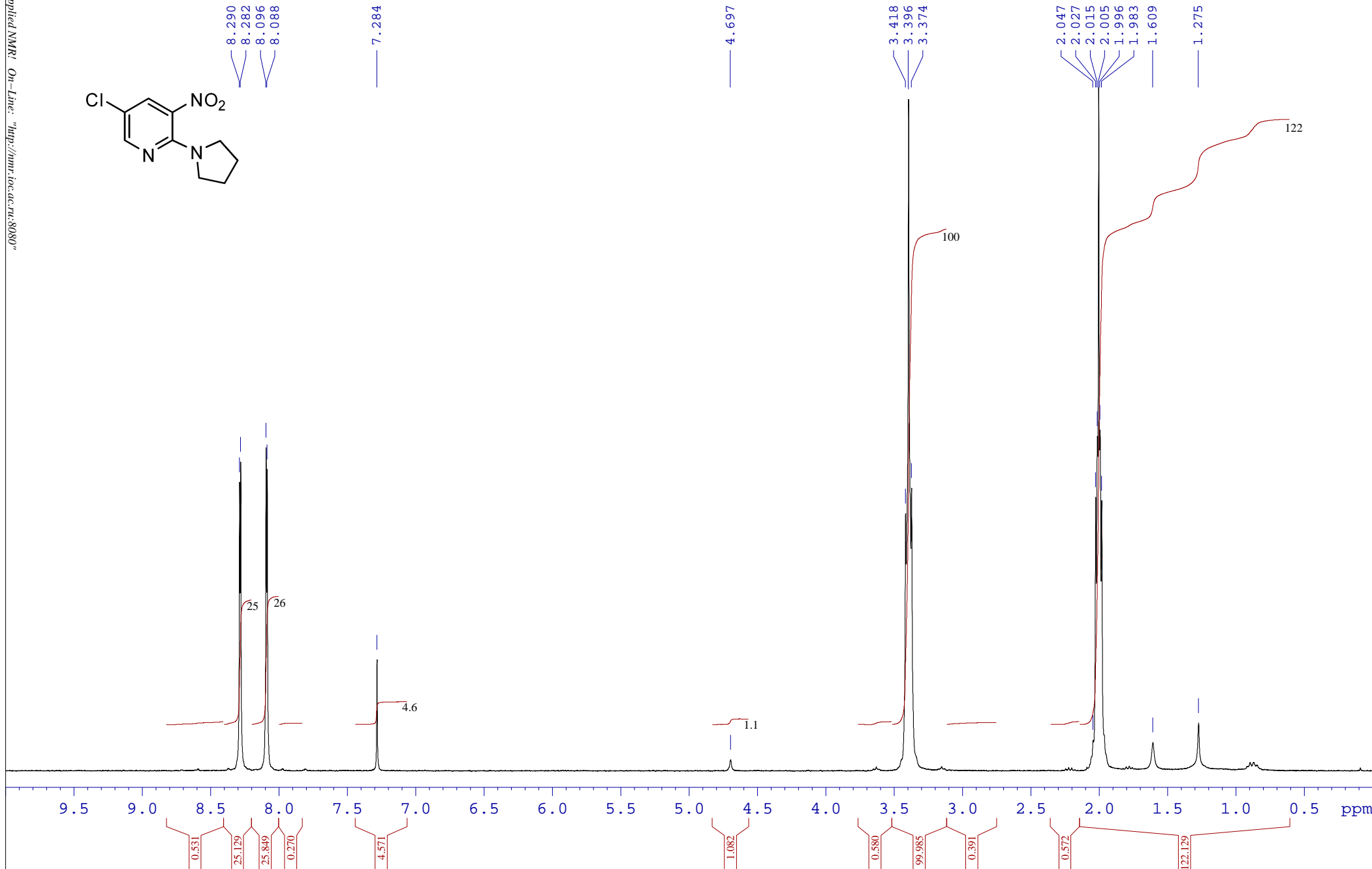
8.290
8.282
8.096
8.088

7.284

4.697

3.418
3.396
3.374

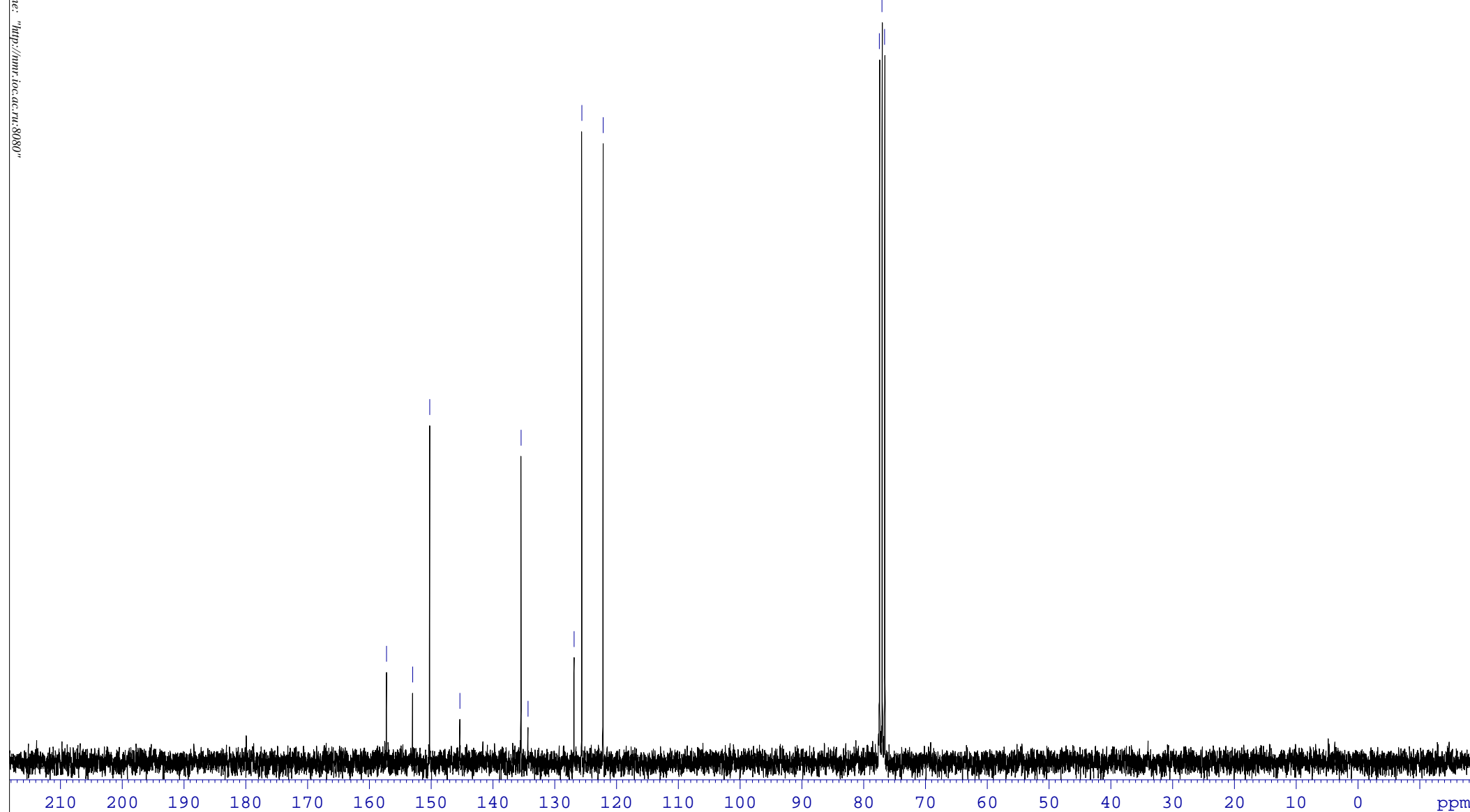
2.047
2.027
2.015
2.005
1.996
1.983
1.609
1.275





/LPIK AF-408.C13

157.228
152.992
150.234
145.351
135.449
134.325
126.870
125.612
122.161
77.468
77.045
76.621



Display Report

Analysis Info

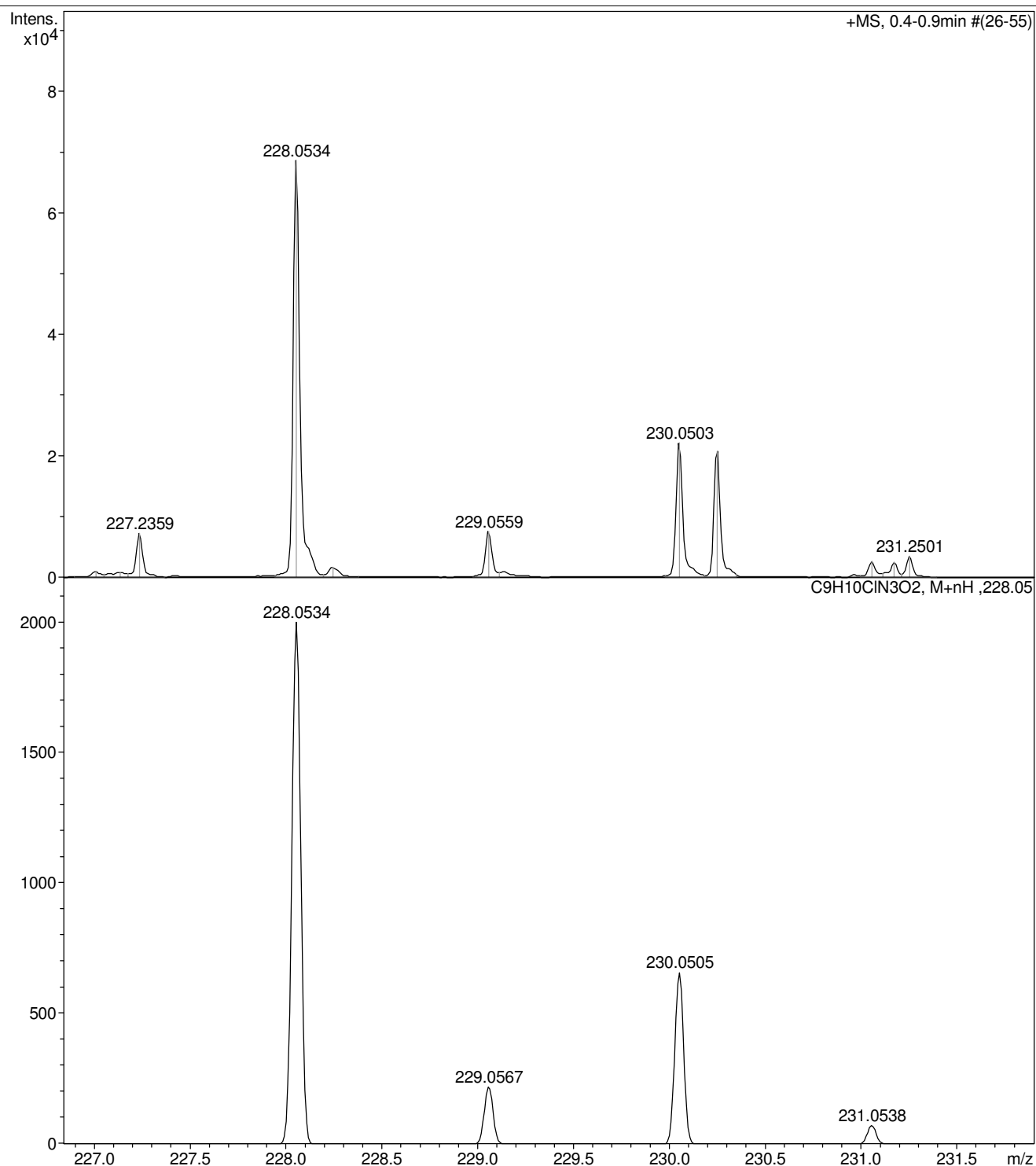
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428021.d
Method tune_50-1600.m
Sample Name /LPIK AF-408
Comment C9H10CIN3O2 mH 228.0534 clb added CH3OH

Acquisition Date 28.04.2021 12:28:48

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

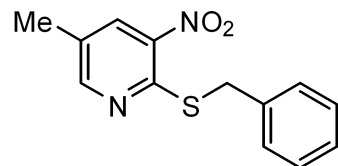
Acquisition Parameter

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





/LPIK AF-416



8.577

8.325

7.457

7.433

7.349

7.326

7.302

7.282

7.262

7.250

4.482

3.626

3.512

2.472

2.431

1.586

122

38

59

19

20

6.5

1.2

7.7

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 ppm

0.432

19.215

1.147

19.709

1.089

0.365

122.134

0.541

0.361

37.972

0.496

0.434

6.508

1.211

0.406

0.515

59.256

0.672

0.391

0.352

7.736

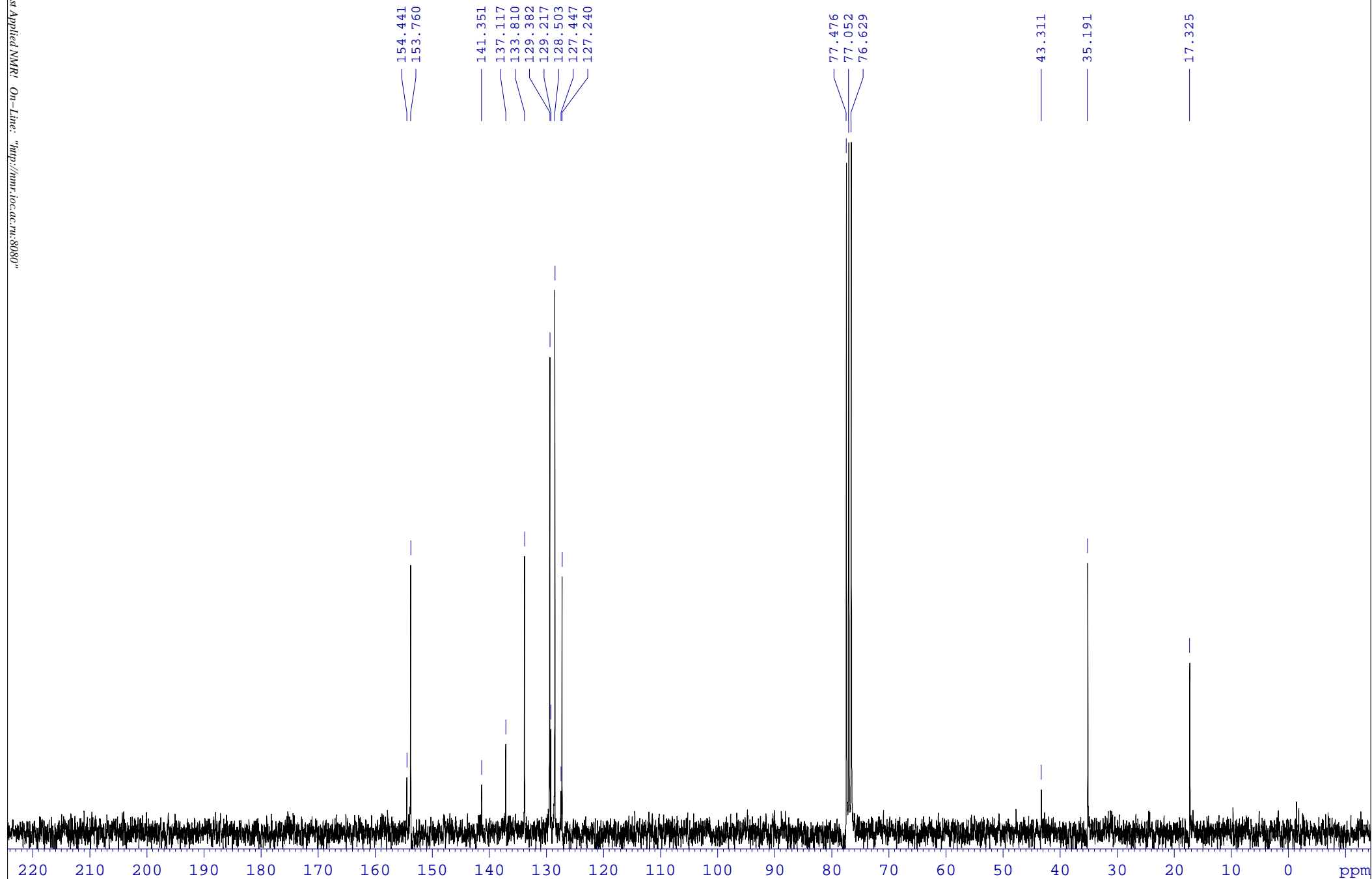
0.735

0.280

0.404



/LPIK AF-416.13 Kokorekin-20259



Display Report

Analysis Info

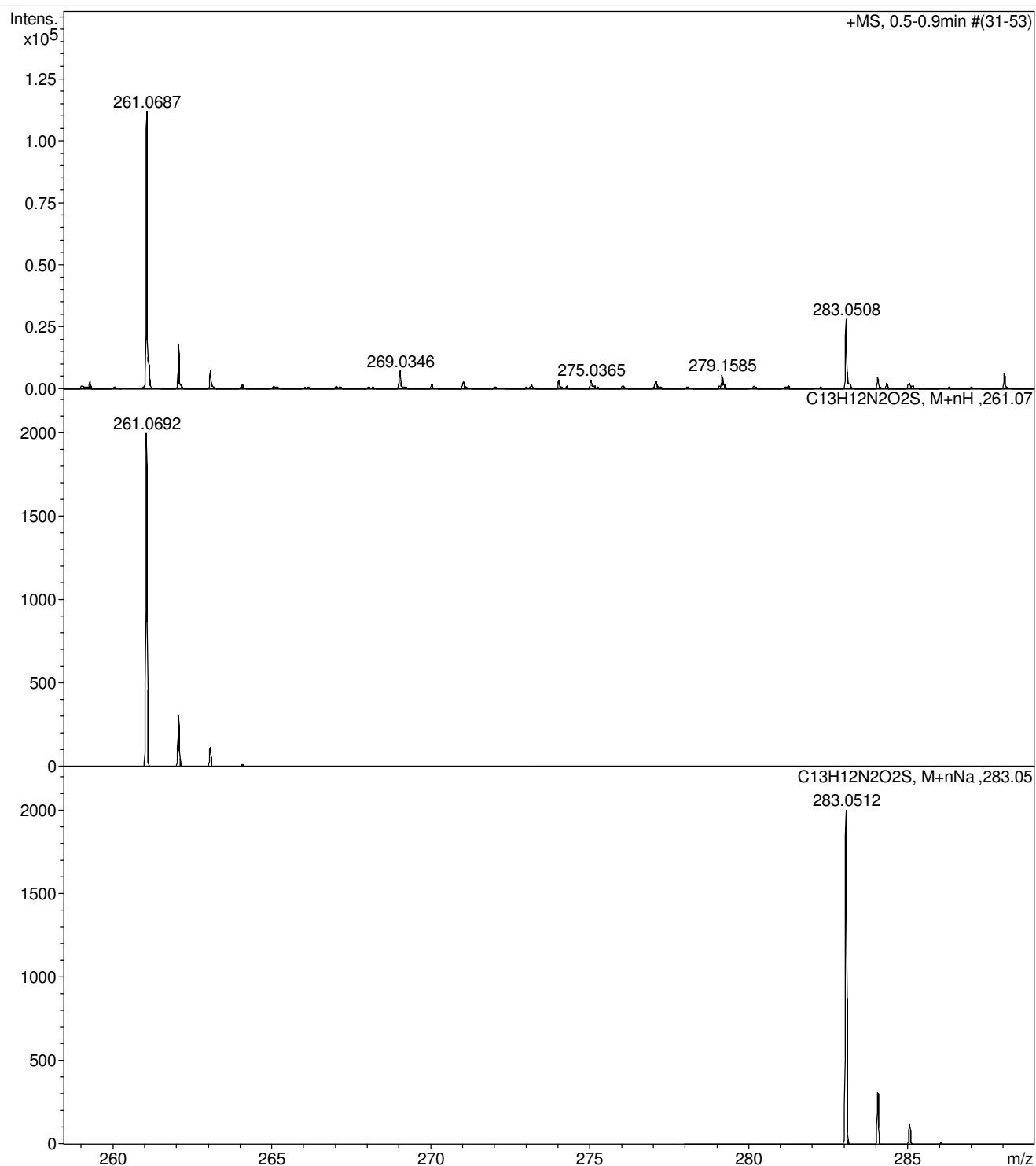
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428022.d
Method tune_50-1600.m
Sample Name /LPIK AF-416
Comment C13H12N2O2S mH 261.0692 clb added CH3OH

Acquisition Date 28.04.2021 12:33:48

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

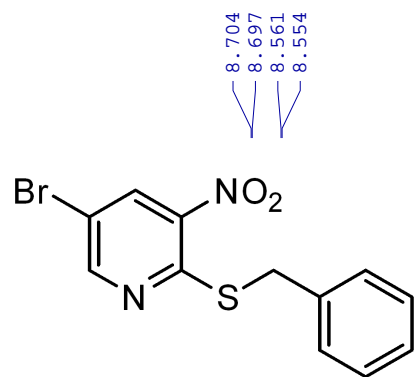
Acquisition Parameter

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





/LPIK AF_421



8.704
8.697
8.561
8.554

7.366
7.342
7.281
7.259
7.234
7.222
7.201
7.176

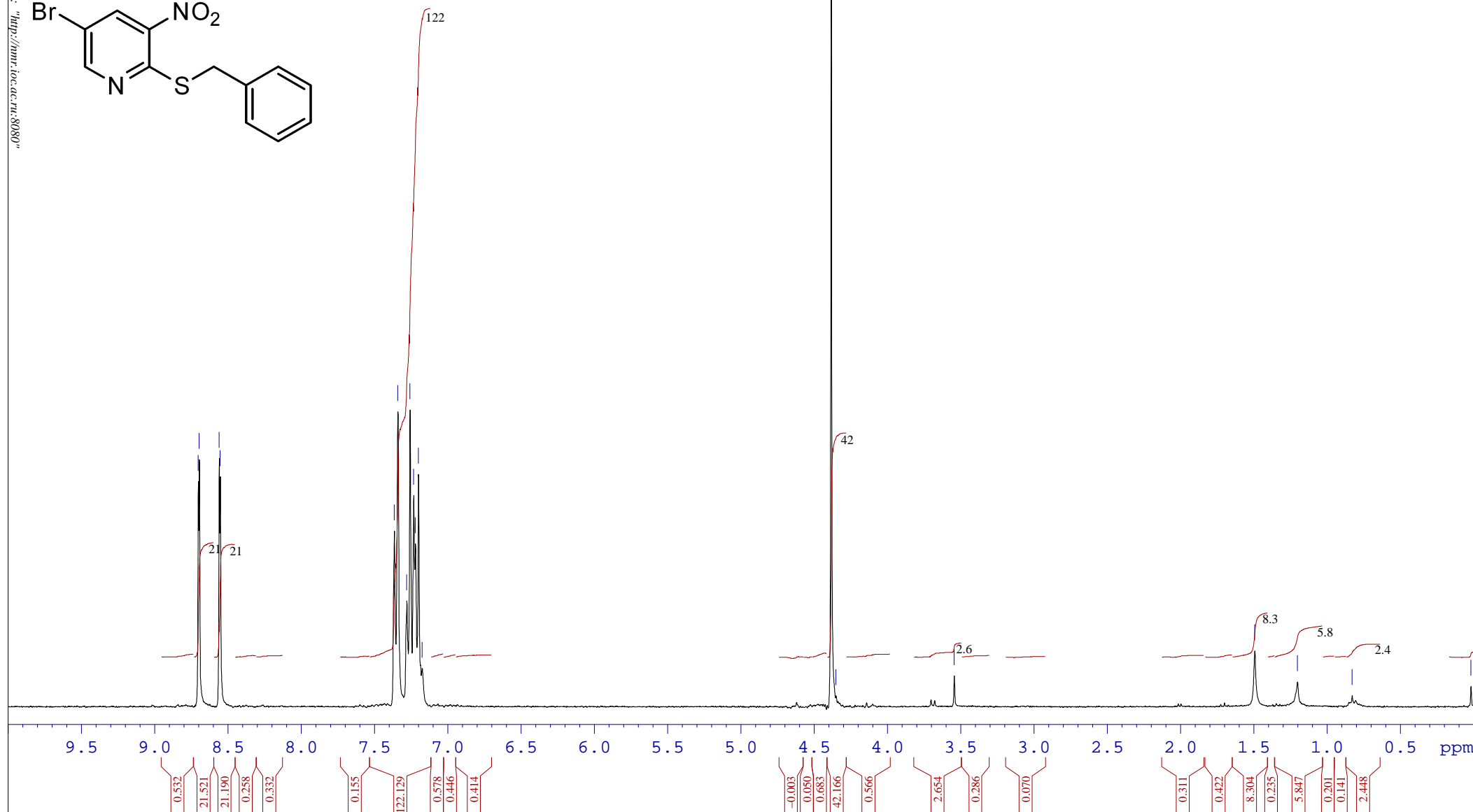
4.385
4.352

3.546

1.495

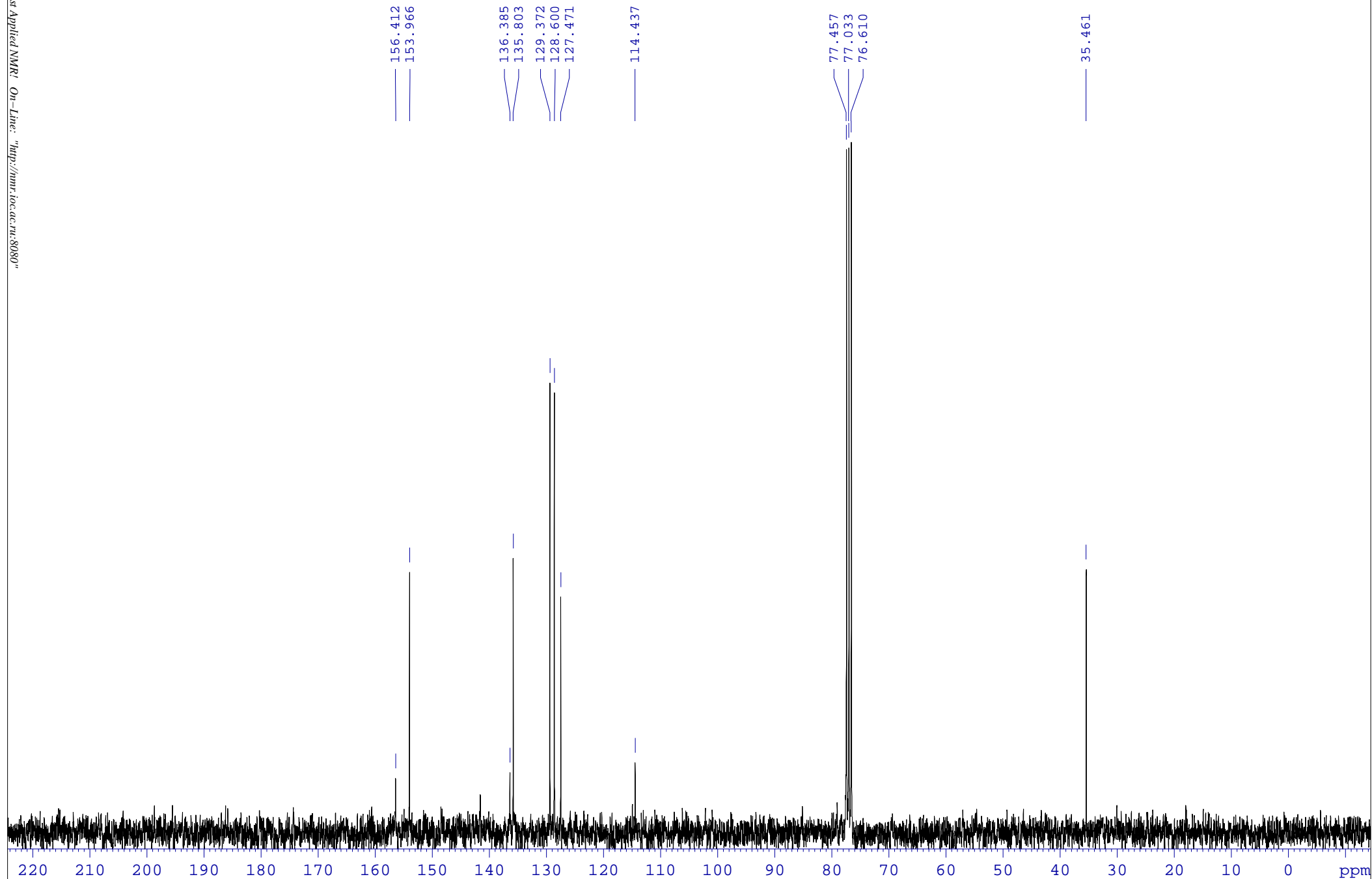
1.203

0.830





/LPIK AF-421.13 Kokorekin-20259



Display Report

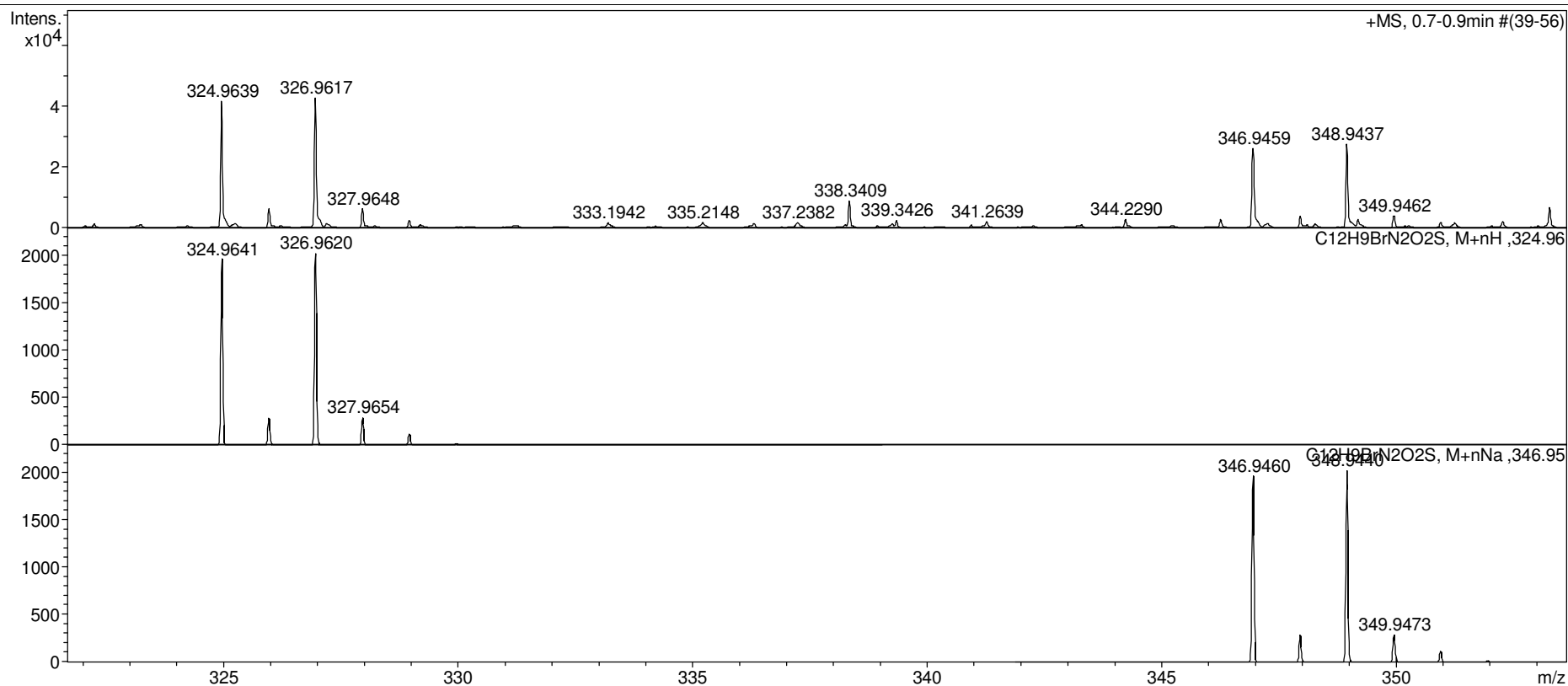
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428023.d
Method tune_50-1600.m
Sample Name /LPIK AF-421
Comment C12H9BrN2O2S mH 324.9640 clb added CH3OH

Acquisition Date 28.04.2021 12:38:09
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

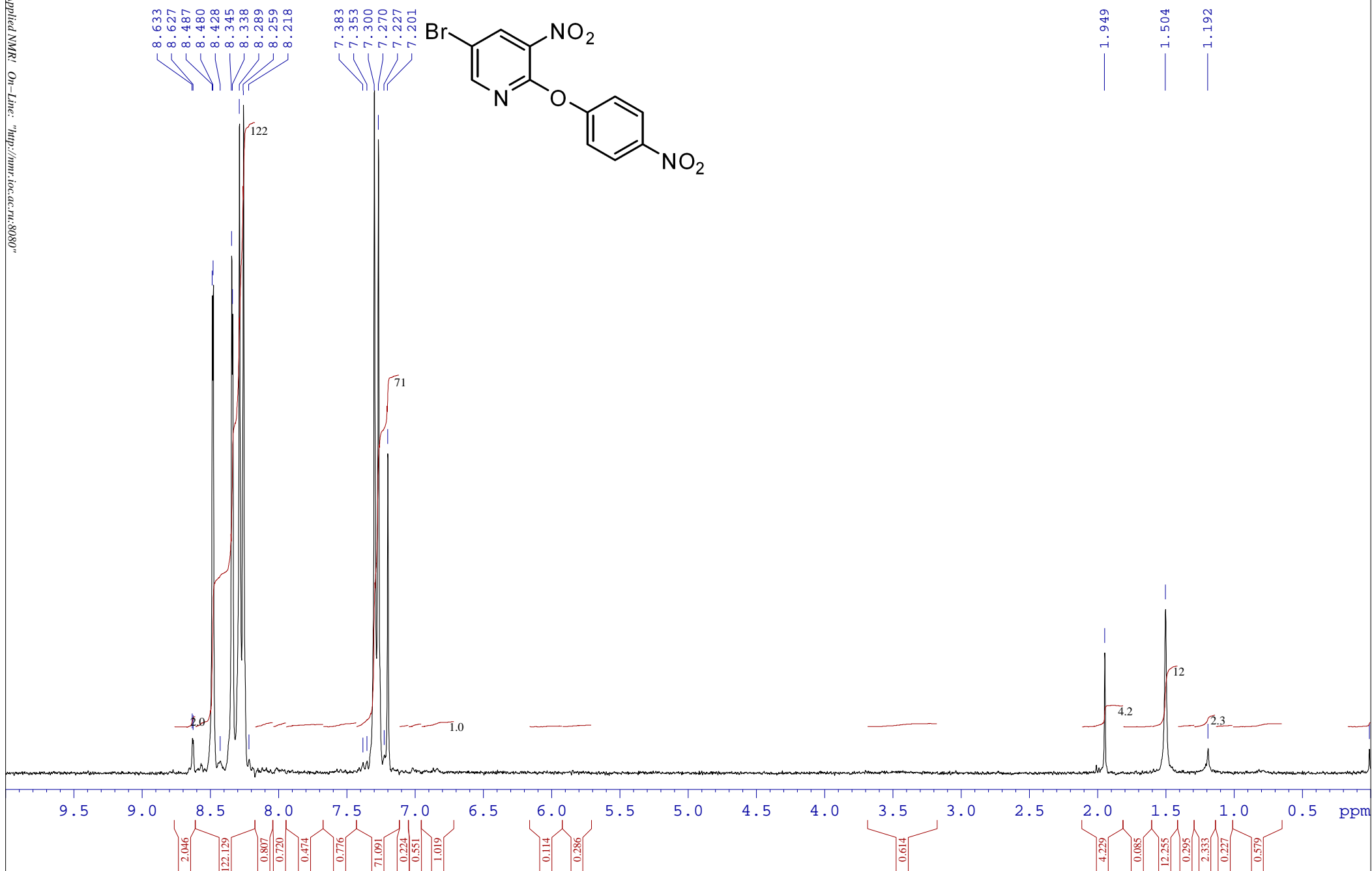
Acquisition Parameter

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





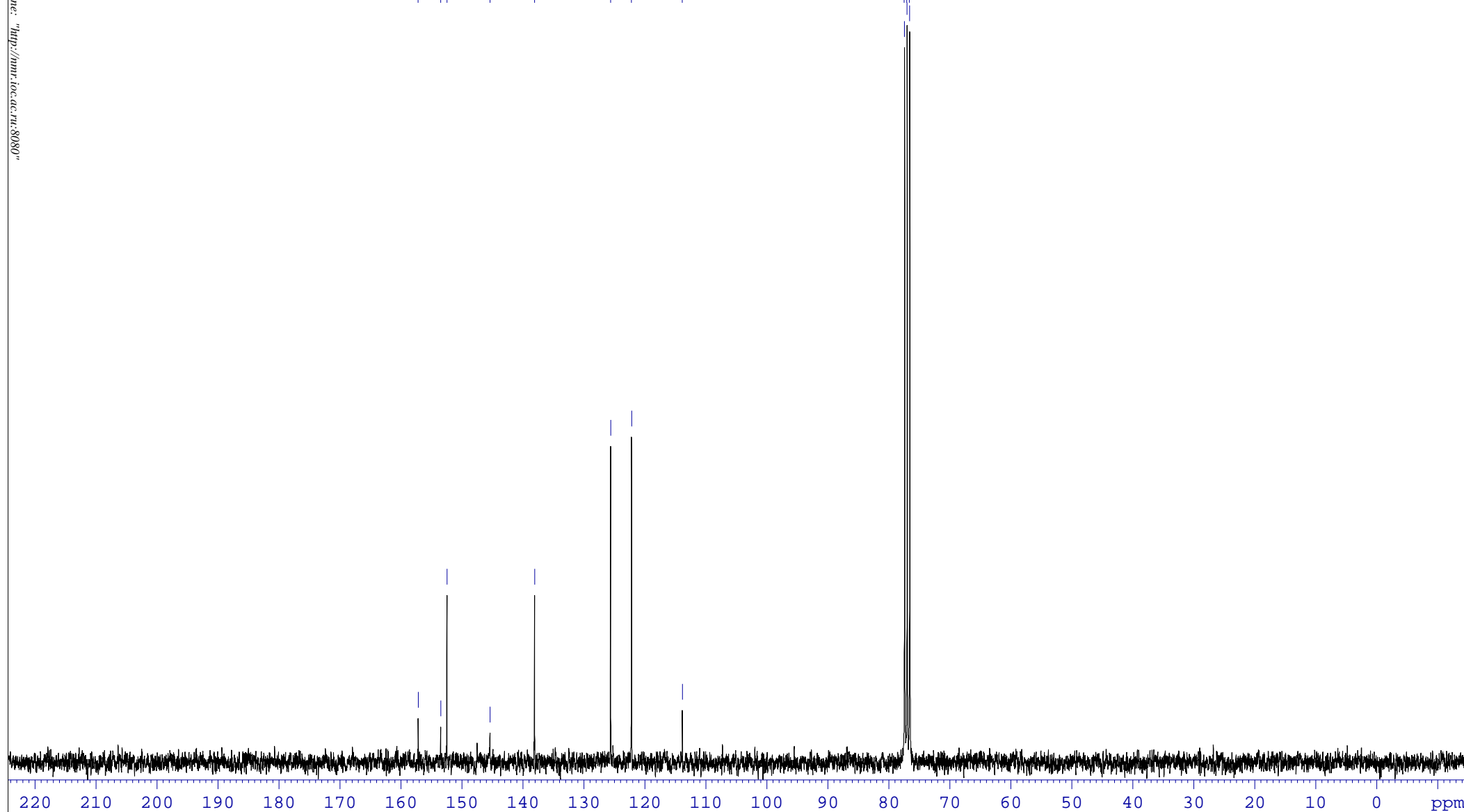
/LPIK AF_422





/LPIK AF-422.13 Kokorekin-20259

157.159
153.466
152.446
145.389
138.071
125.601
122.164
113.846
77.451
77.027
76.604



Display Report

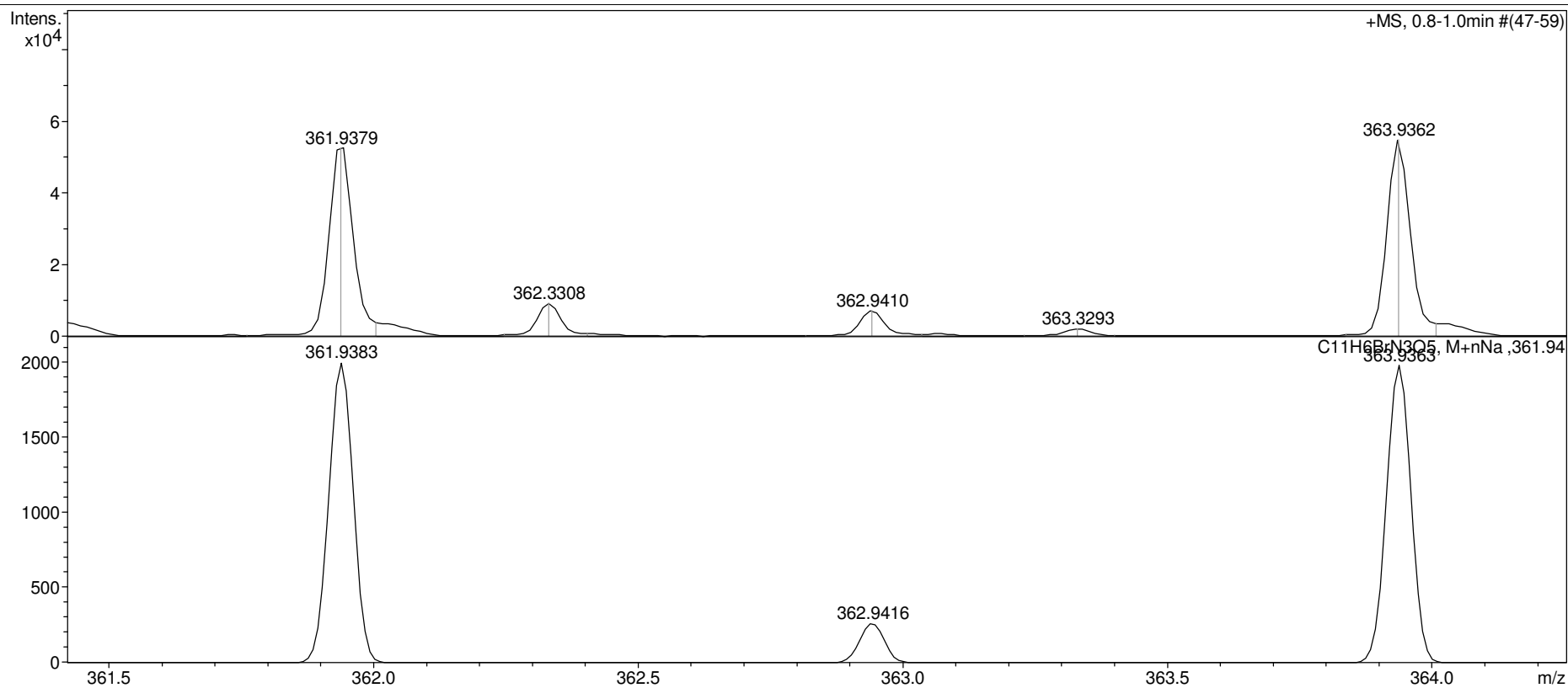
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428024.d
Method tune_50-1600.m
Sample Name /LPIK AF-422
Comment C11H6BrN3O5 mH 339.9563 clb added CH3OH

Acquisition Date 28.04.2021 12:42:53
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



Display Report

Analysis Info

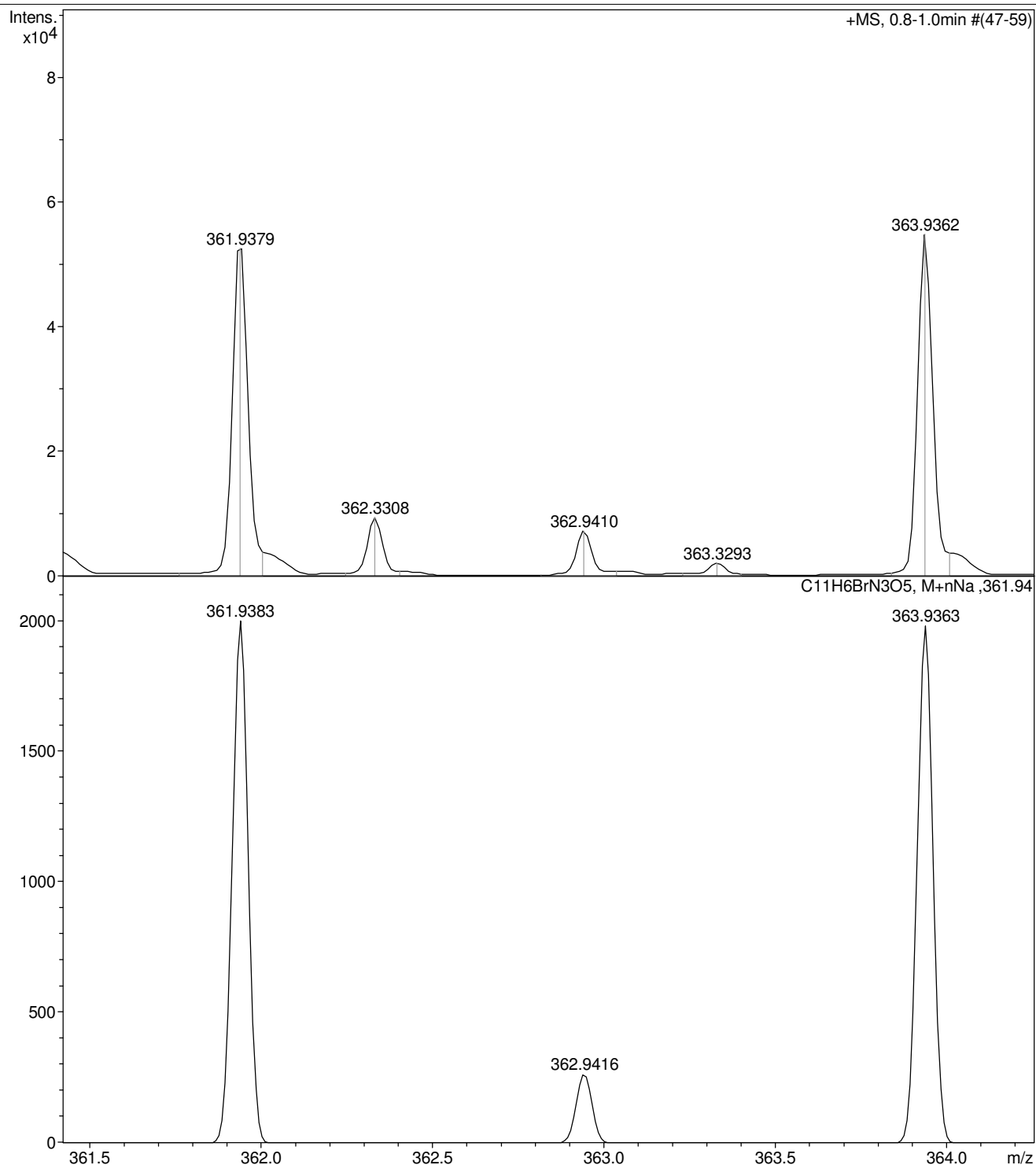
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Method tune_50-1600.m
Sample Name /LPIK AF-422
Comment C11H6BrN3O5 mH 339.9563 clb added CH3OH

Acquisition Date 28.04.2021 12:42:53

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

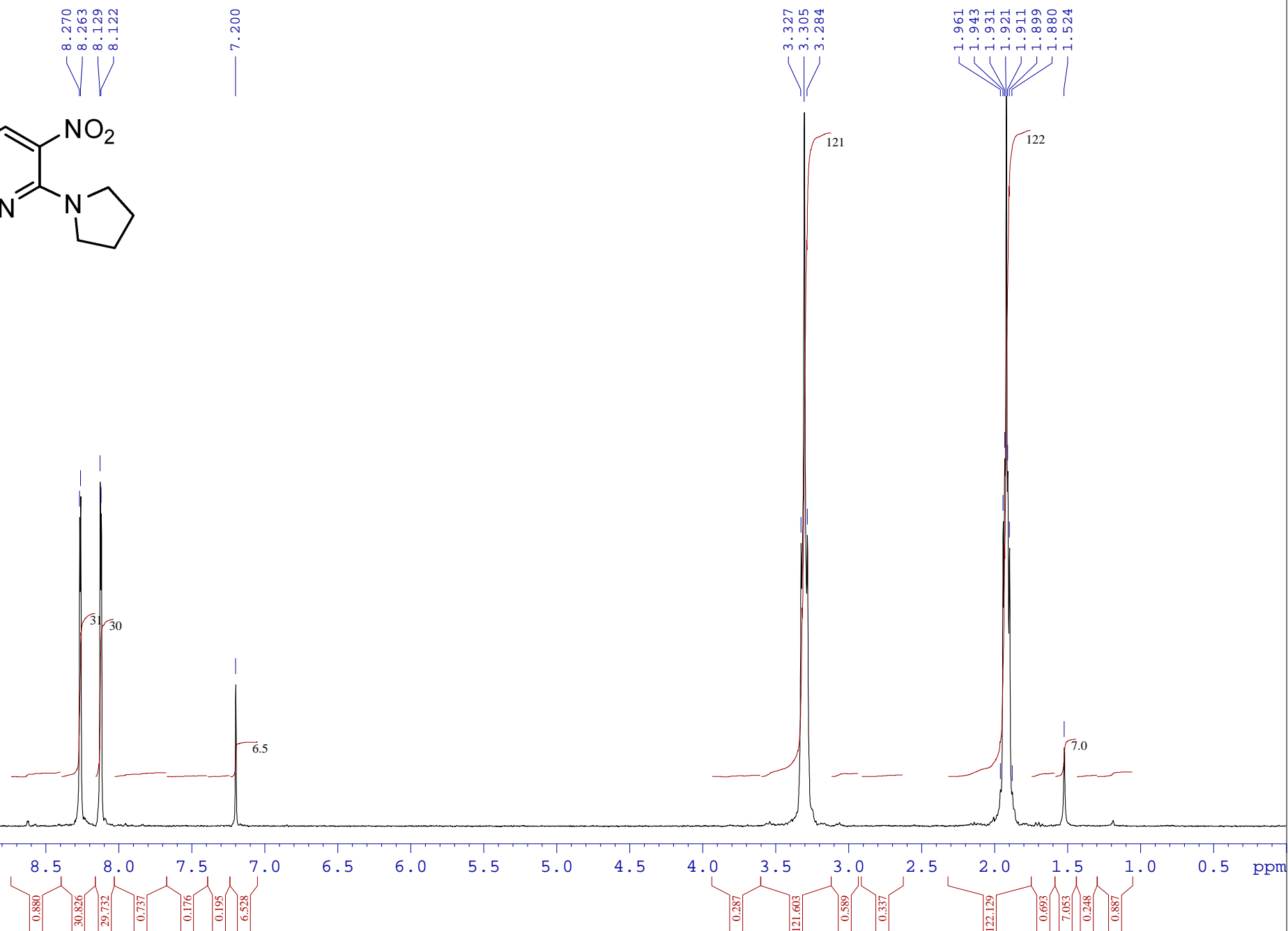
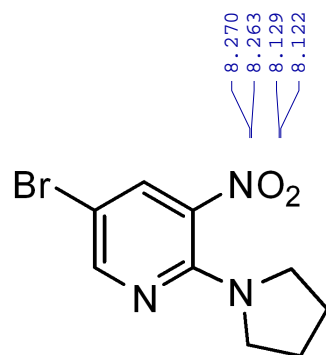
Acquisition Parameter

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



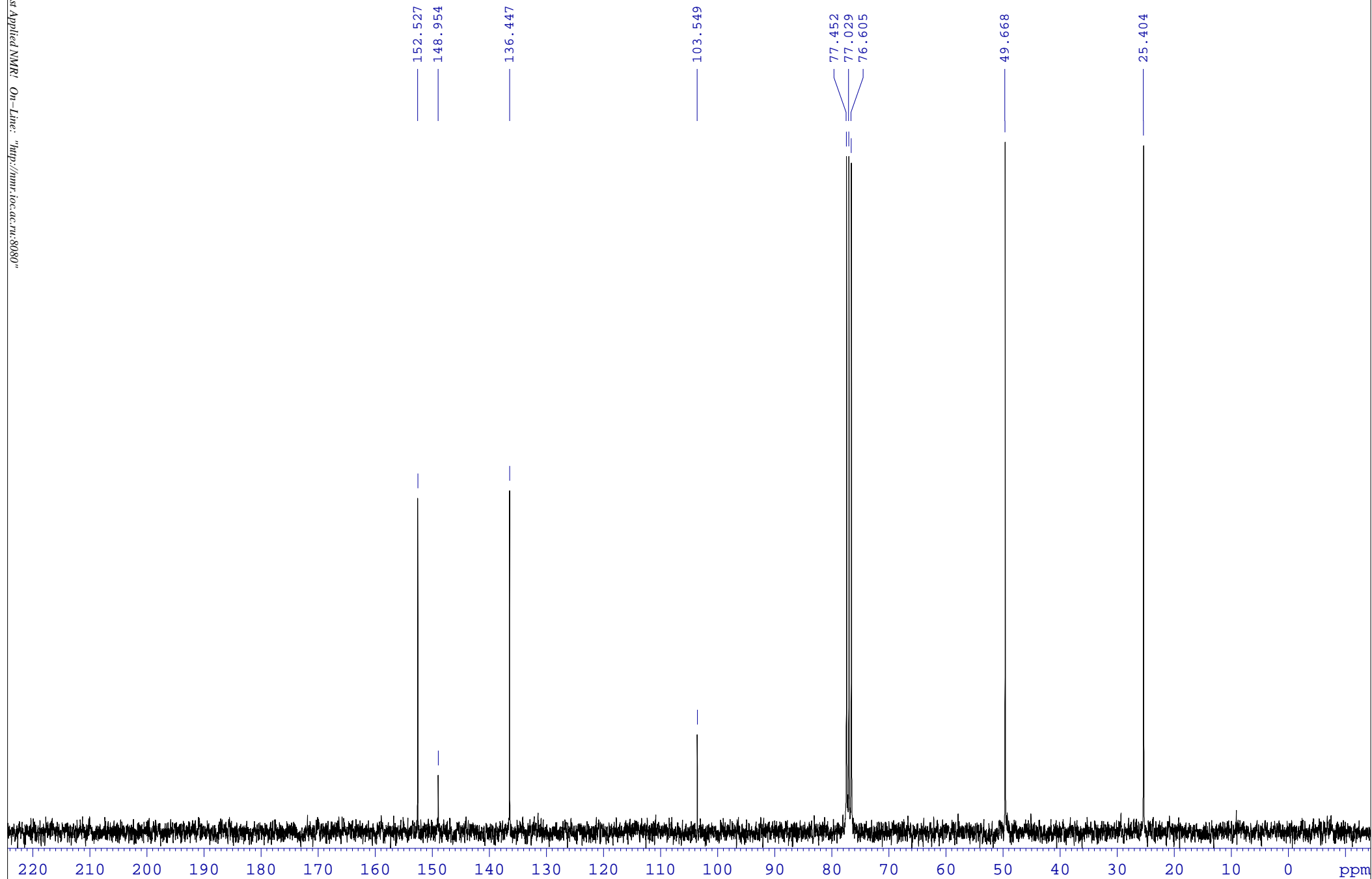


/LPIK AF_423





/LPIK AF-423.13 Kokorekin-20259



Display Report

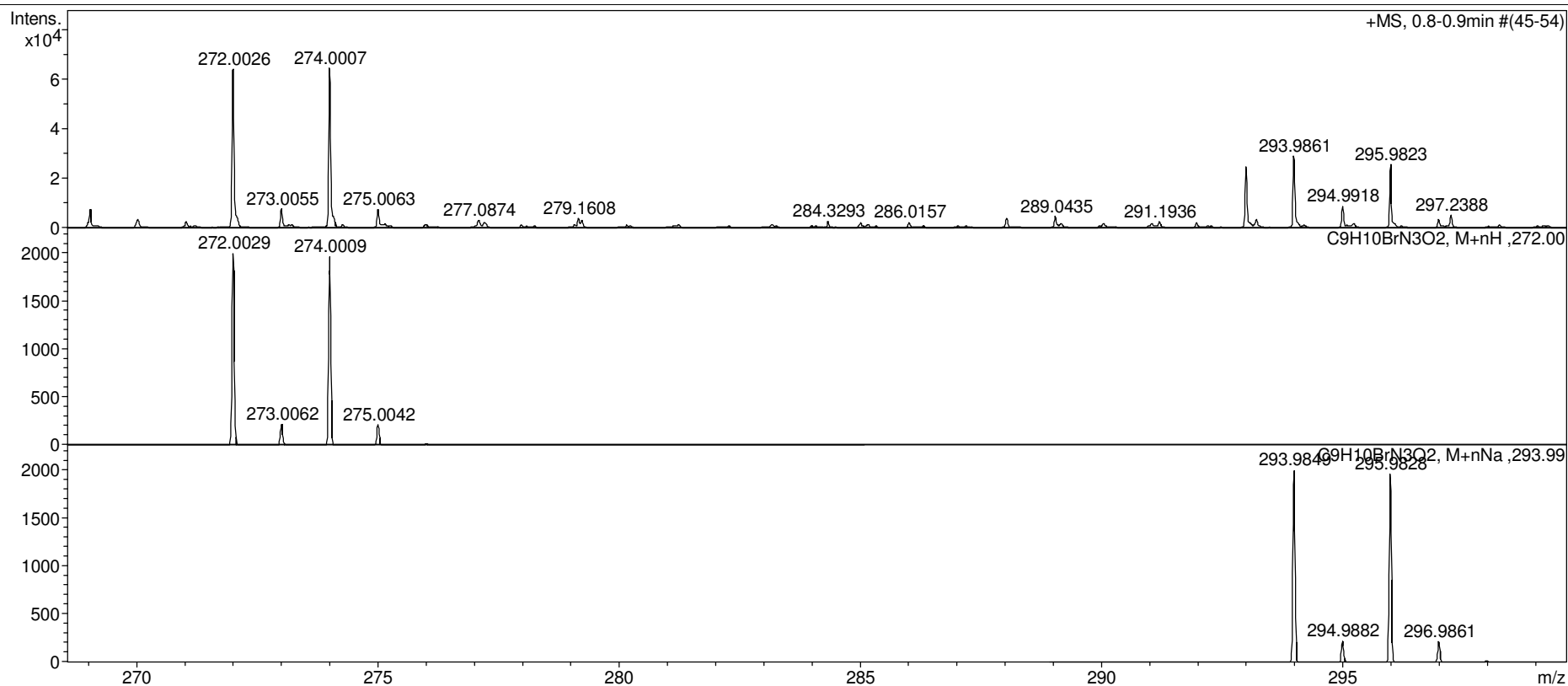
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428025.d
Method tune_50-1600.m
Sample Name /LPIK AF-423
Comment C9H10BrN3O2 mH 272.0029clb added CH3OH

Acquisition Date 28.04.2021 12:51:19
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

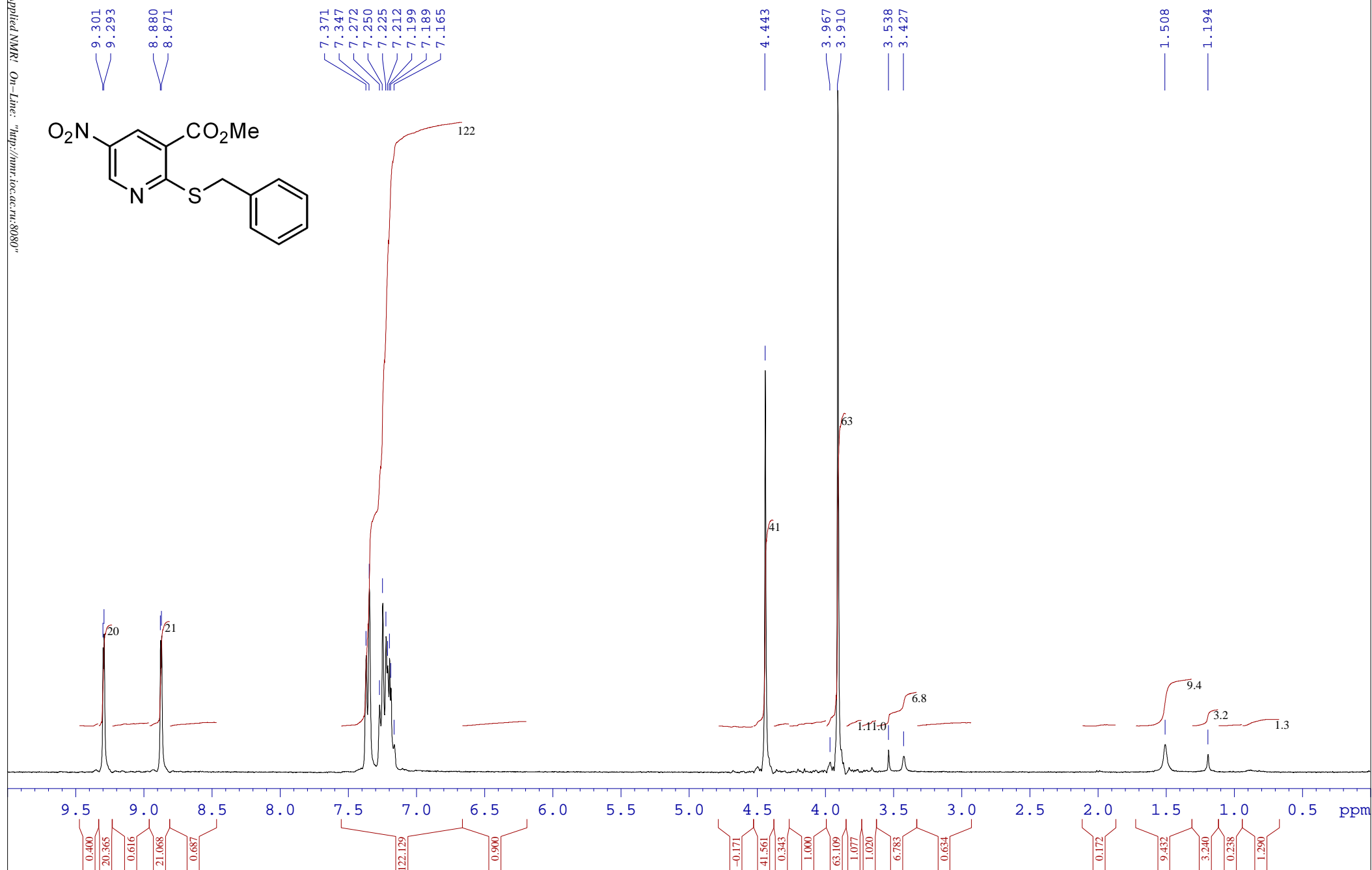
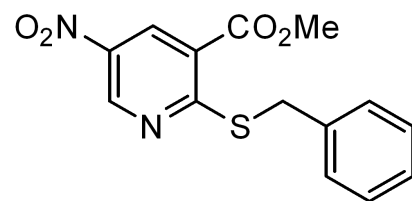
Acquisition Parameter

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





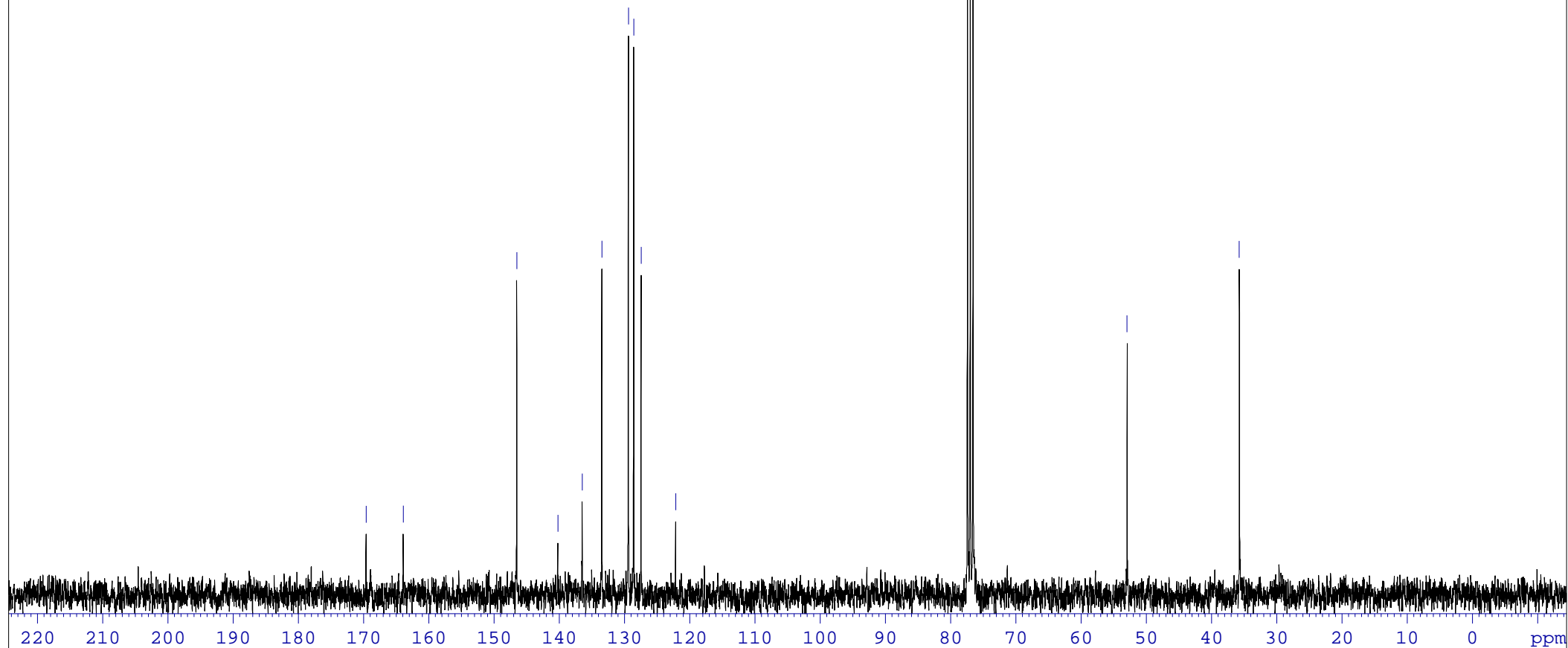
/LPIK AF426





/LPIK AF-426.13 Kokorekin-20259

169.606
163.912
146.504
140.204
136.477
133.463
129.386
128.575
127.440
122.141
77.465
77.041
76.617
52.972
35.770



Display Report

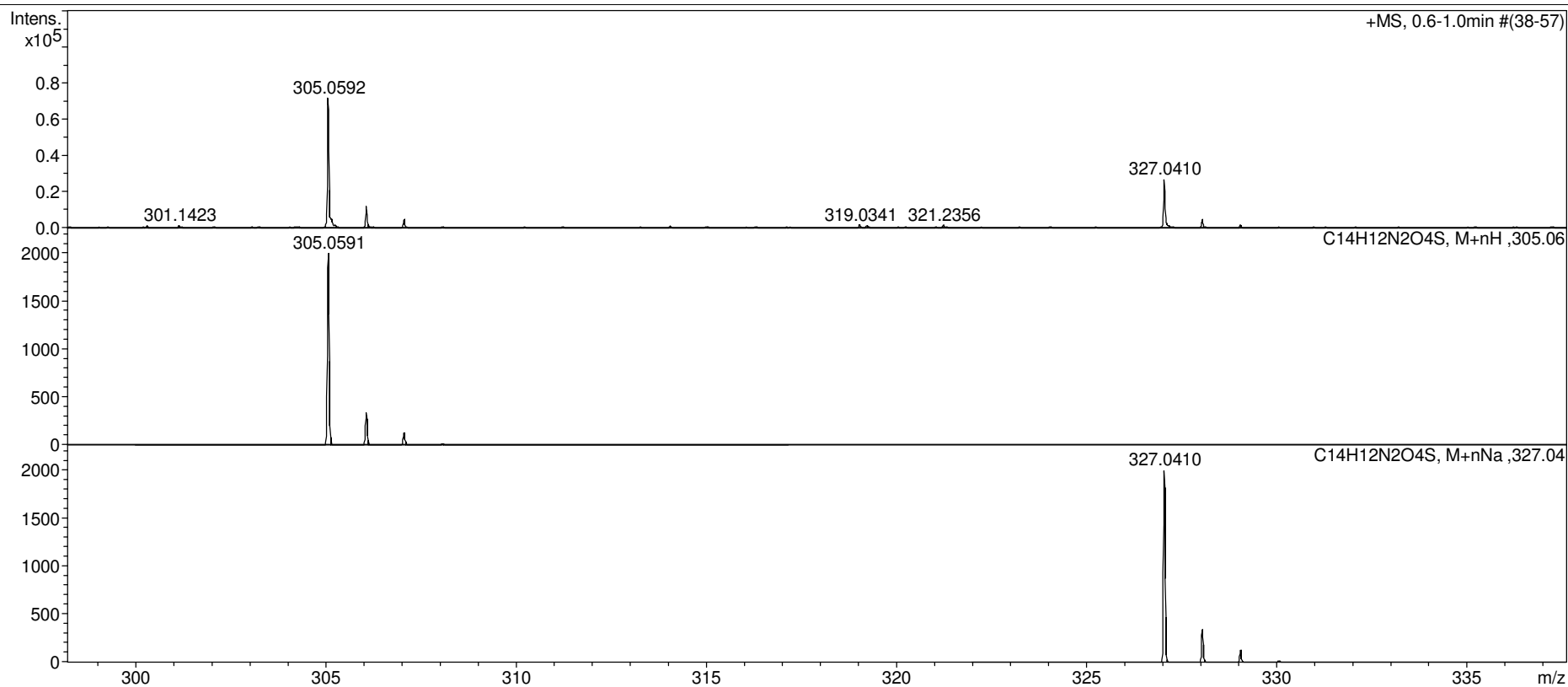
Analysis Info

Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428026.d
Method tune_50-1600.m
Sample Name /LPIK AF-426
Comment C14H12N2O4S mH 305.0590 clb added CH3OH

Acquisition Date 28.04.2021 12:56:11
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

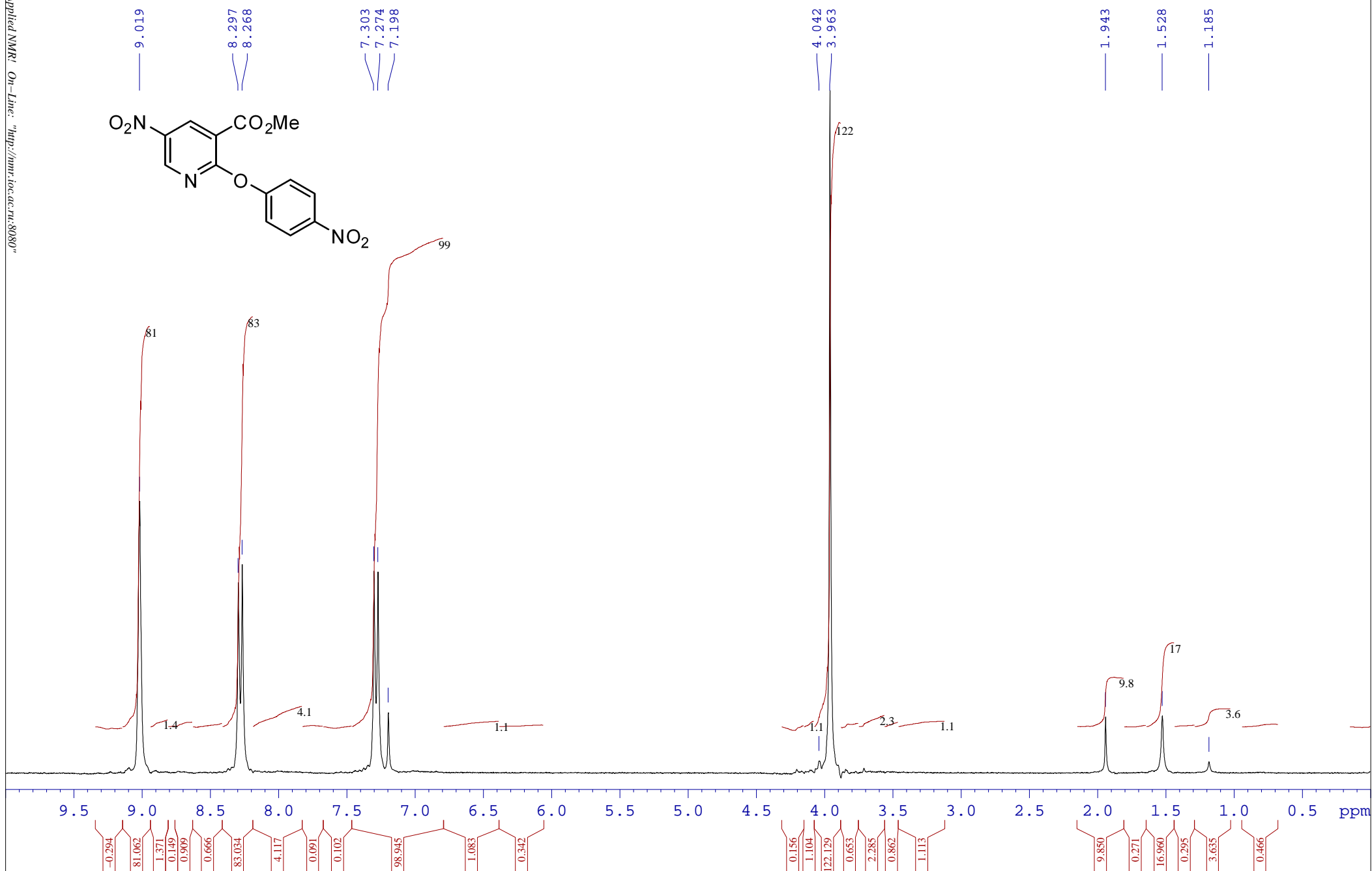
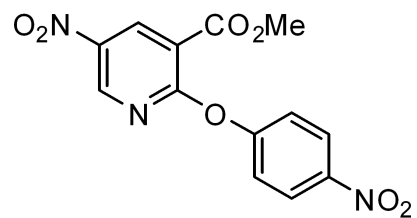
Acquisition Parameter

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





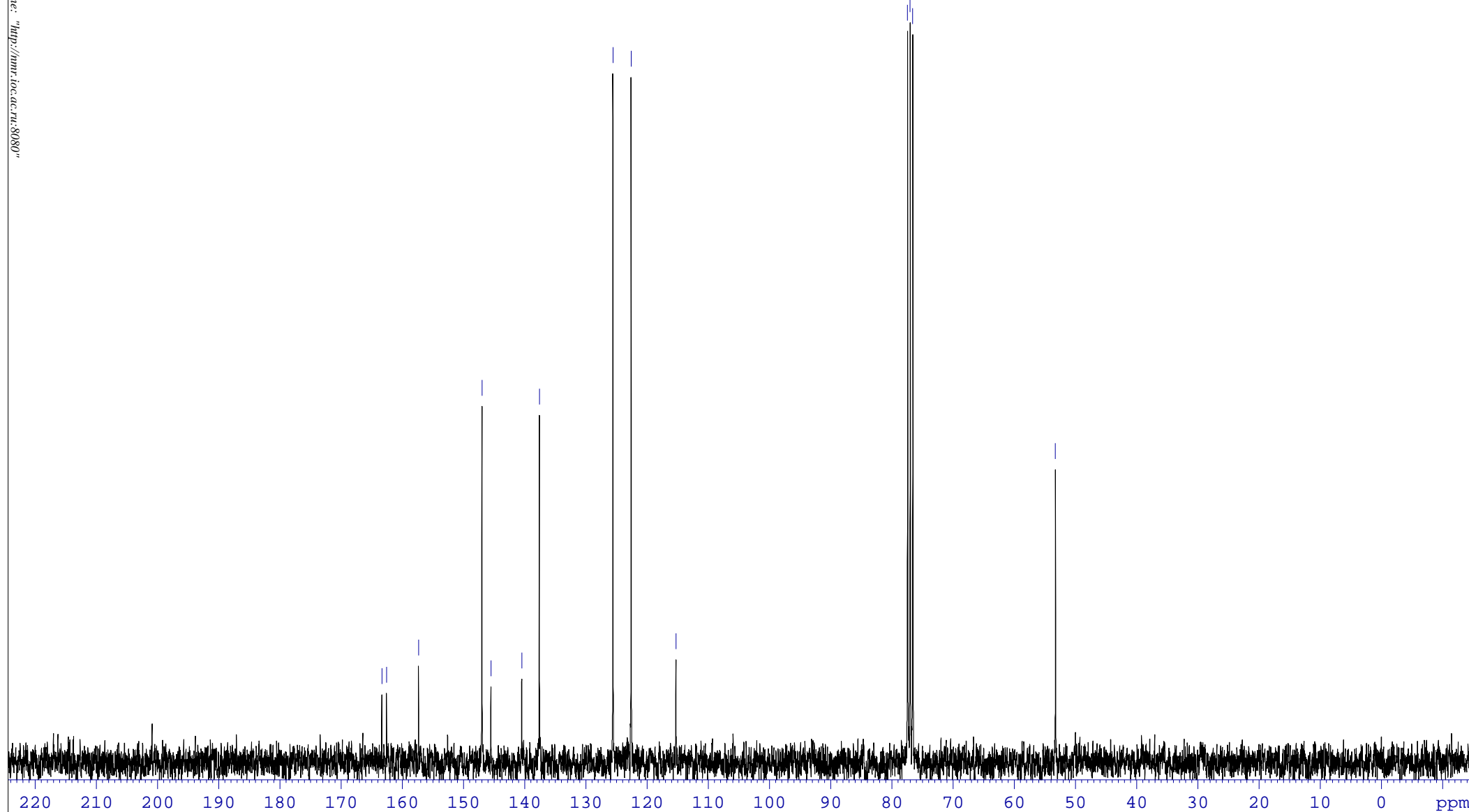
/LPIK AF427





/LPIK AF-427.13 Kokorekin-20259

163.325
162.573
157.338
146.968
145.506
140.466
137.587
125.568
122.598
115.275
77.465
77.042
76.618
53.303



Display Report

Analysis Info

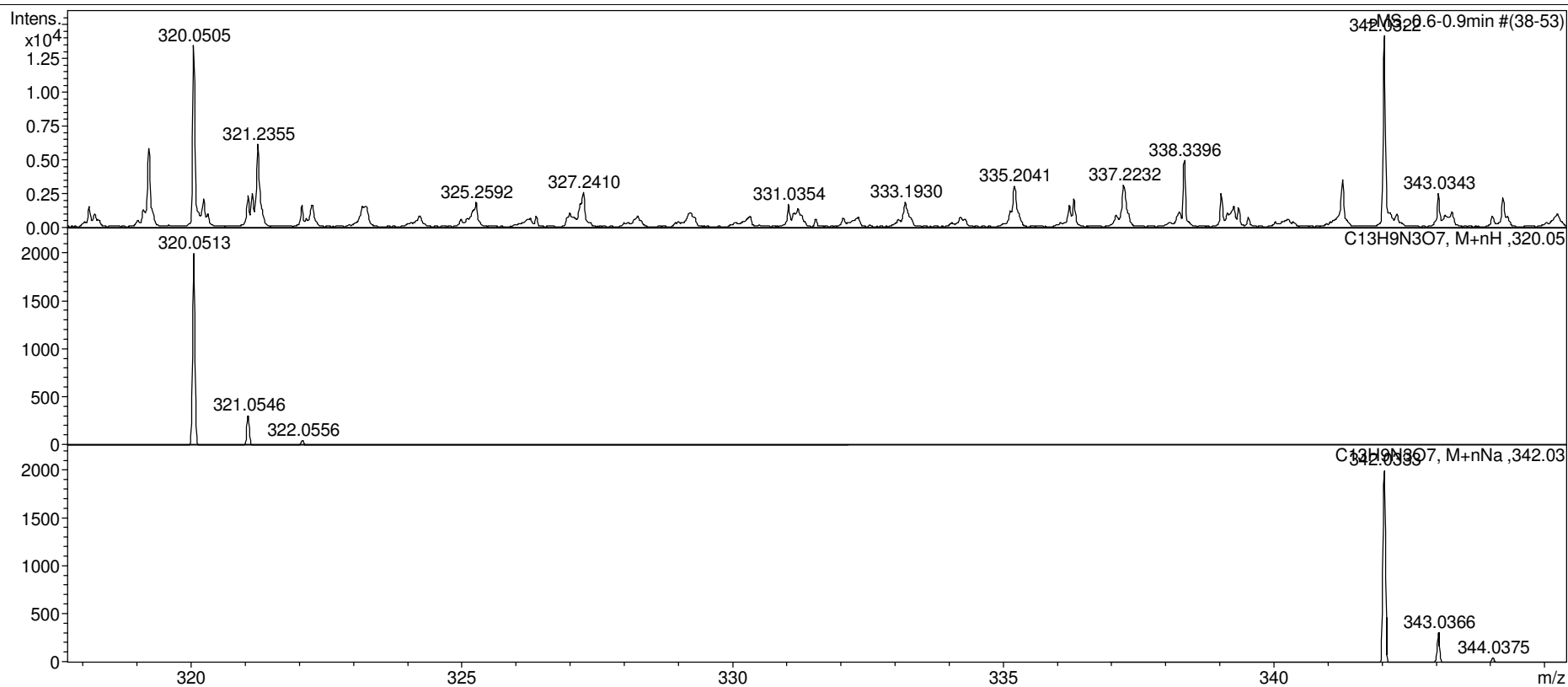
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428027.d
Method tune_50-1600.m
Sample Name /LPIK AF-427
Comment C13H9N3O7 mH 320.0513 clb added CH3OH

Acquisition Date 28.04.2021 13:01:04

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



Display Report

Analysis Info

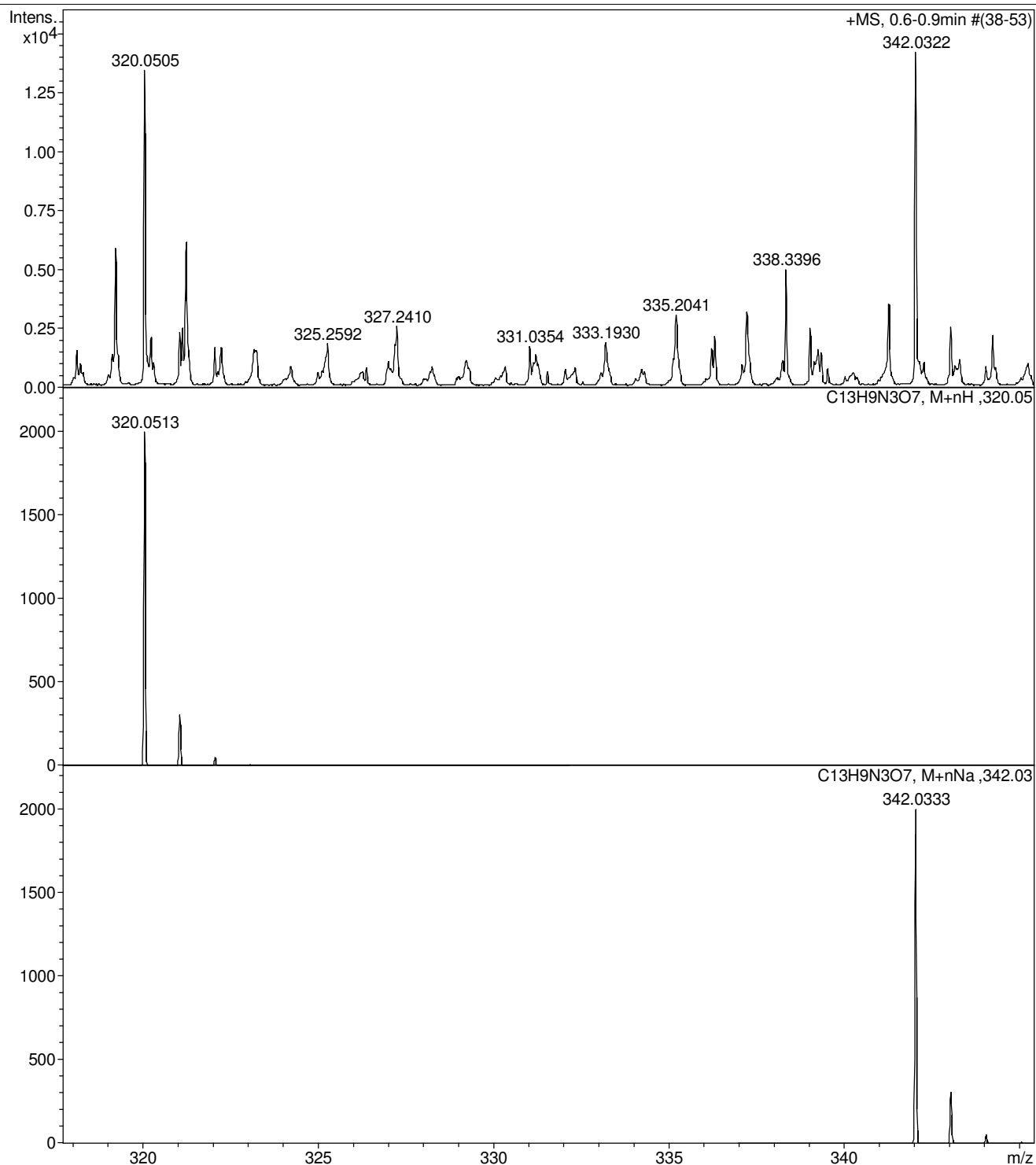
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428027.d
Method tune_50-1600.m
Sample Name /LPIK AF-427
Comment C13H9N3O7 mH 320.0513 clb added CH3OH

Acquisition Date 28.04.2021 13:01:04

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

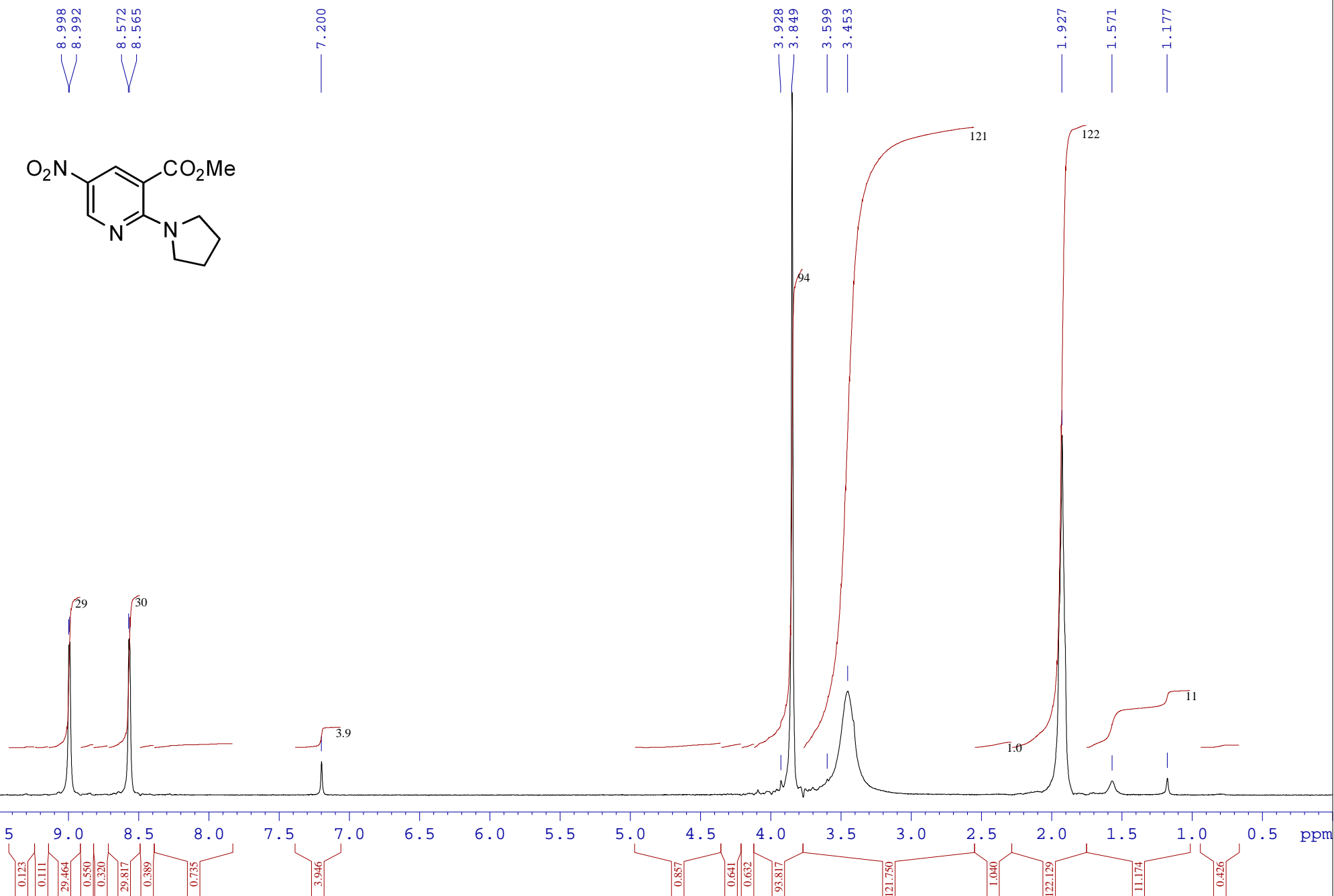
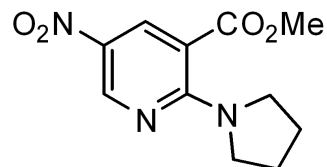
Acquisition Parameter

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



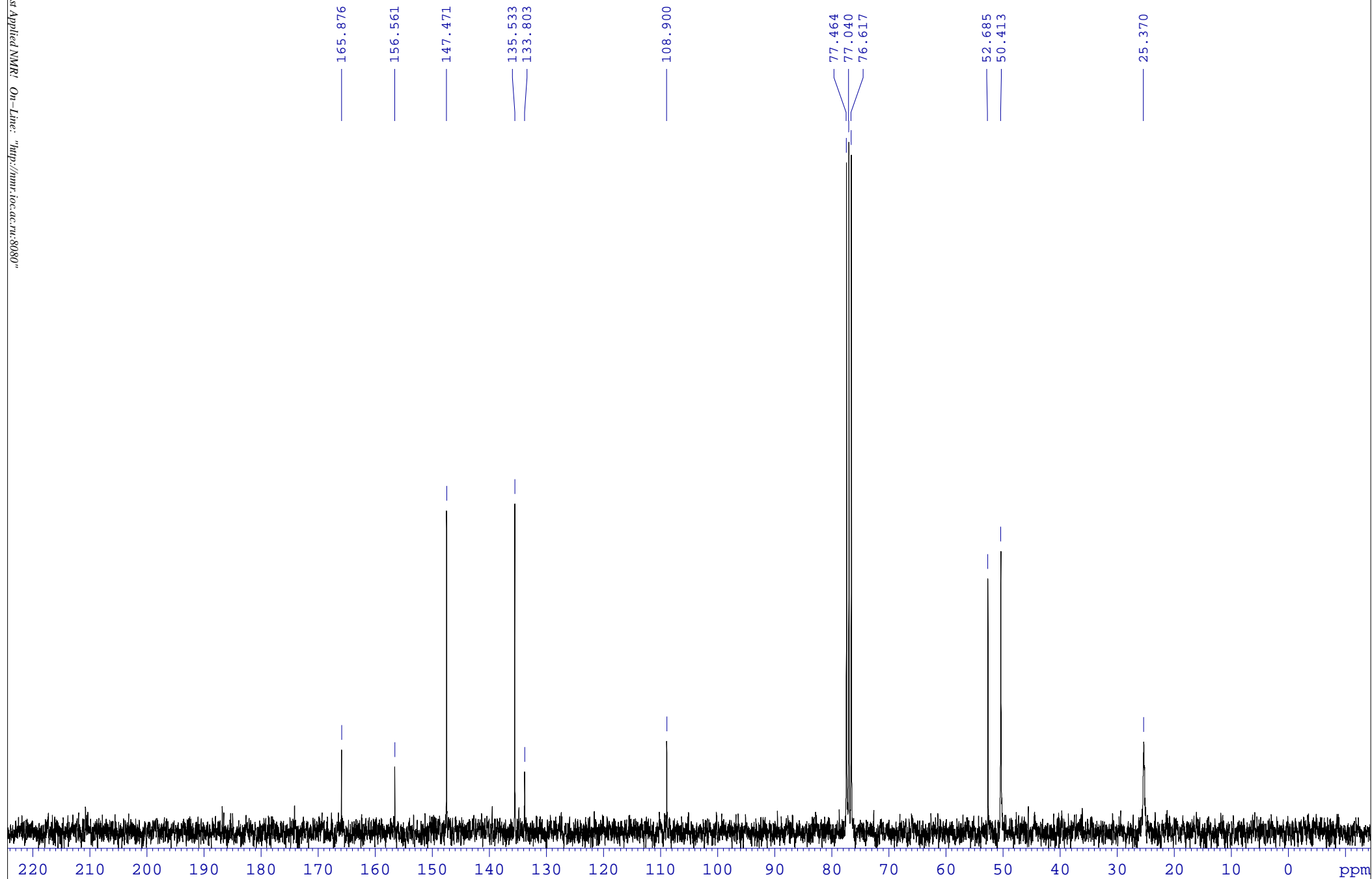


/LPIK AF428





/LPIK AF-428.13 Kokorekin-20259



Display Report

Analysis Info

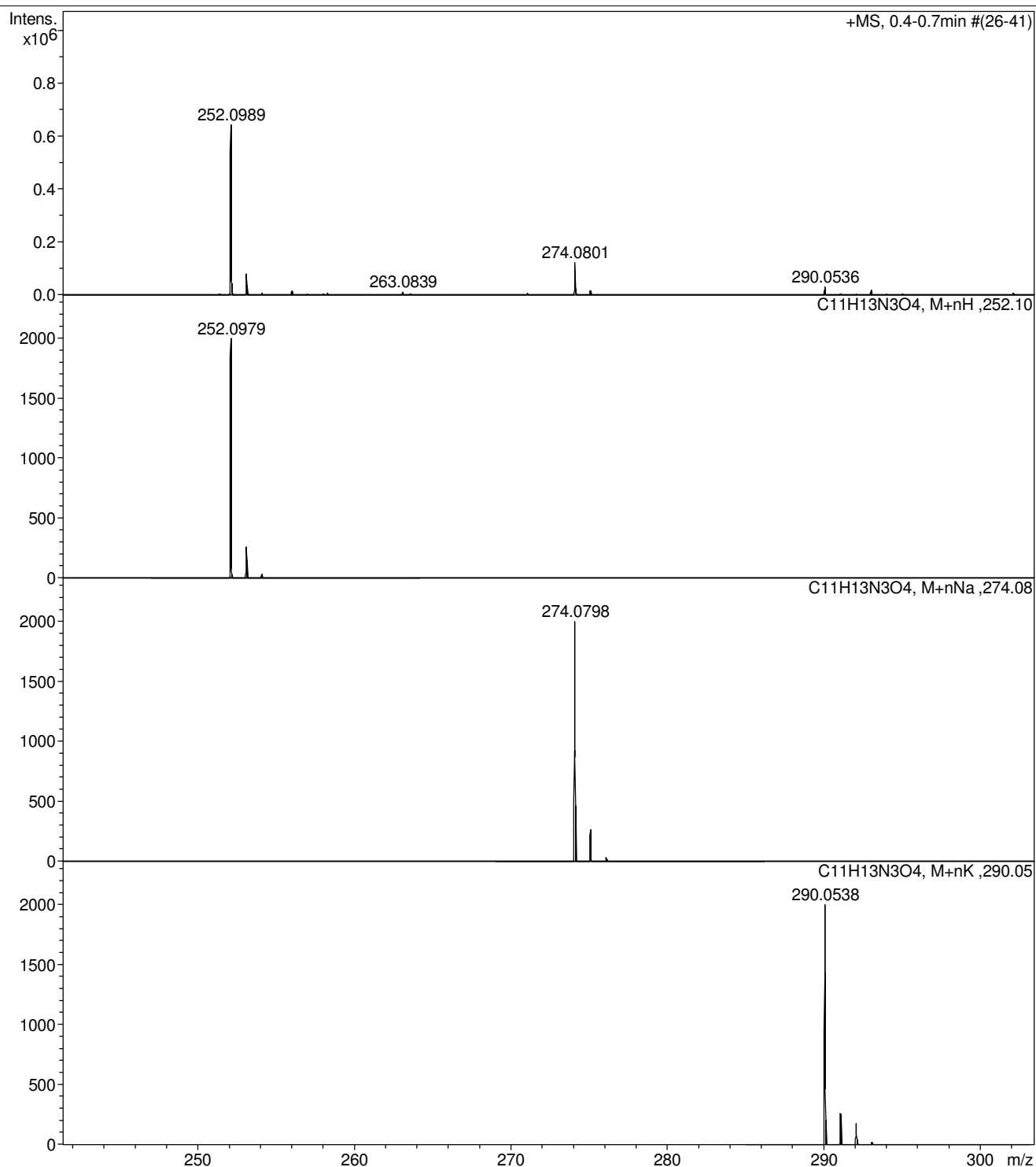
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428028.d
Method tune_50-1600.m
Sample Name /LPIK AF-428
Comment C11H13N3O4 mH 252.0978 clb added CH3OH

Acquisition Date 28.04.2021 13:16:27

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

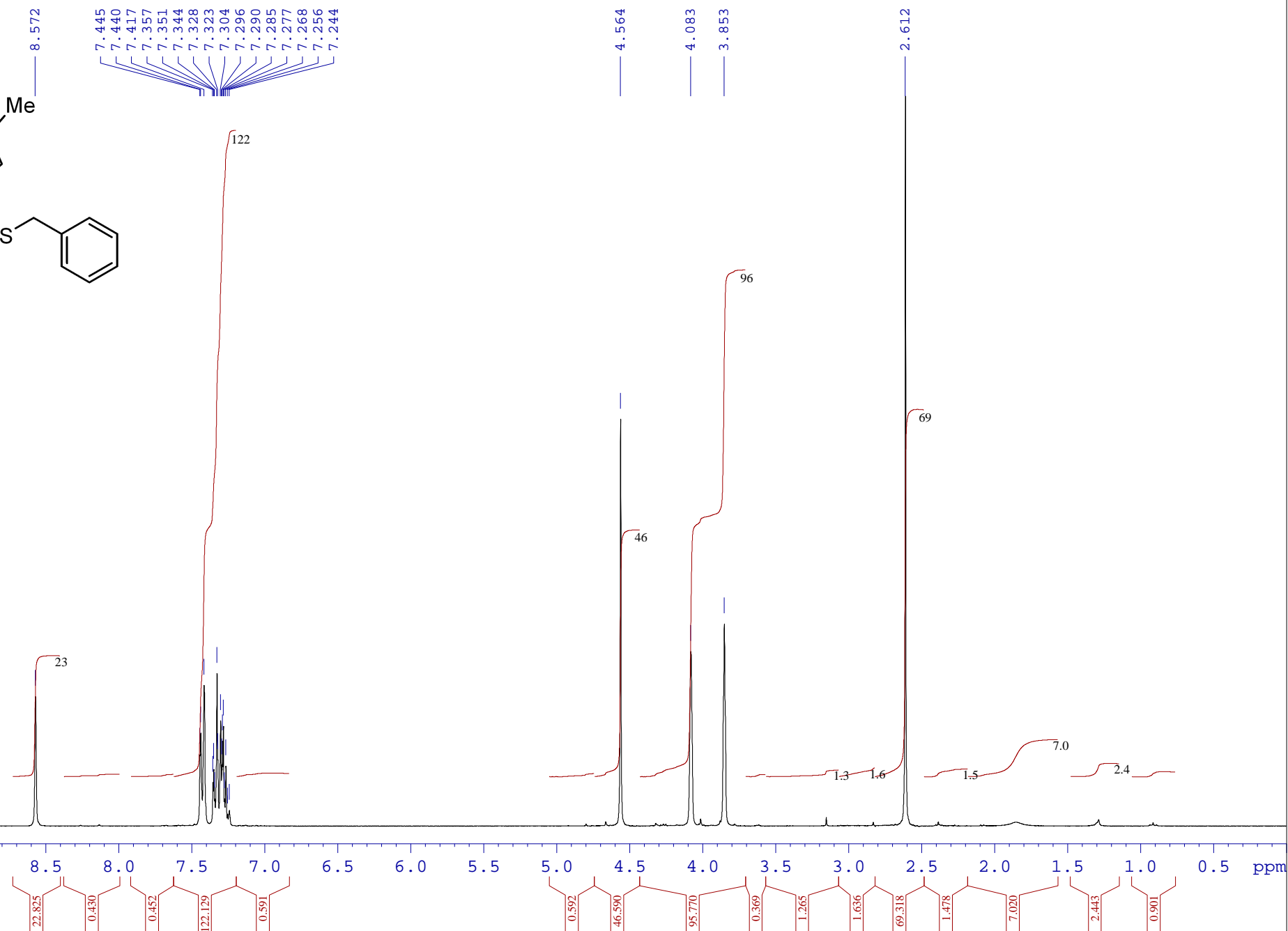
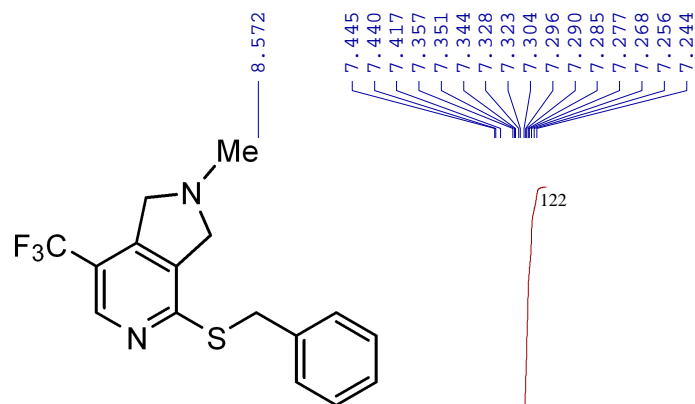
Acquisition Parameter

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



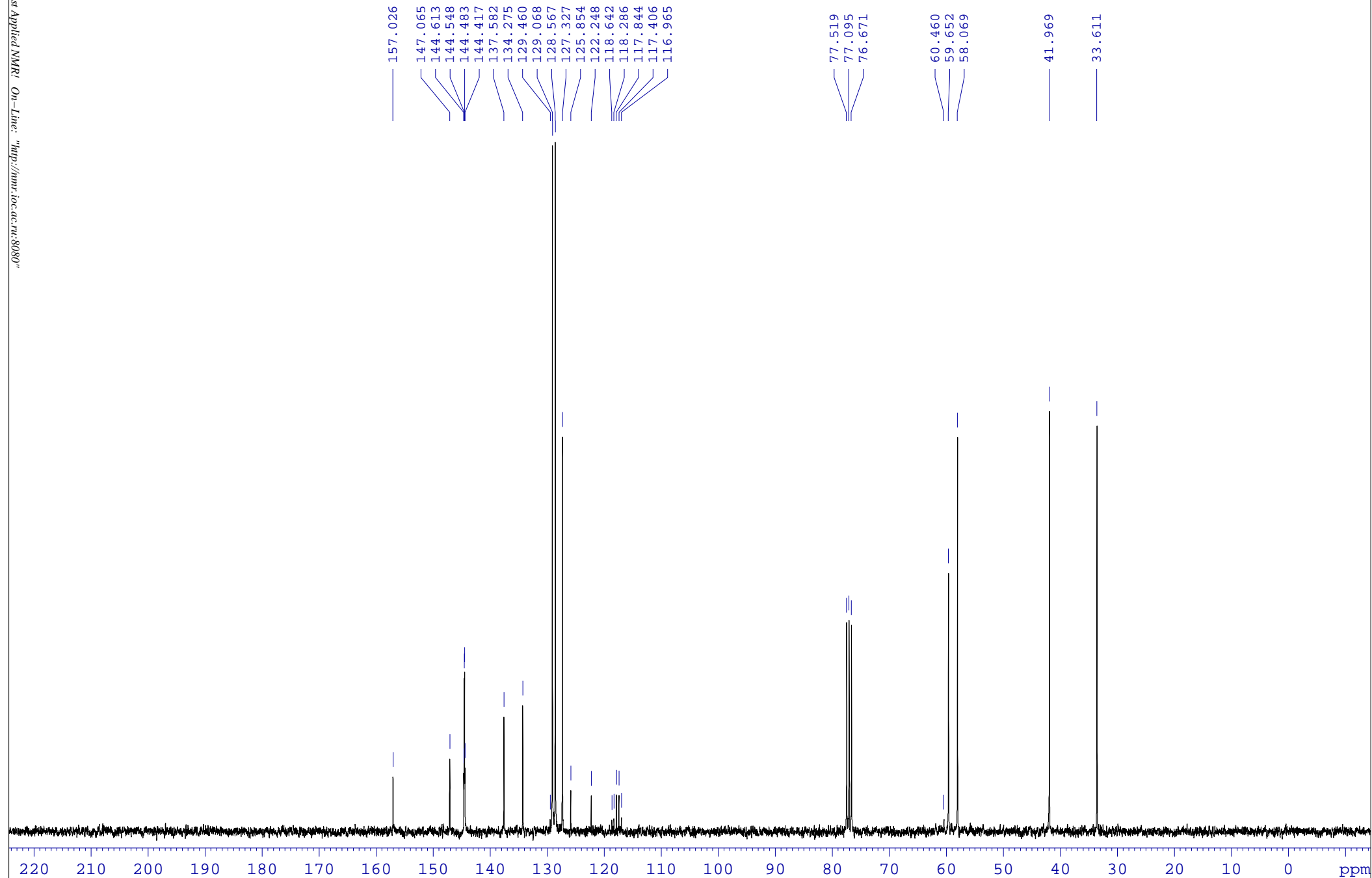


/LPIK AF-365.3 Kokorekin-20259





/LPIK AF-365.1.13 Kokorekin-20259



Display Report

Analysis Info

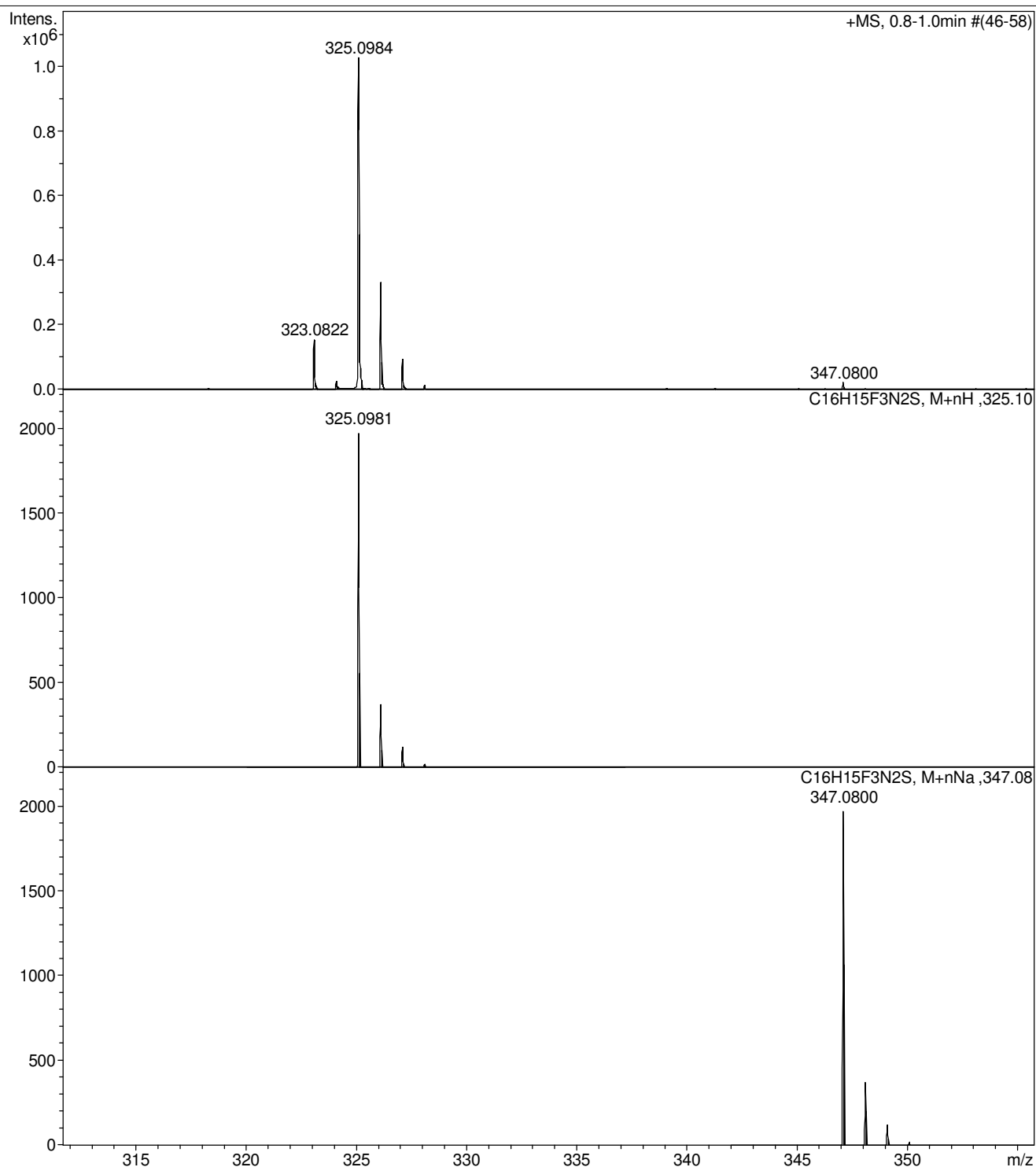
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0211015.d
Method tune_50-1600.m
Sample Name /lpik AF-365
Comment C16H15F3N2S mH 325.0980 alibrant added CH3OH

Acquisition Date 11.02.2021 11:47:29

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

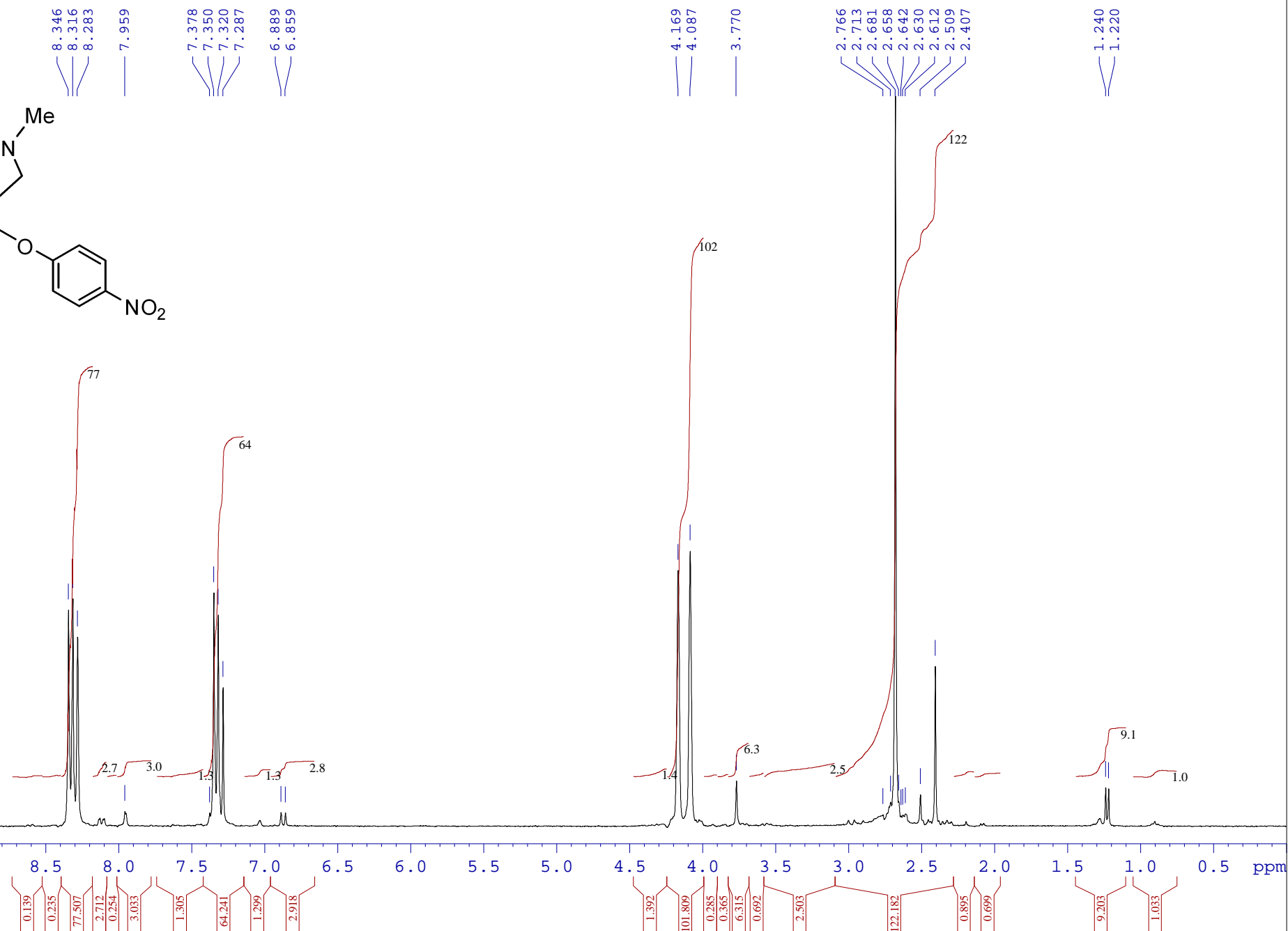
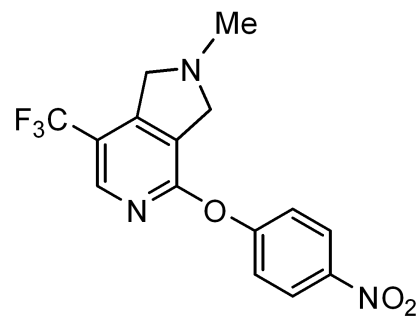
Acquisition Parameter

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





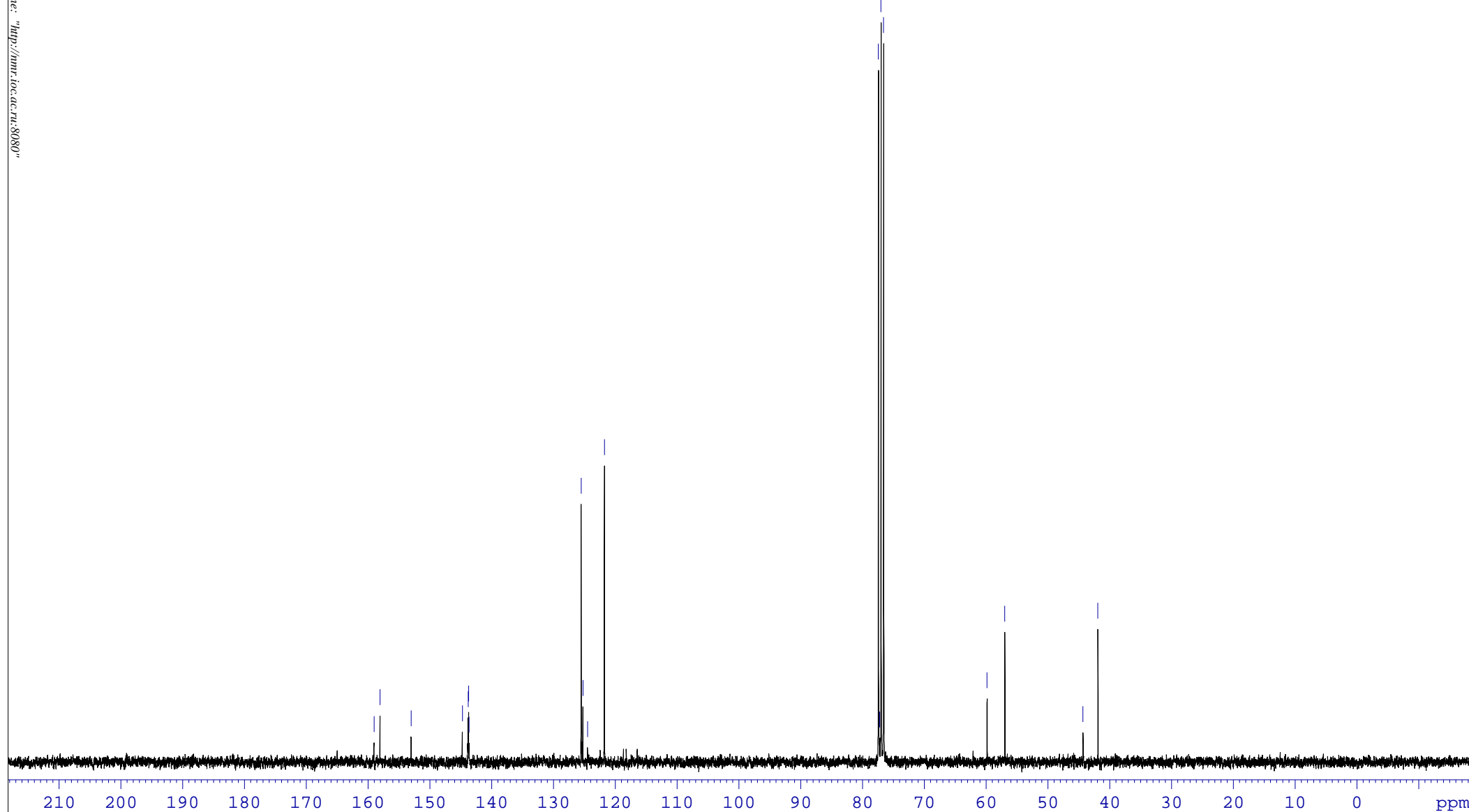
/LPIK AF-367.R





/LPIK AF-367.C13 CDCl3 13C 20mg 1024scans

159.021
158.066
153.031
144.728
143.801
143.732
143.665
125.514
125.223
124.485
121.750
77.453
77.228
77.029
76.606
59.866
56.996
44.345
41.937



Display Report

Analysis Info

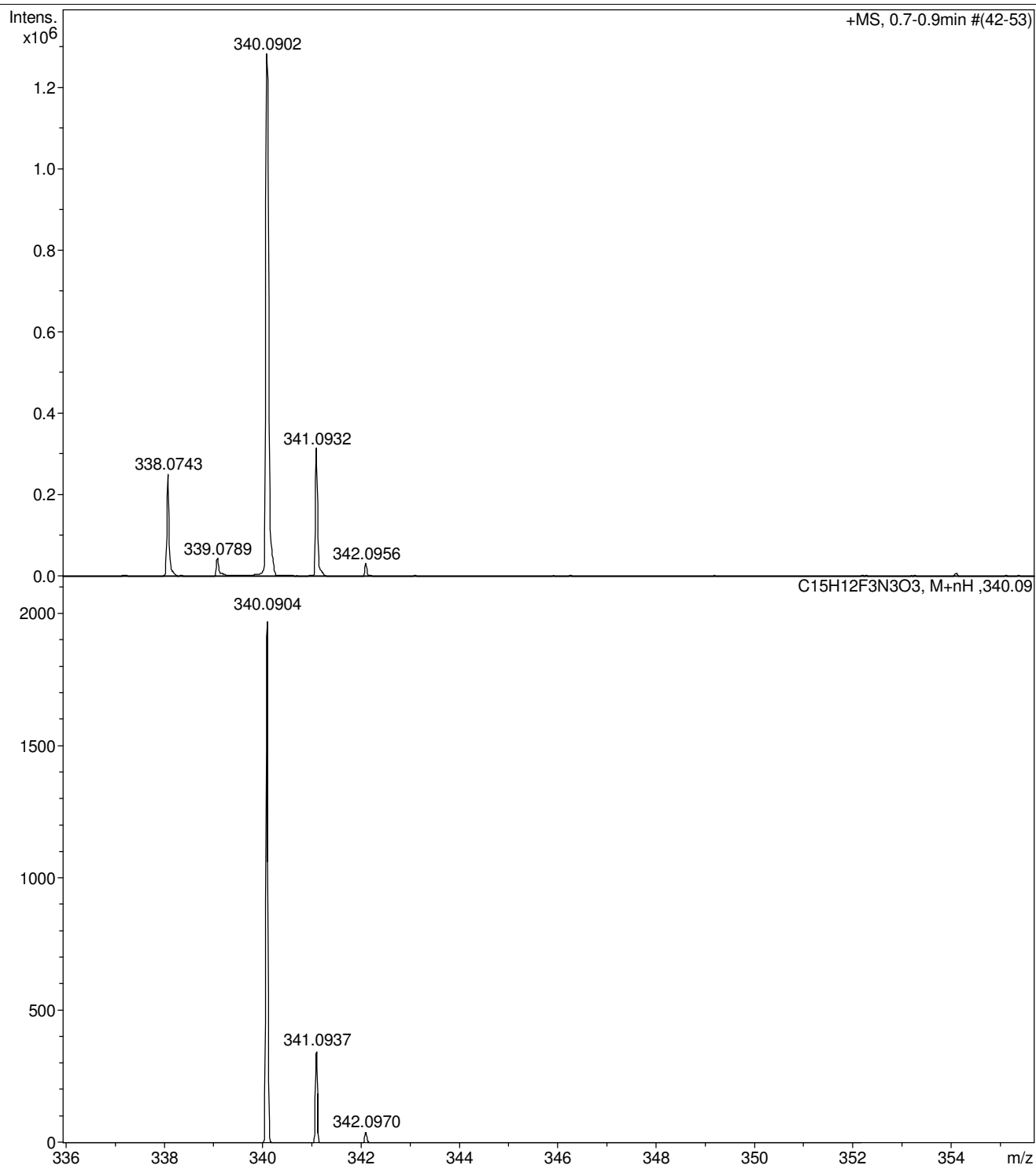
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0211016.d
Method tune_50-1600.m
Sample Name /lpik AF-367
Comment C15H12F3N3O3 mH 340.0903 alibrant added CH3OH

Acquisition Date 11.02.2021 11:56:34

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

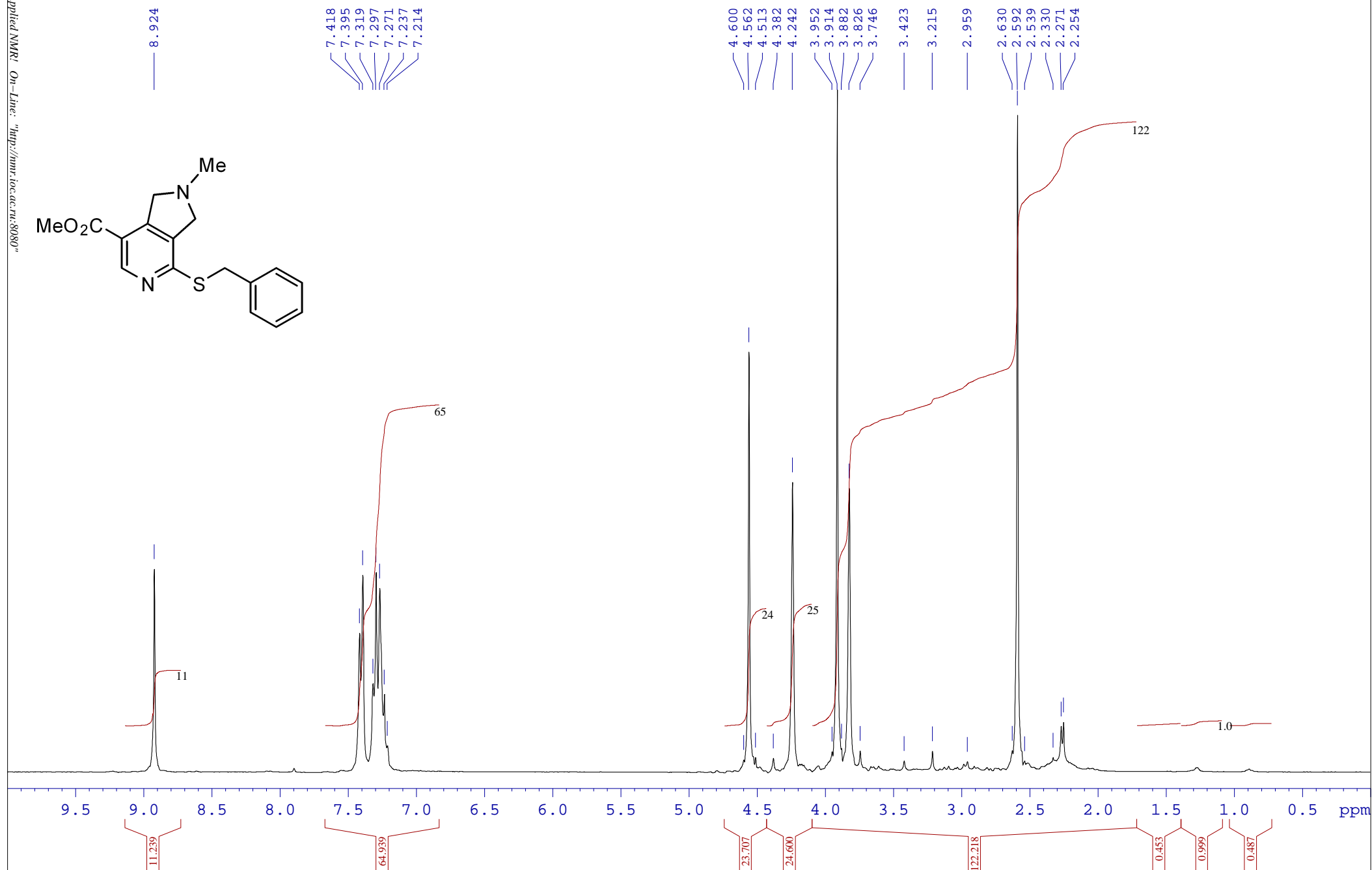
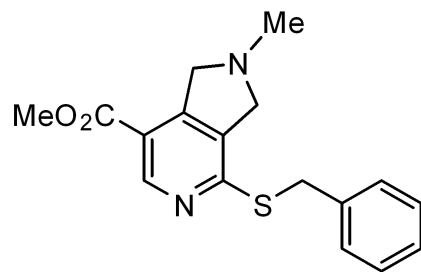
Acquisition Parameter

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



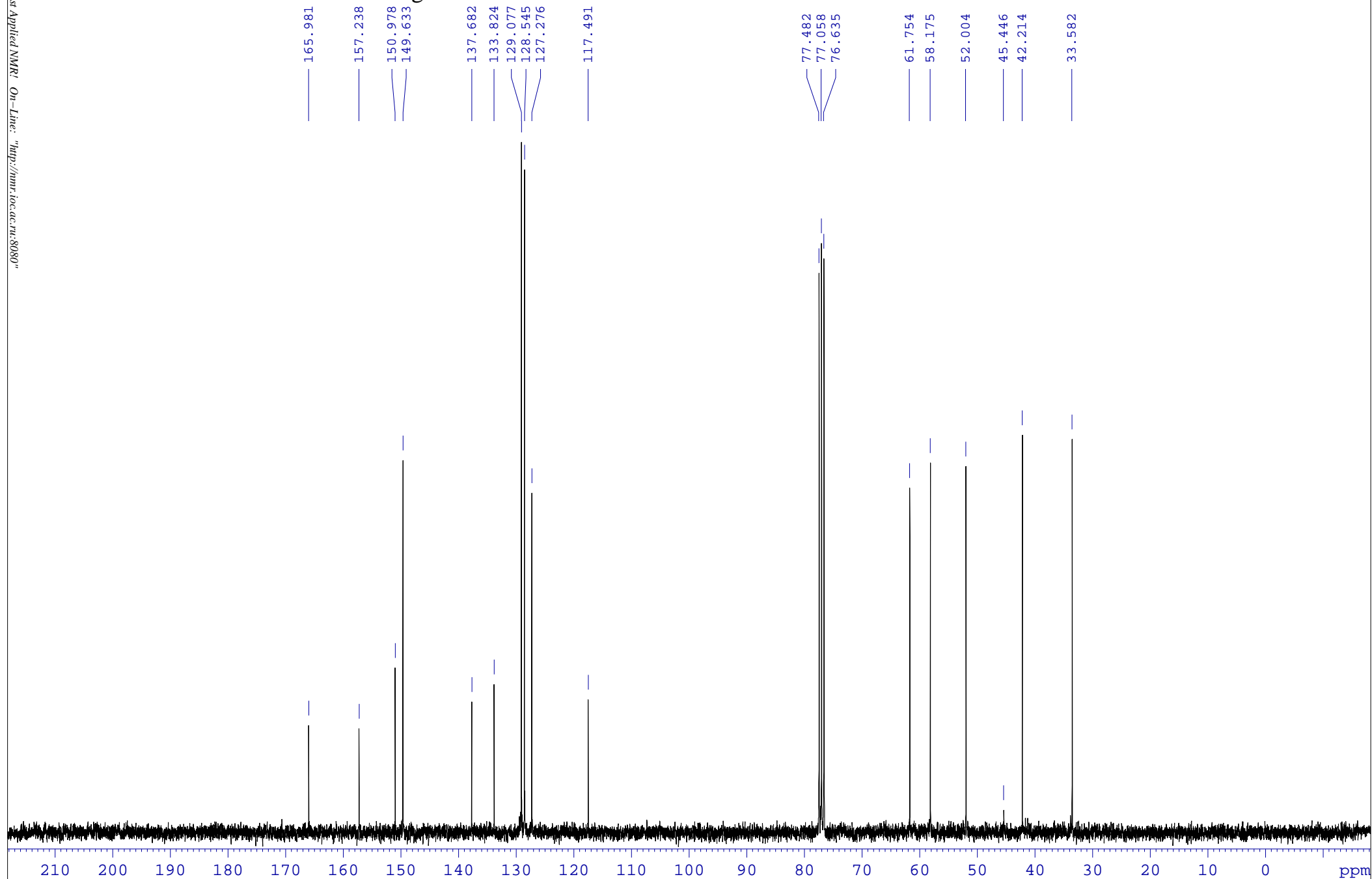


/LPIK AF-388





/LPIK AF-388.C13 CDCl3 13C 25mg 512scans



Display Report

Analysis Info

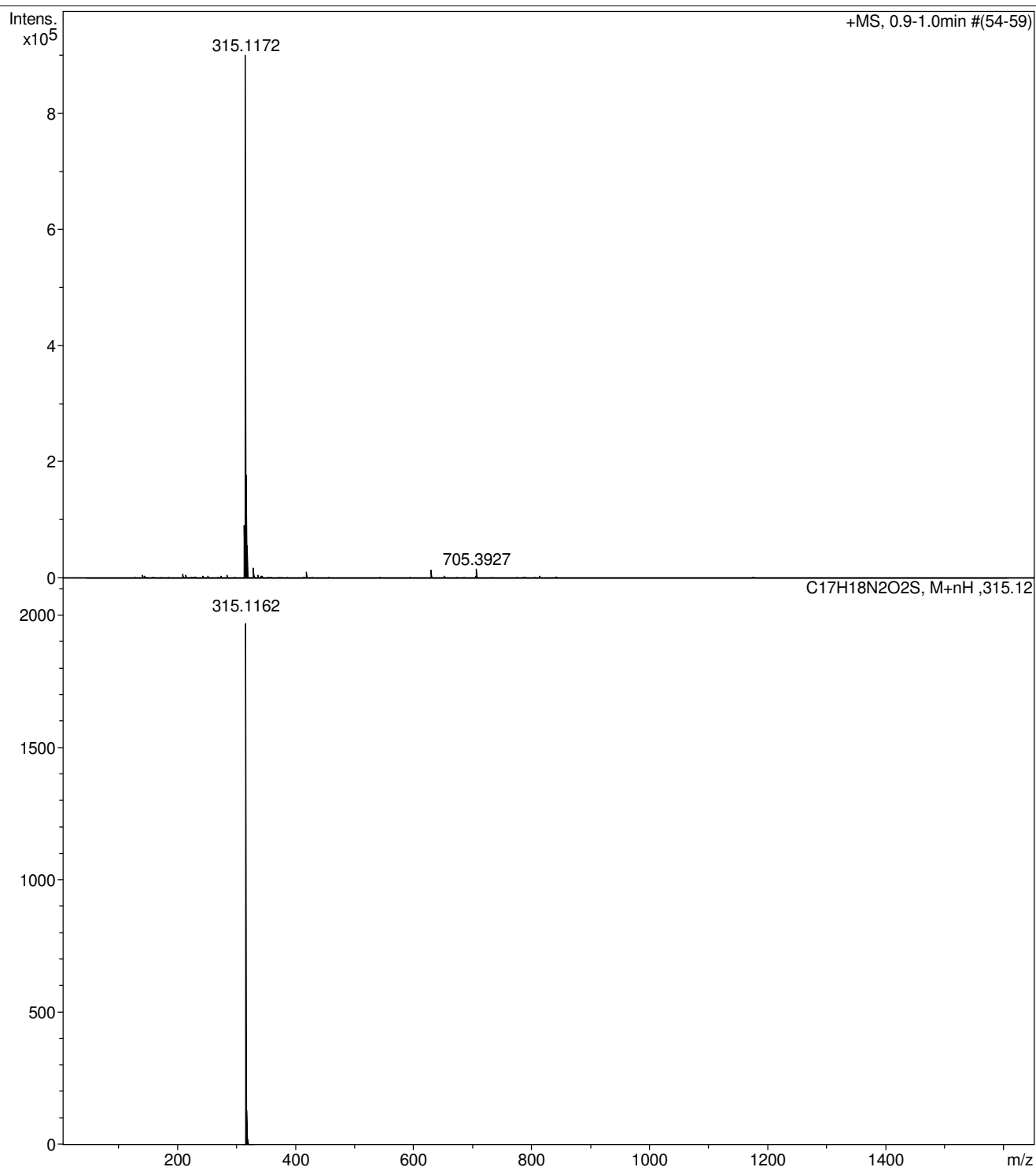
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0210030.d
Method tune_50-1600.m
Sample Name /LPIK AF-388
Comment C17H18N2O2S mH 315.0061 calibrant added CH3CN

Acquisition Date 10.02.2021 21:06:14

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

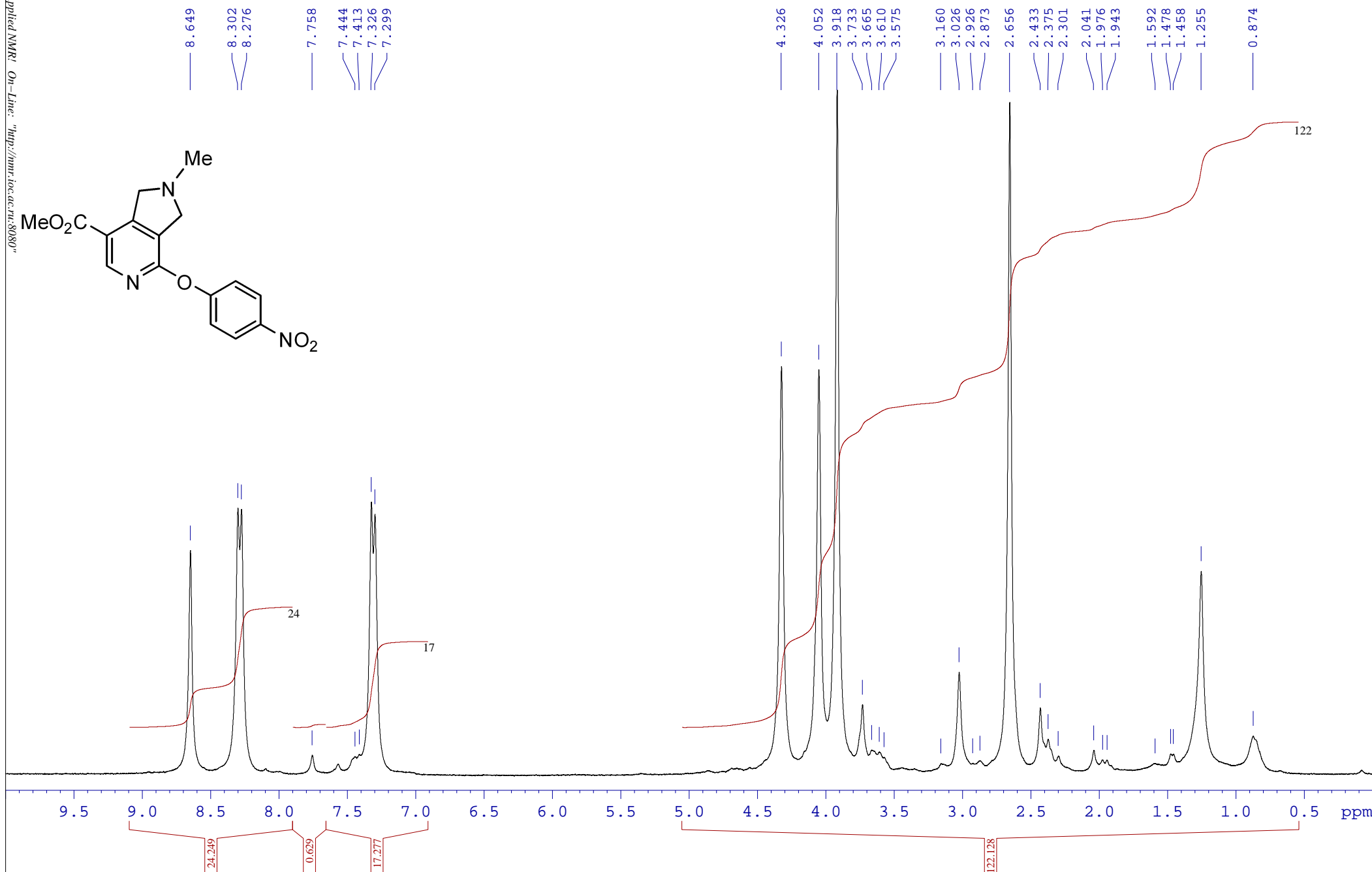
Acquisition Parameter

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





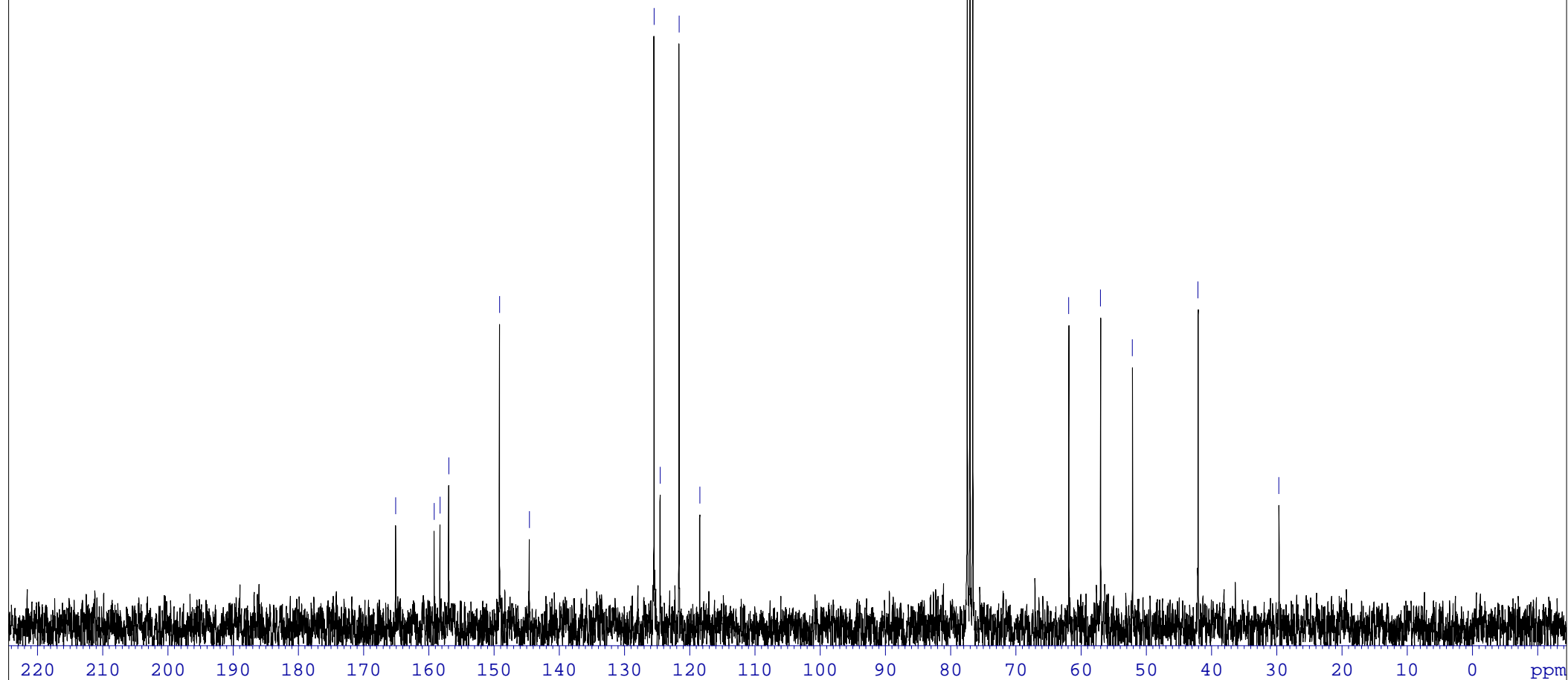
/LPIK AF-402.2 Kokorekin-20259





/LPIK AF-402.2.13 Kokorekin-20259

165.087
159.179
158.278
156.934
149.152
144.579
125.464
124.531
121.624
118.448
77.483
77.060
76.636
61.911
57.037
52.153
42.092
29.693



Display Report

Analysis Info

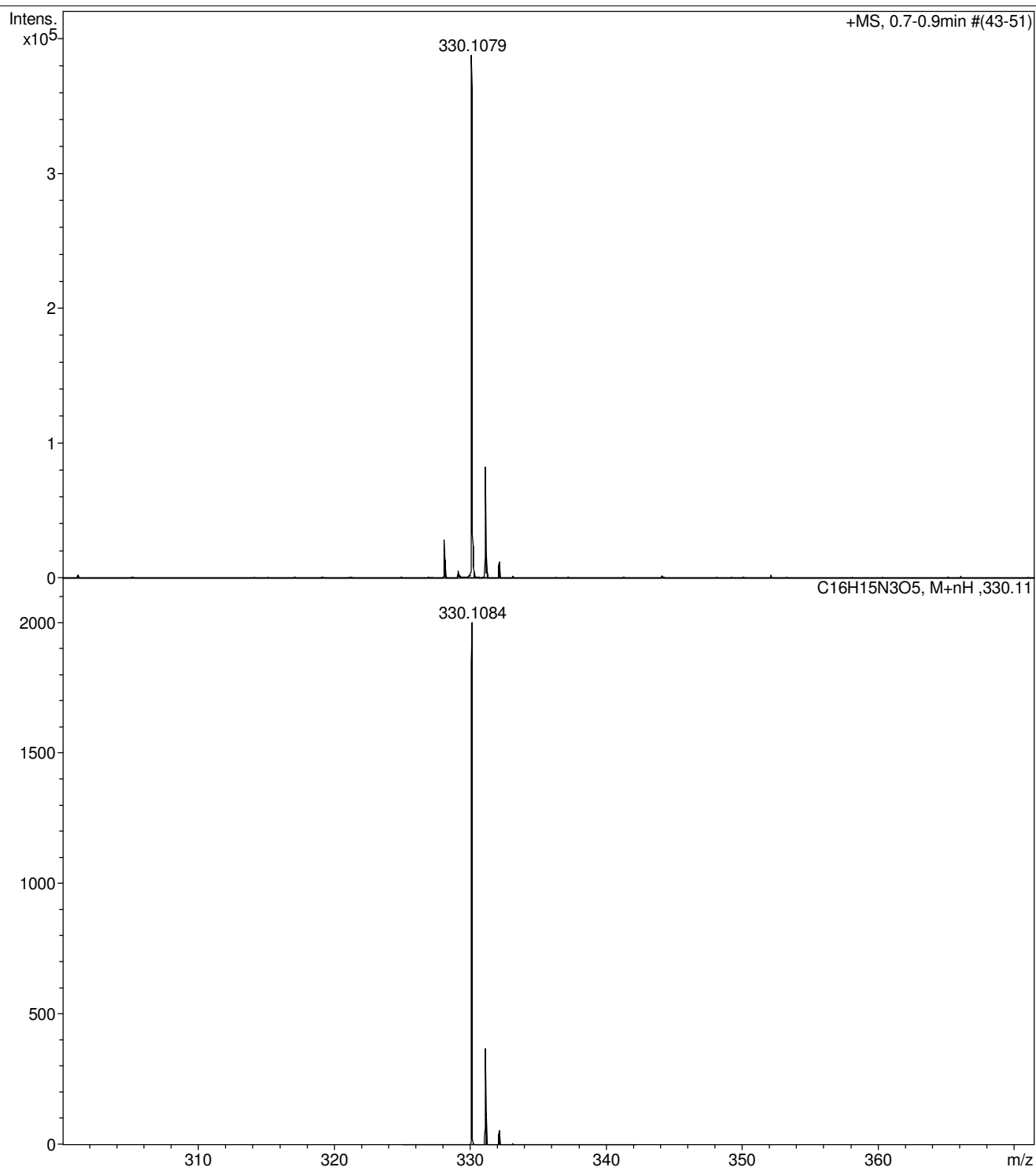
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0428029.d
Method tune_50-1600.m
Sample Name /LPIK AF-402
Comment C16H15N3O5 mH 330.1084 clb added CH3OH

Acquisition Date 28.04.2021 13:21:03

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

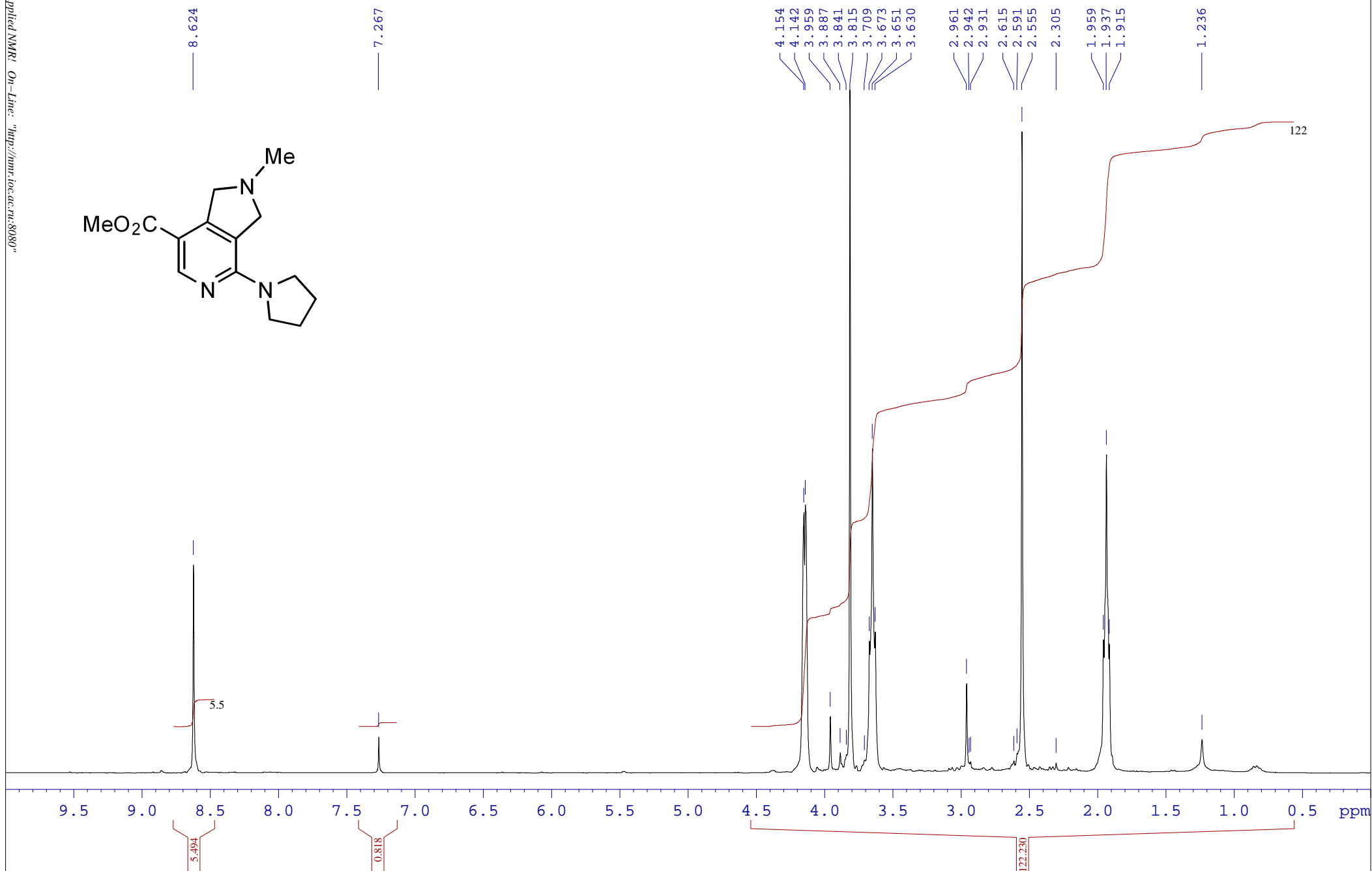
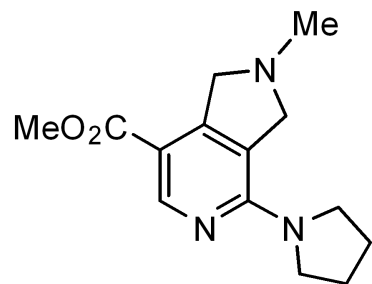
Acquisition Parameter

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



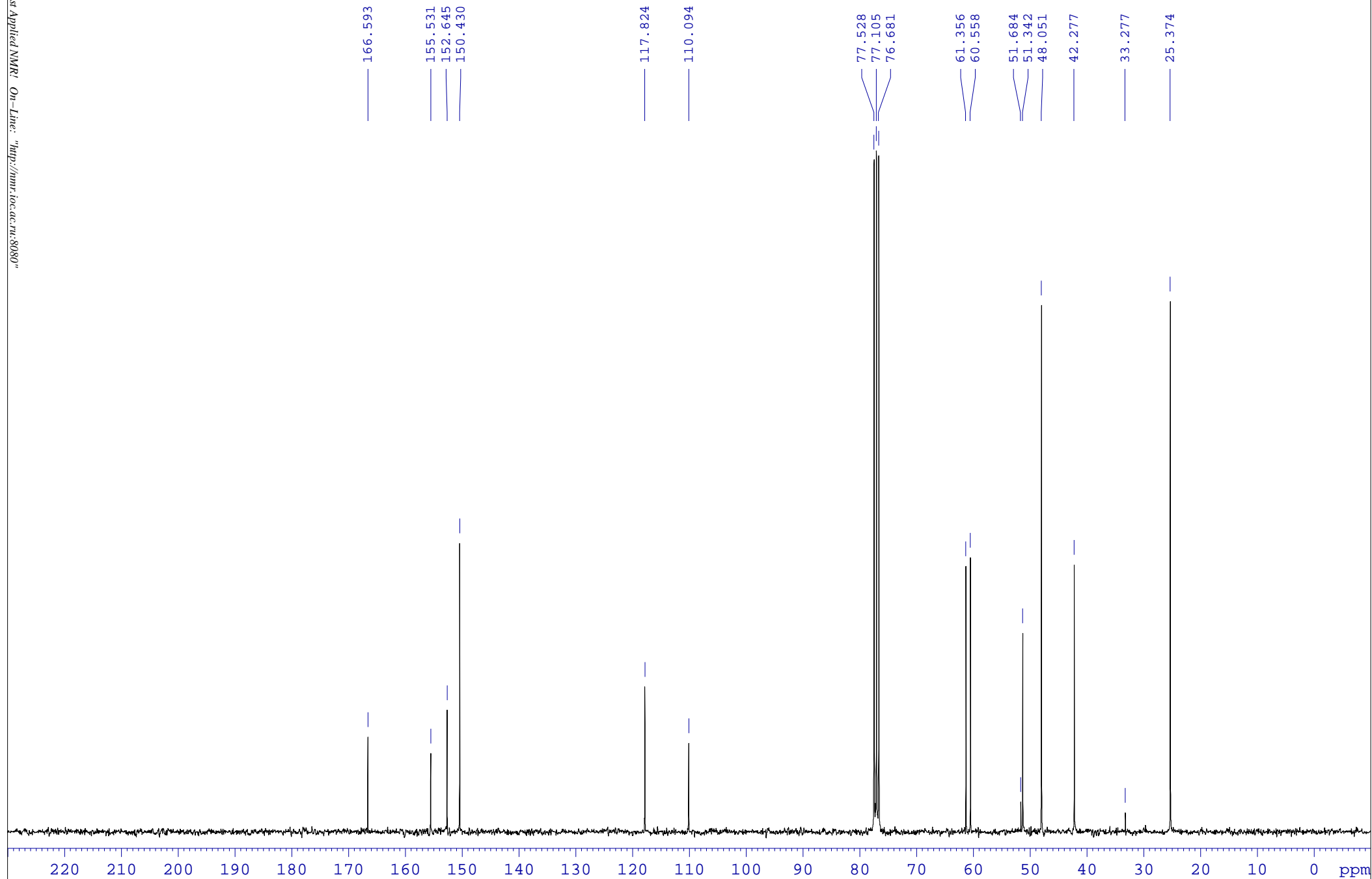


/LPIK AF-393.2





/LPIK AF-393.2.C13



Display Report

Analysis Info

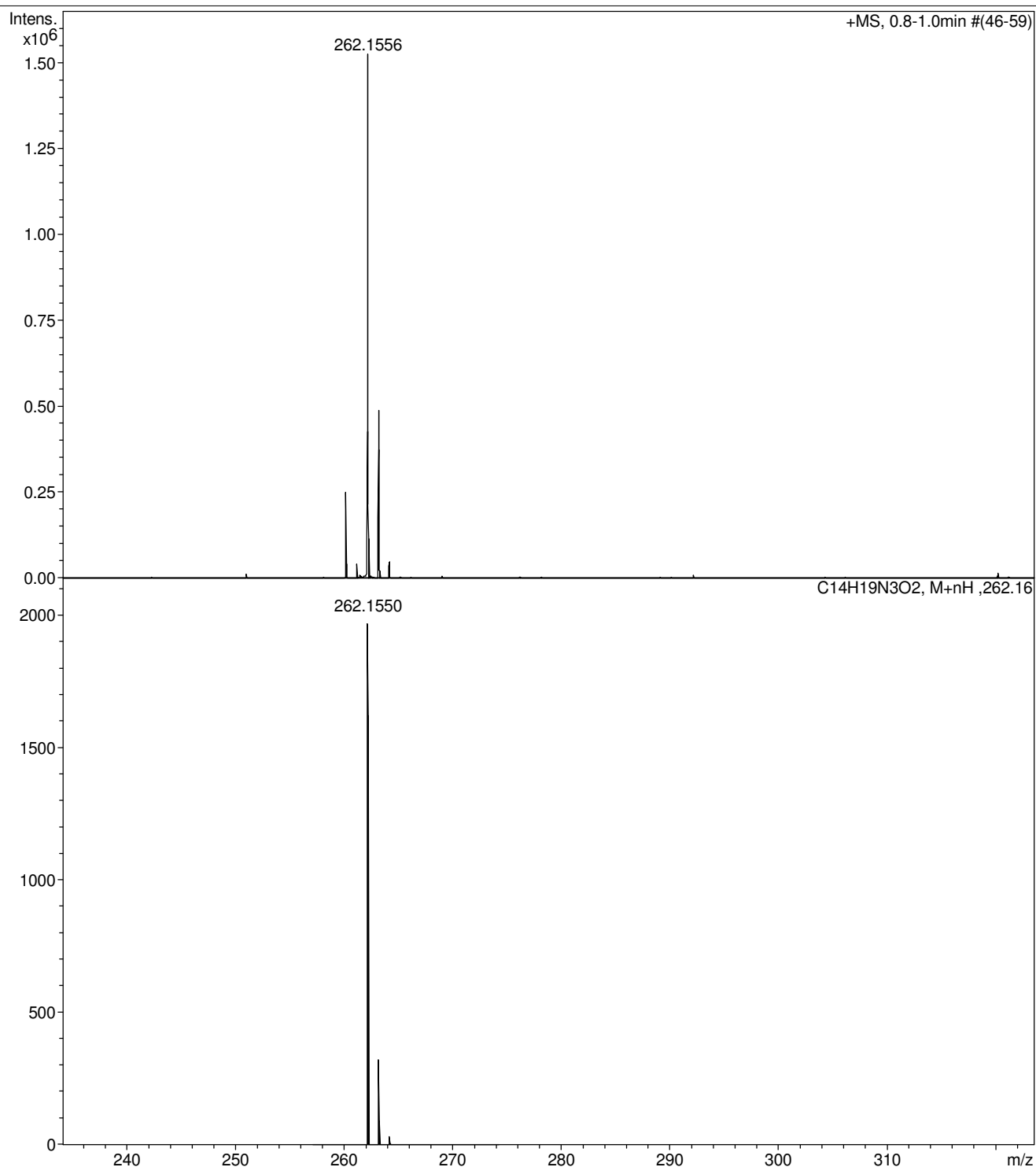
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0211021.d
Method tune_50-1600.m
Sample Name /LPIK AF-393.2
Comment C14H19N3O2 mH 262.1550alibrant added CH3OH

Acquisition Date 11.02.2021 12:48:04

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

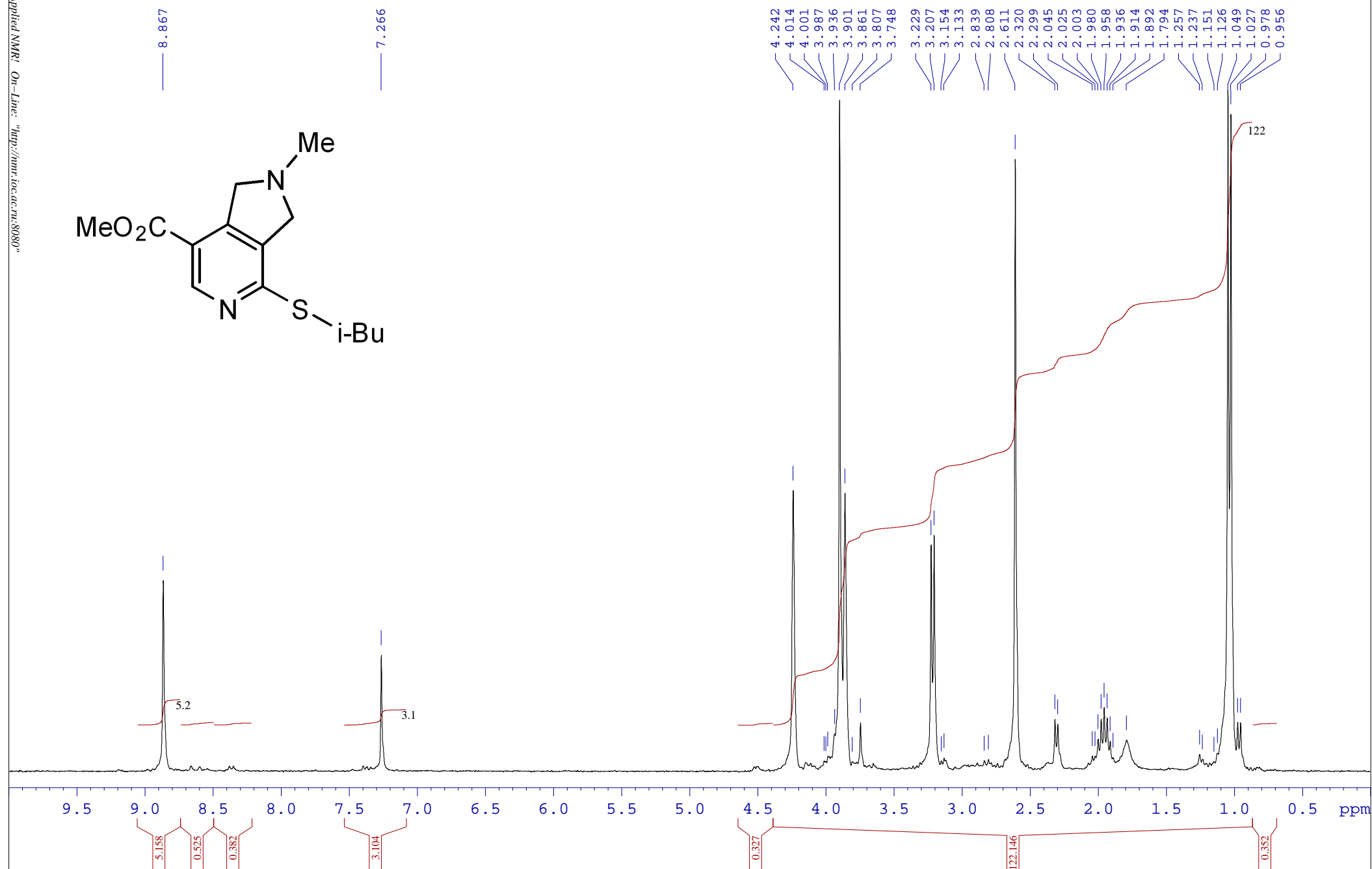
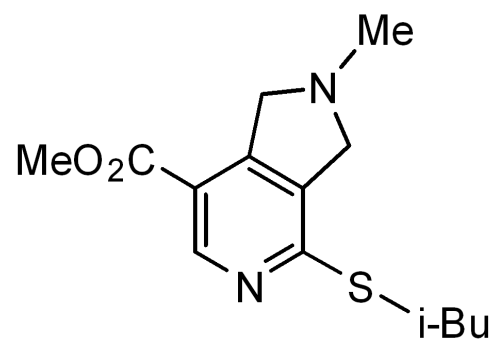
Acquisition Parameter

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



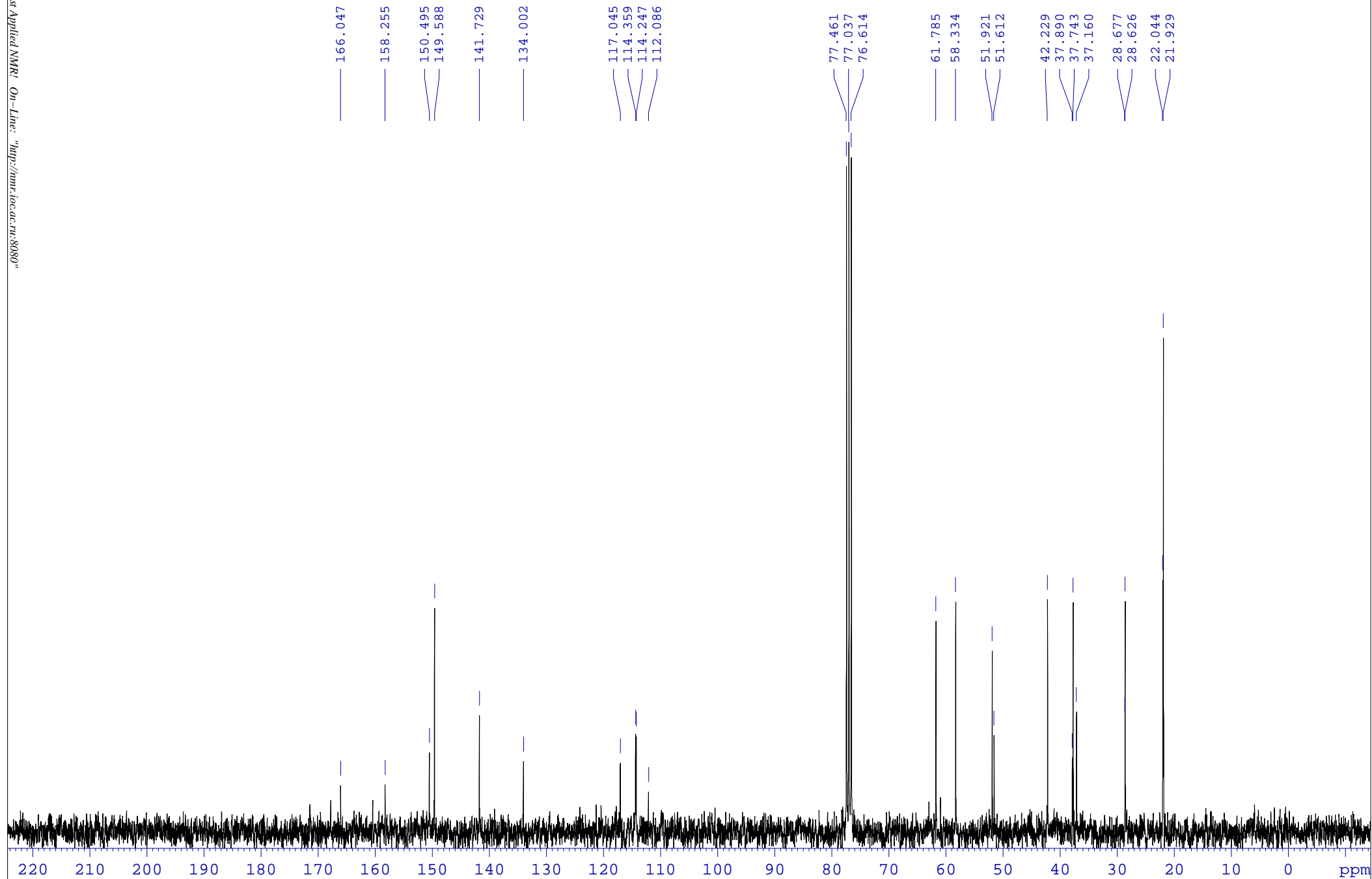


/LPIK AF-400.R





/LPIK AF-400.1.13 Kokorekin-20259



Display Report

Analysis Info

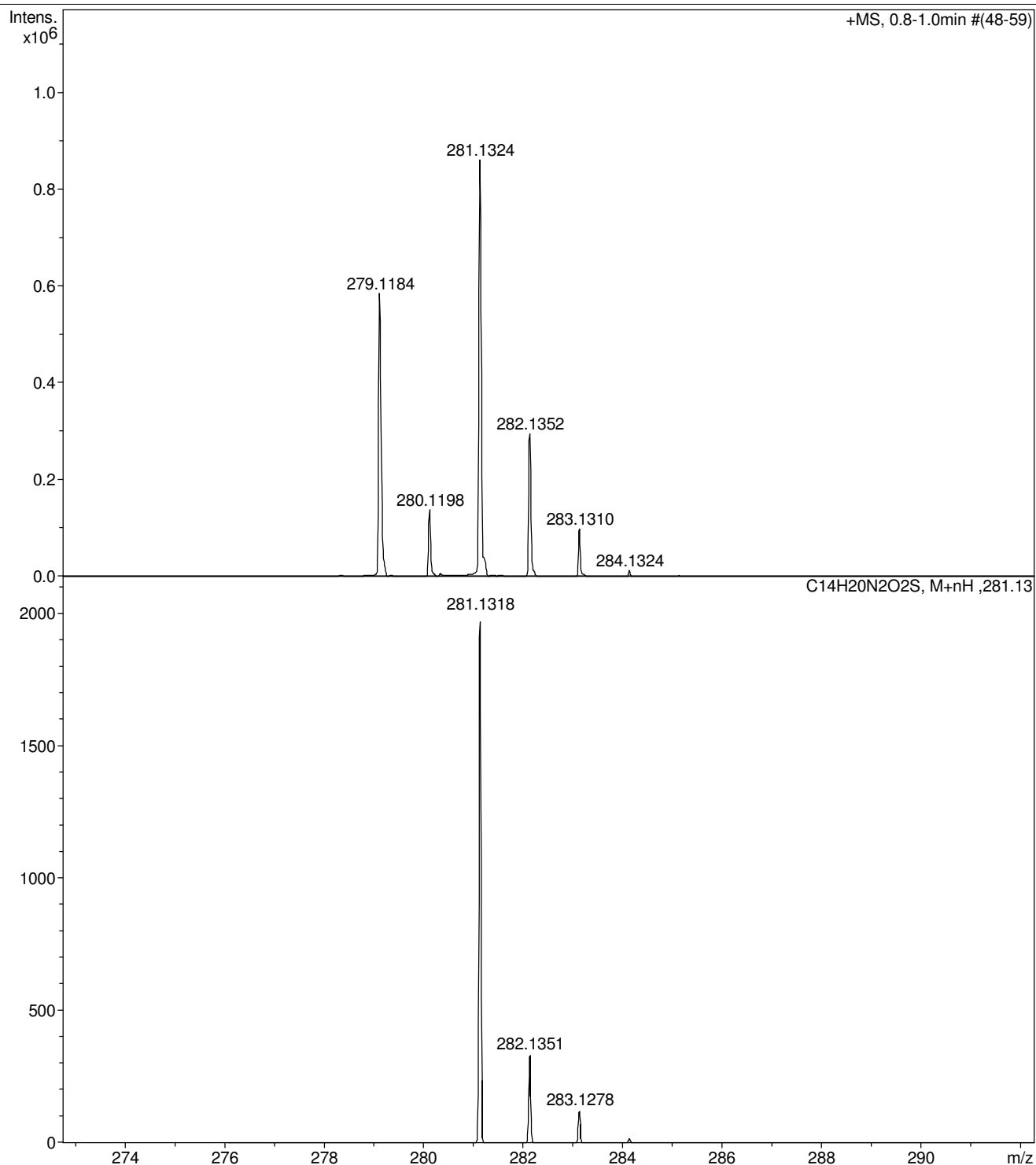
Analysis Name D:\Data\Kolotyrkina\2021\Bastrakov\0211023.d
Method tune_50-1600.m
Sample Name /LPIK AF-400
Comment C14H20N2O2S mH 281.1318 calibrant added CH3OH

Acquisition Date 11.02.2021 13:03:54

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

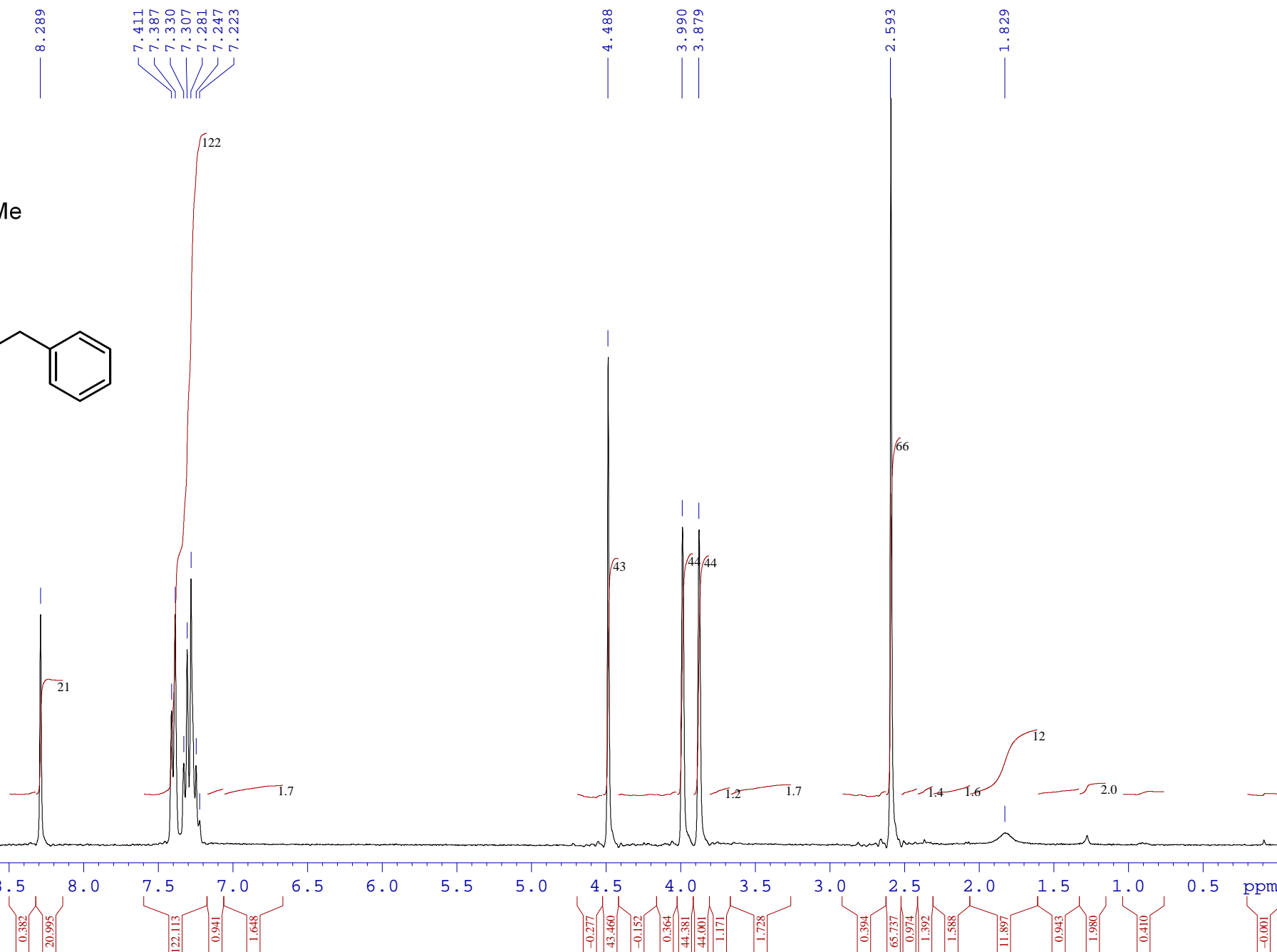
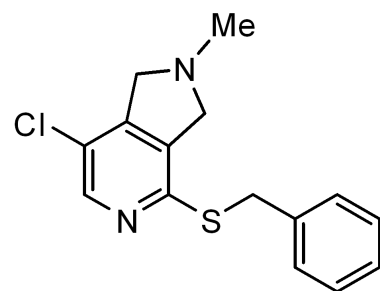
Acquisition Parameter

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



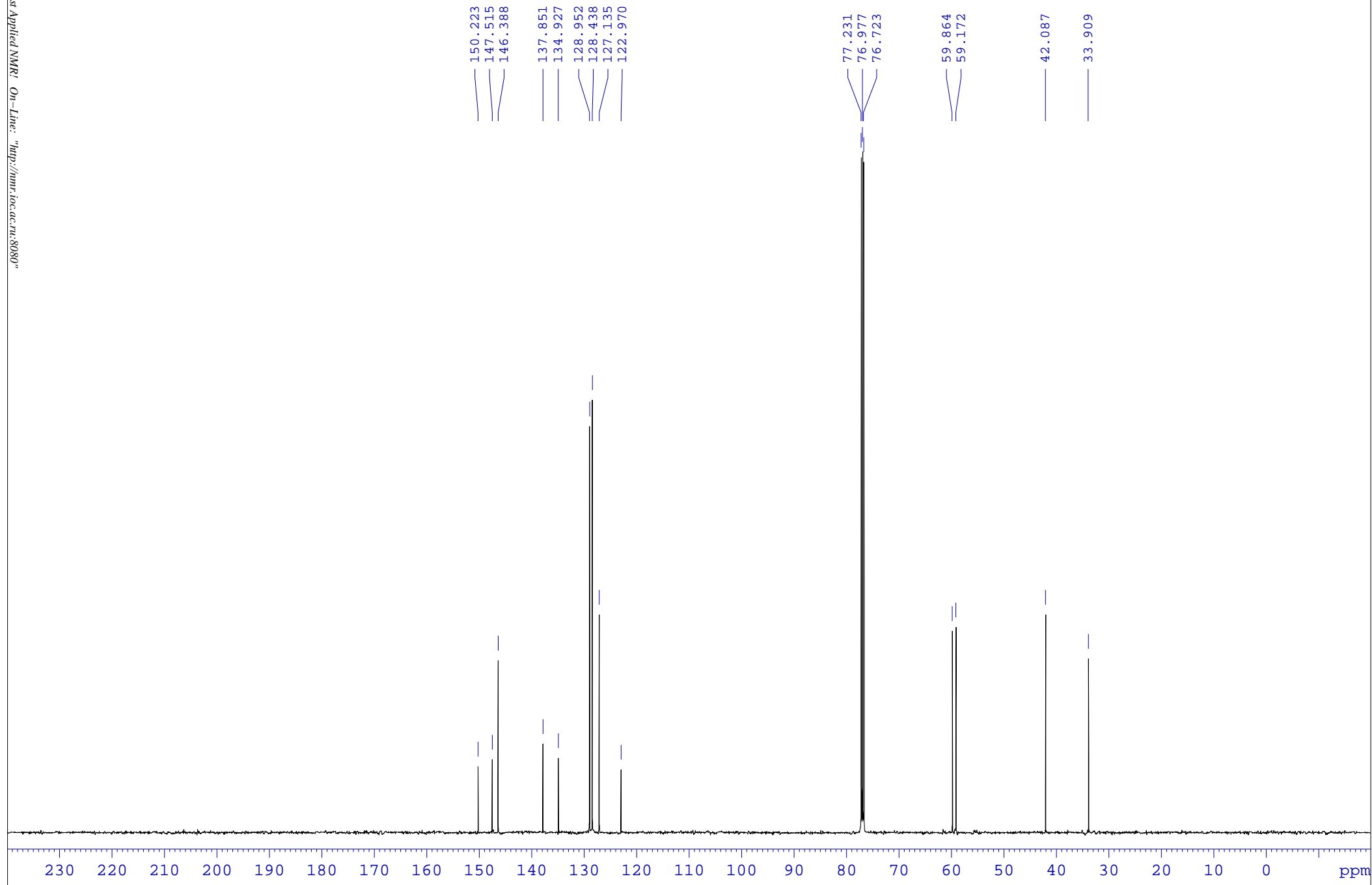


/LPIK AF-409





/LPIK AF-409.C13



Display Report

Analysis Info

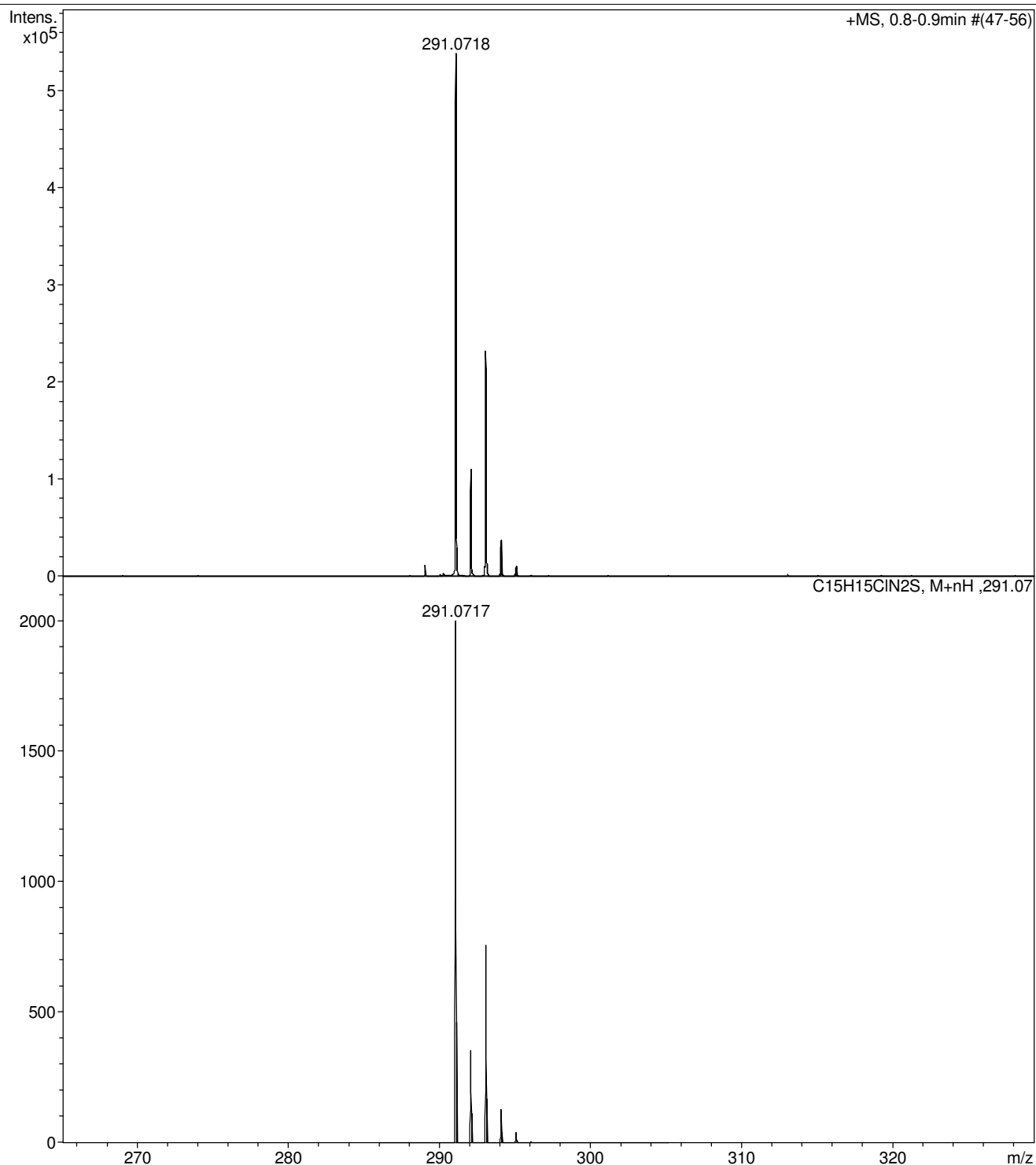
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Method tune_50-1600.m
Sample Name /LPIK AF-409
Comment C15H15ClN2S mH 291.0717 clb added CH3OH

Acquisition Date 28.04.2021 13:26:23

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

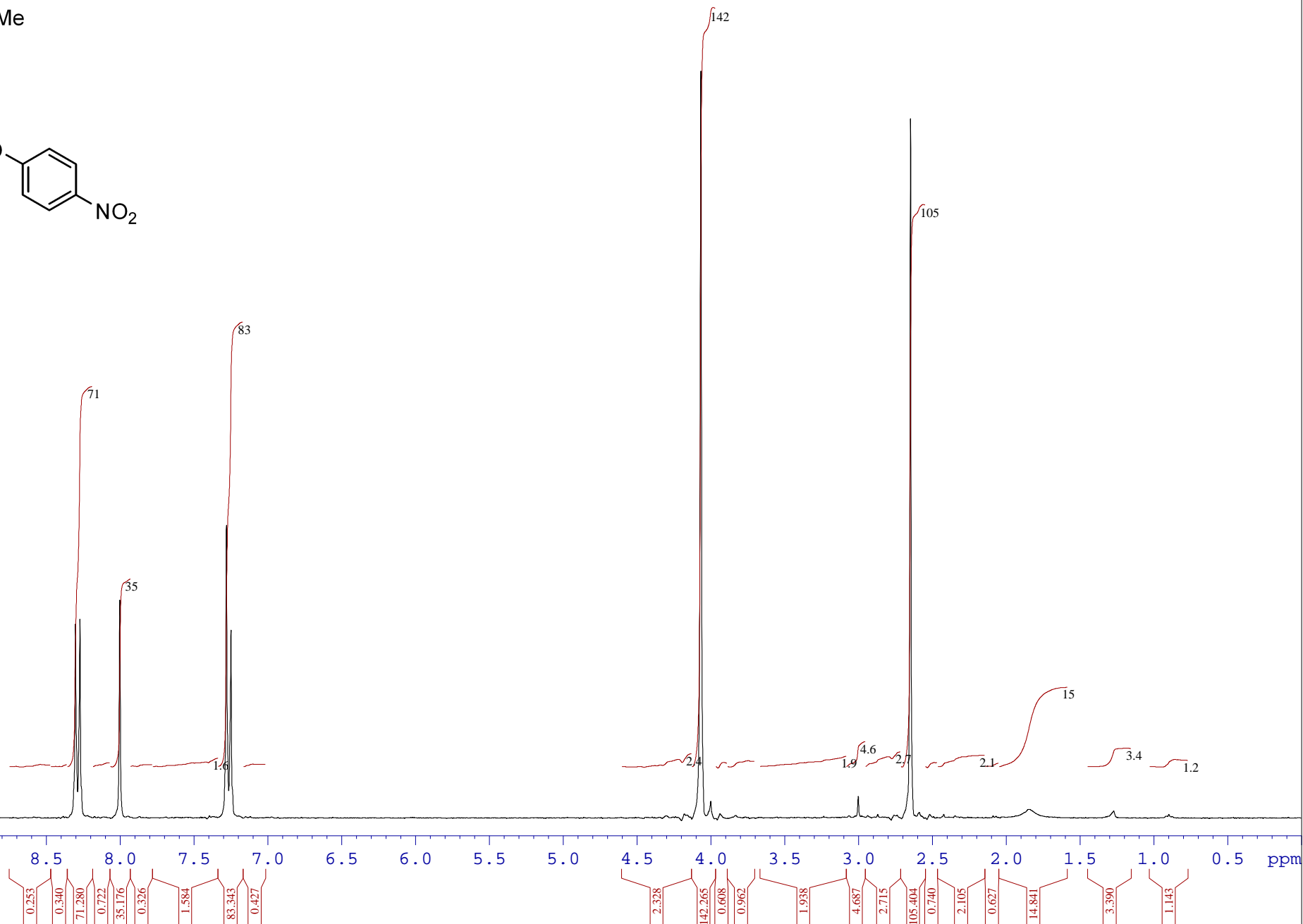
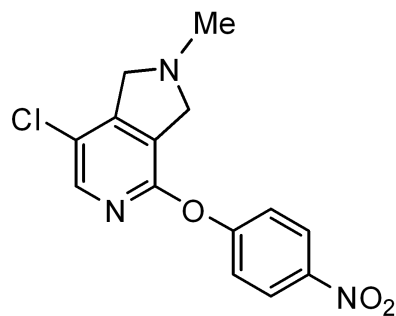
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
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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



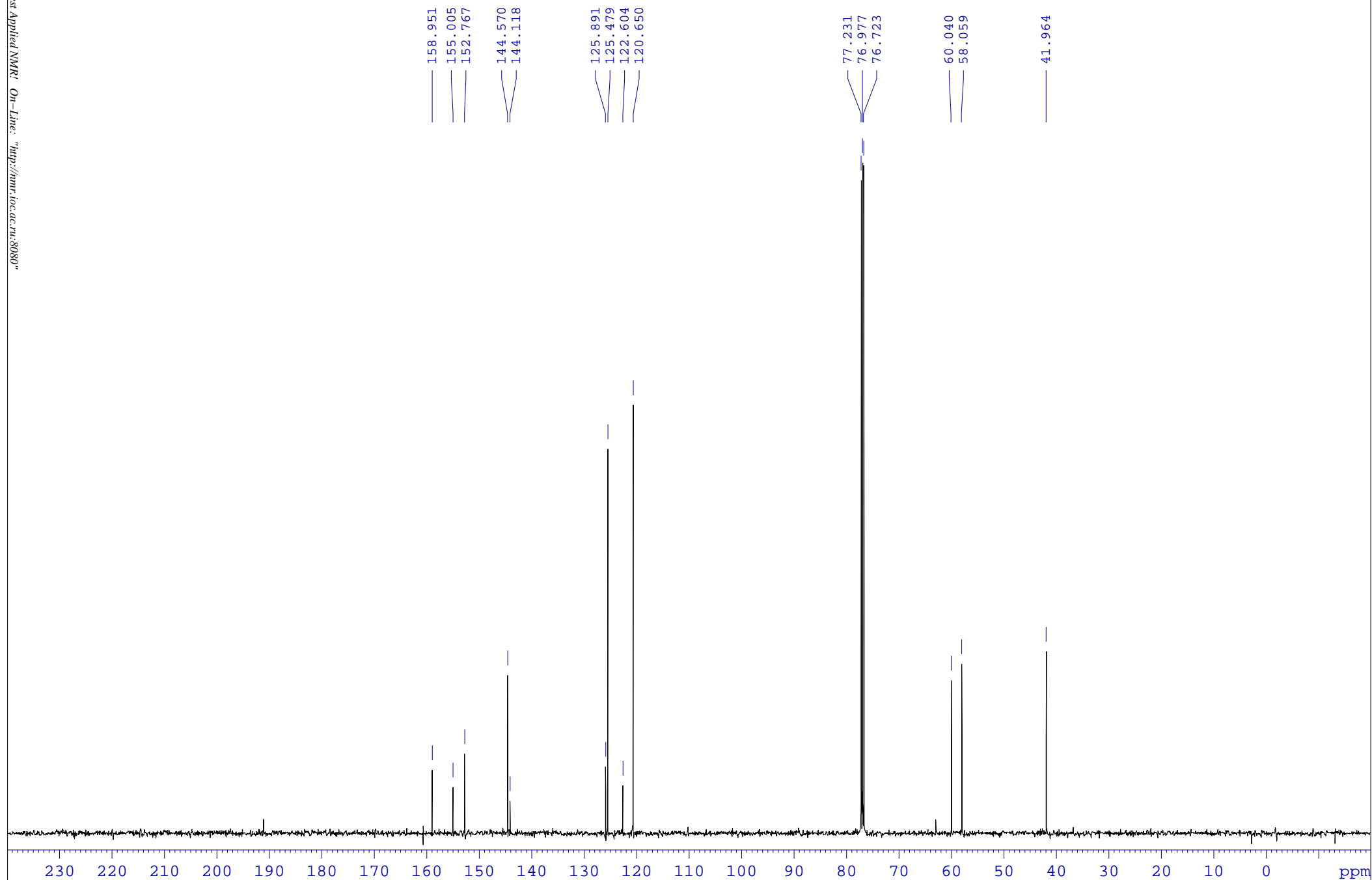


/LPIK AF-413





/LPIK AF-413.C13



Display Report

Analysis Info

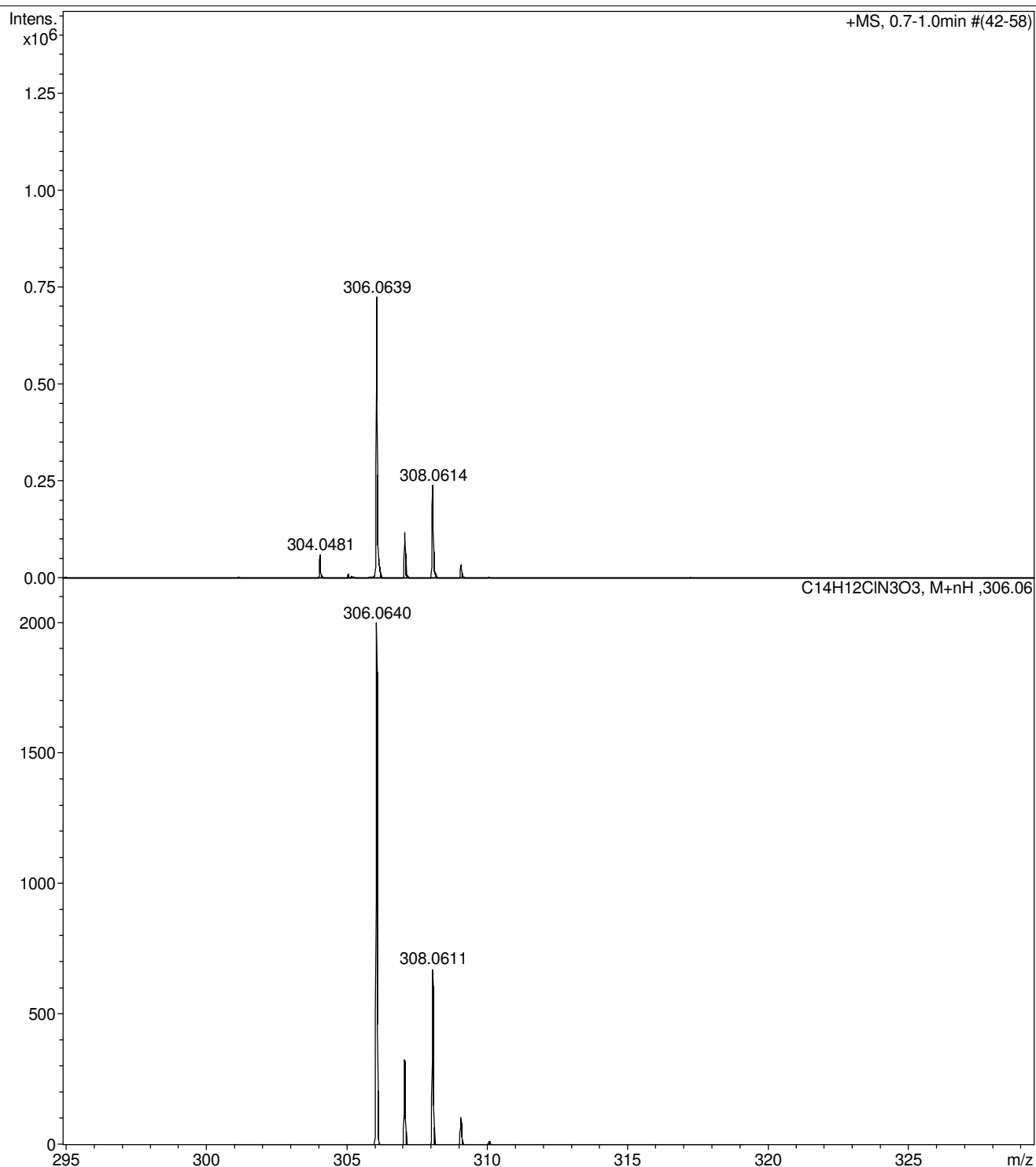
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Method tune_50-1600.m
Sample Name /LPIK AF-413
Comment C14H12CIN3O3 mH 306.0639 clb added CH3OH

Acquisition Date 29.04.2021 17:57:27

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

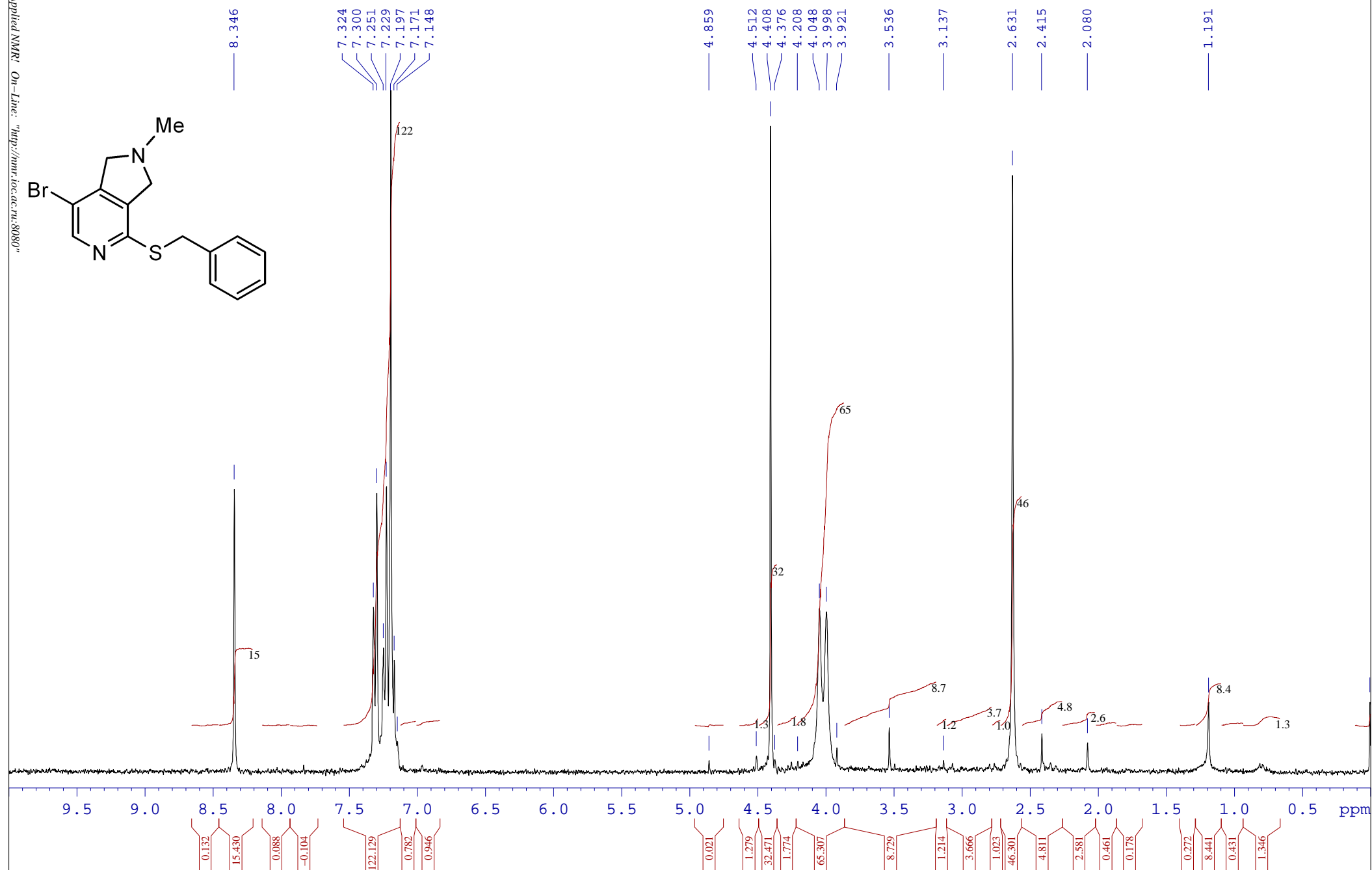
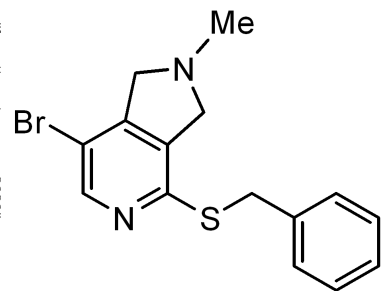
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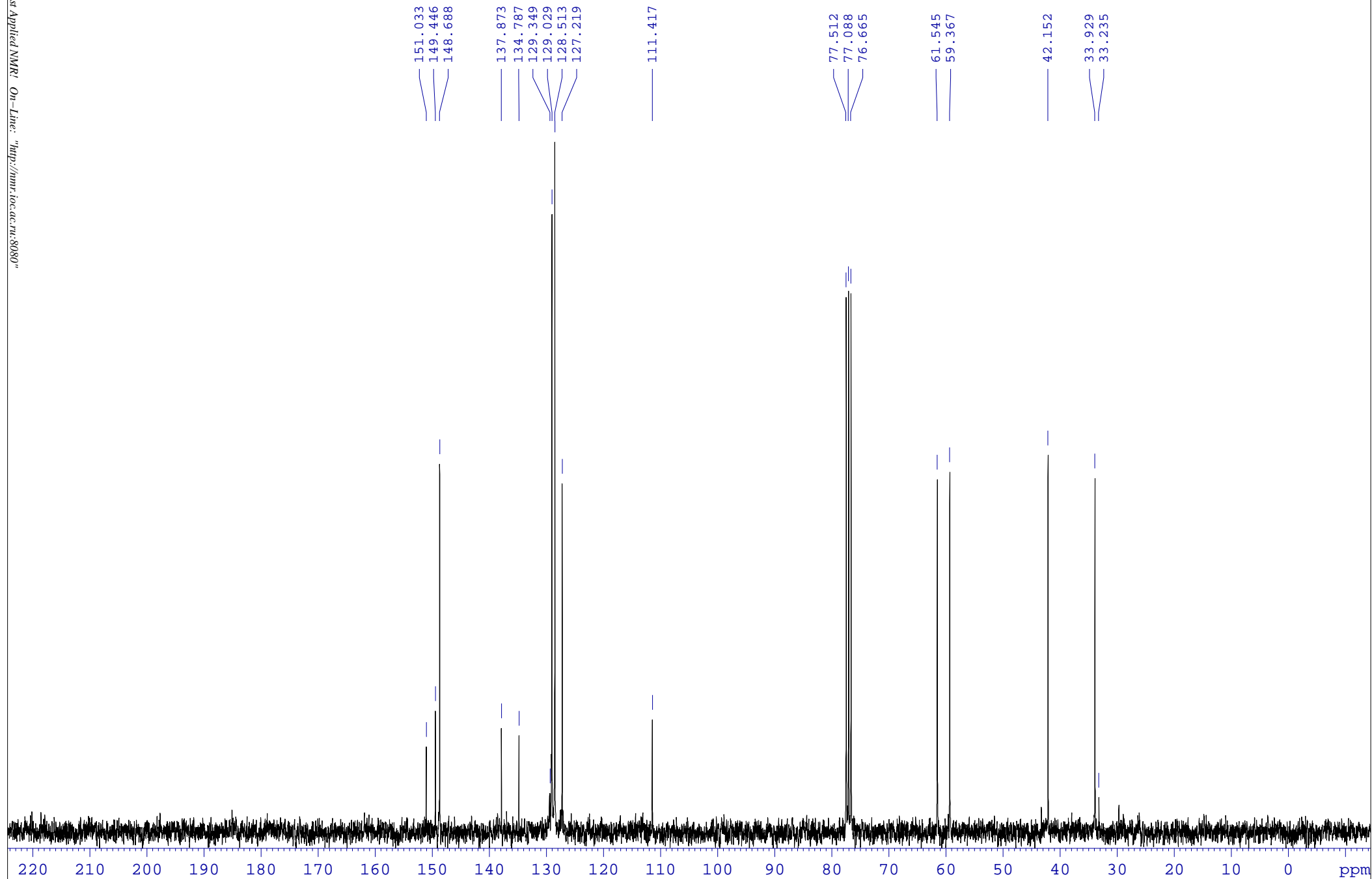


/LPIK AF-429





/LPIK AF-429.1.13 Kokorekin-20259



Display Report

Analysis Info

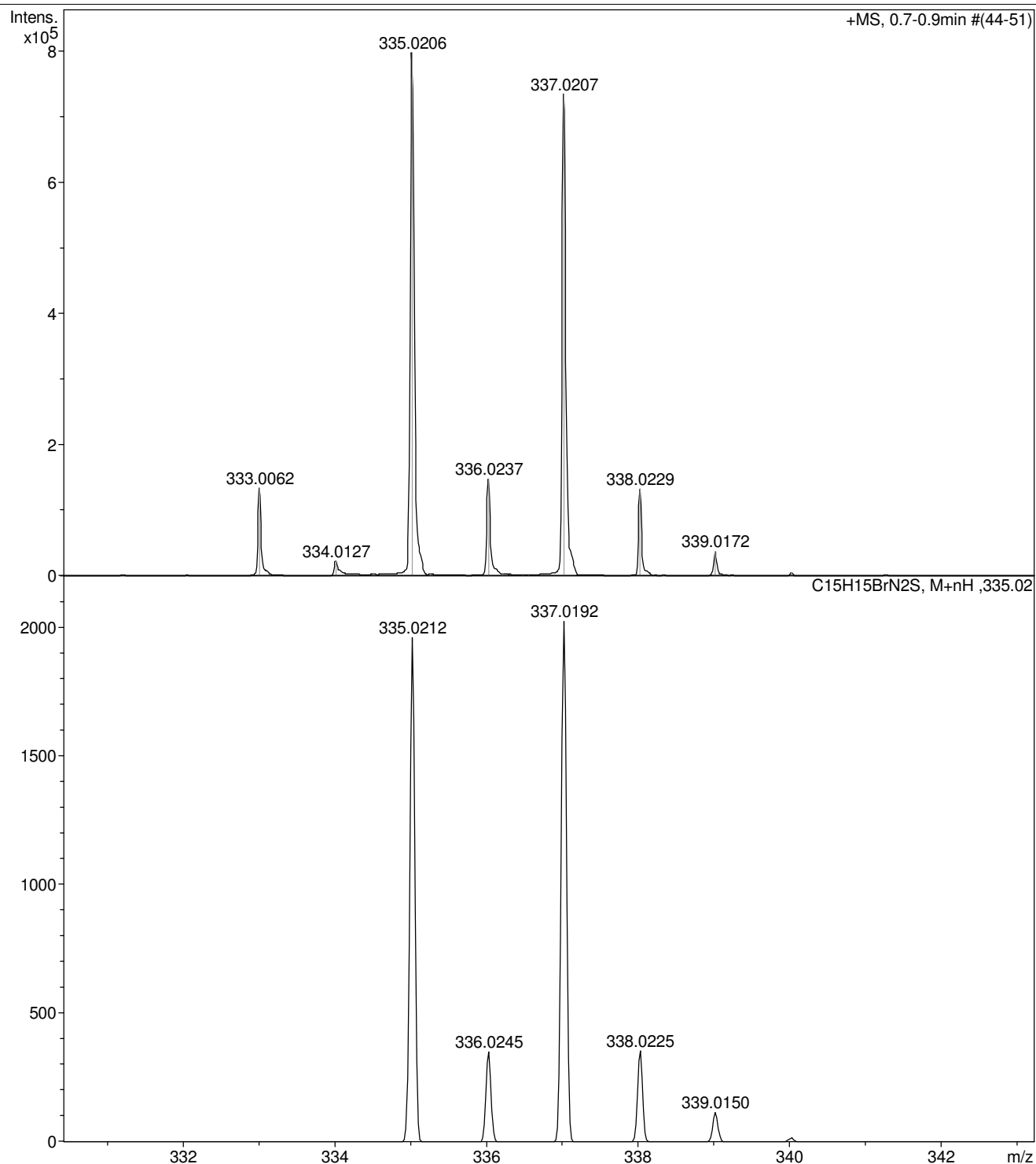
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Sample Name /LPIK AF-429P
Comment C15H15BrN2S mH 335.0212 calibrant added, CH3OH

Acquisition Date 07.07.2021 16:12:07

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

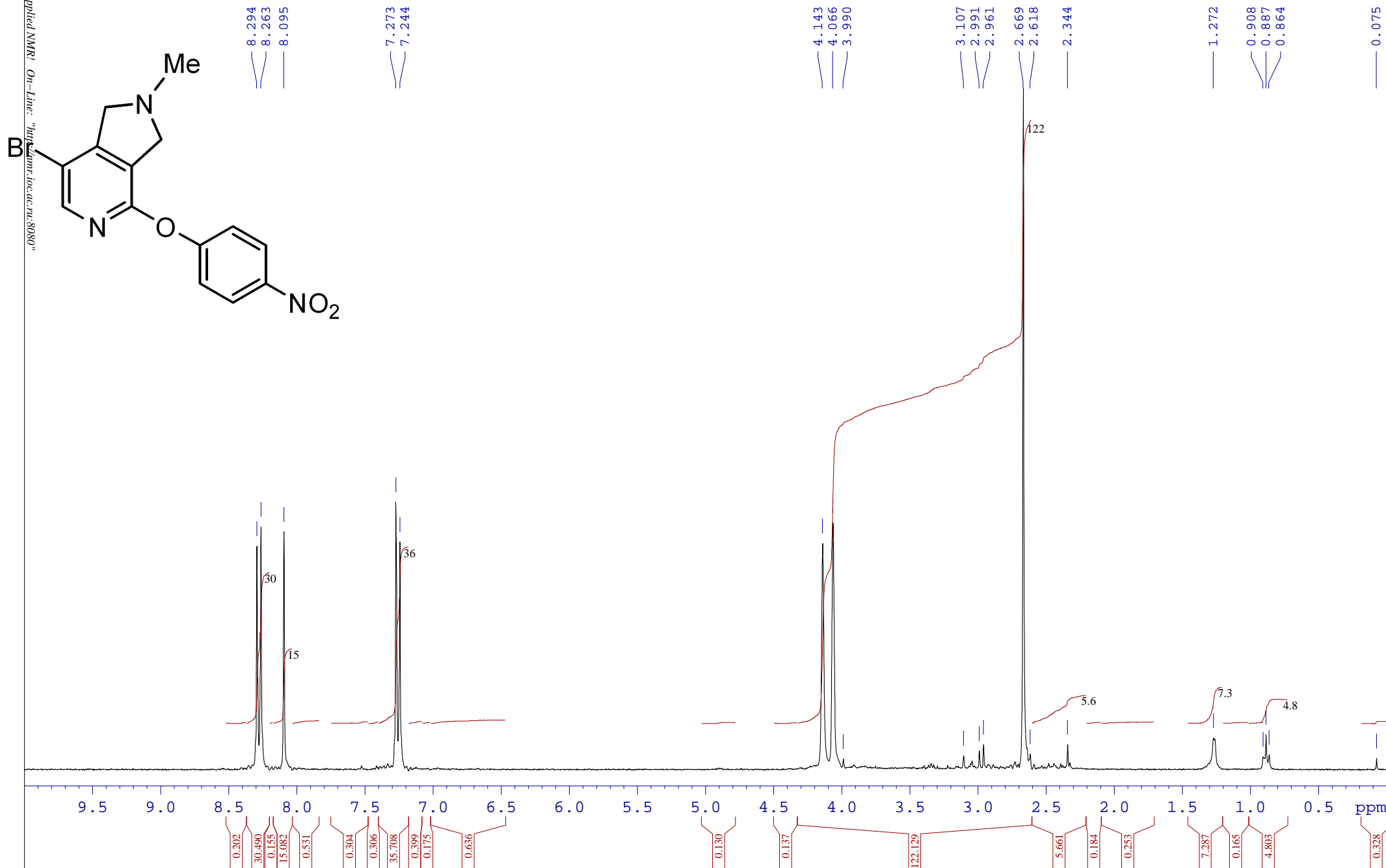
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Focus	Not active			Set Dry Heater	200 °C
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Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



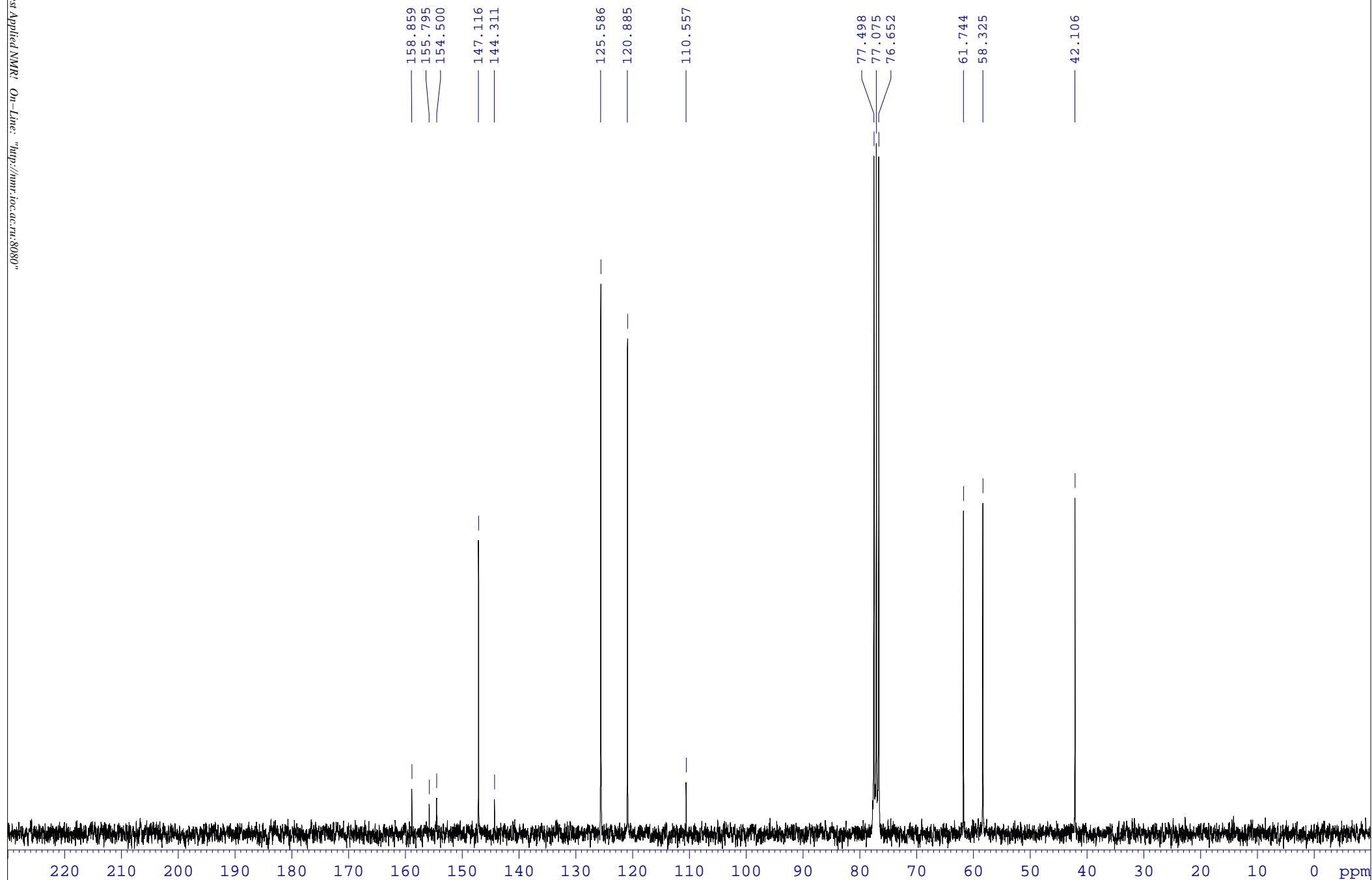


/LPIK AF-430





/LPIK AF-430.C13



Display Report

Analysis Info

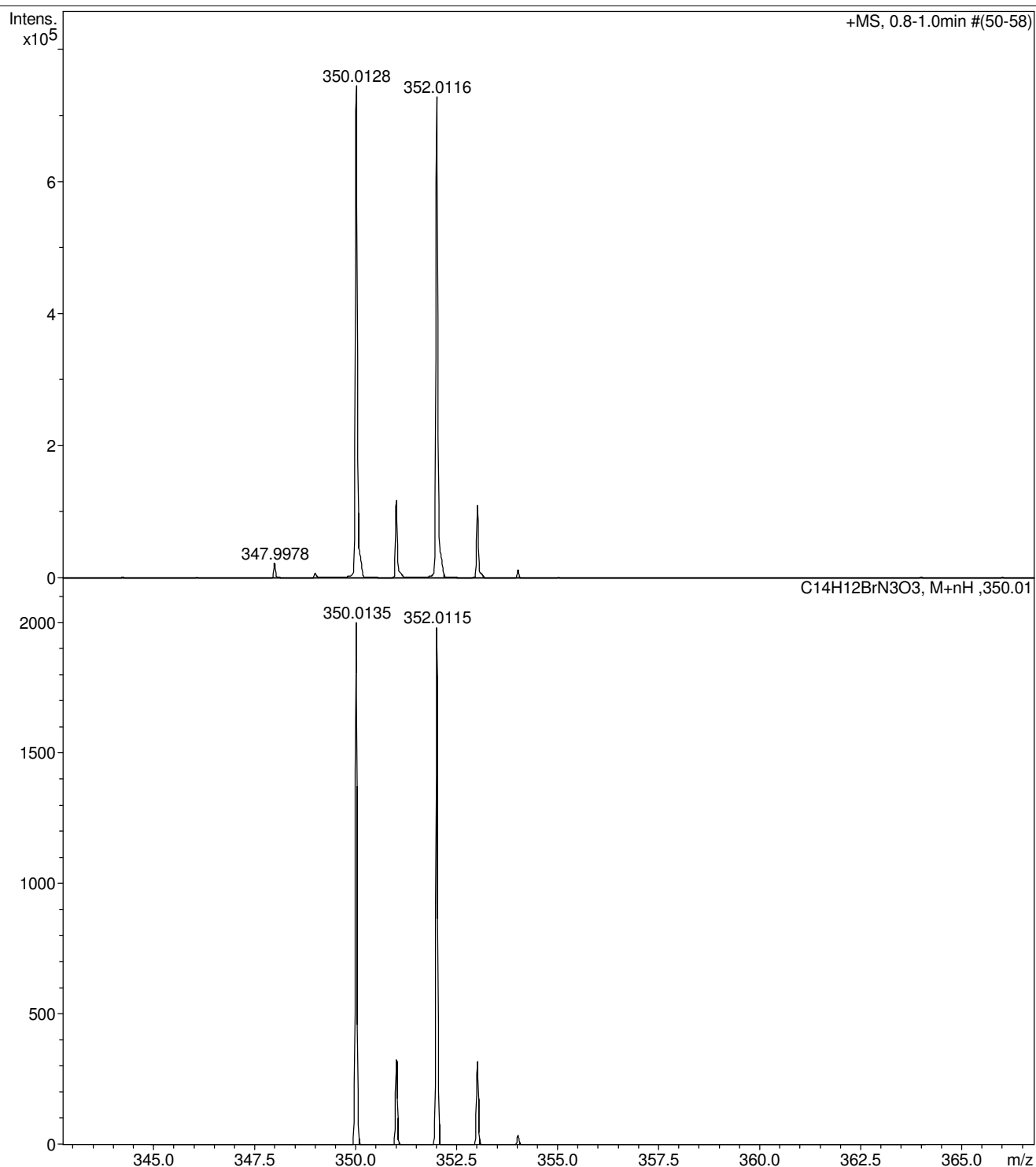
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Method tune_50-1600.m
Sample Name /LPIK AF-430
Comment C14H12BrN3O3 mH 350.0134clb added CH3OH

Acquisition Date 29.04.2021 18:06:30

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

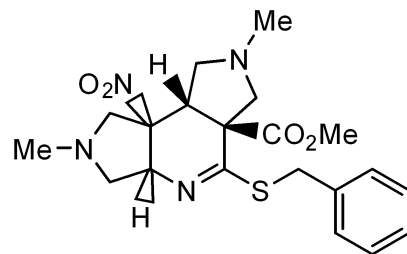
Acquisition Parameter

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





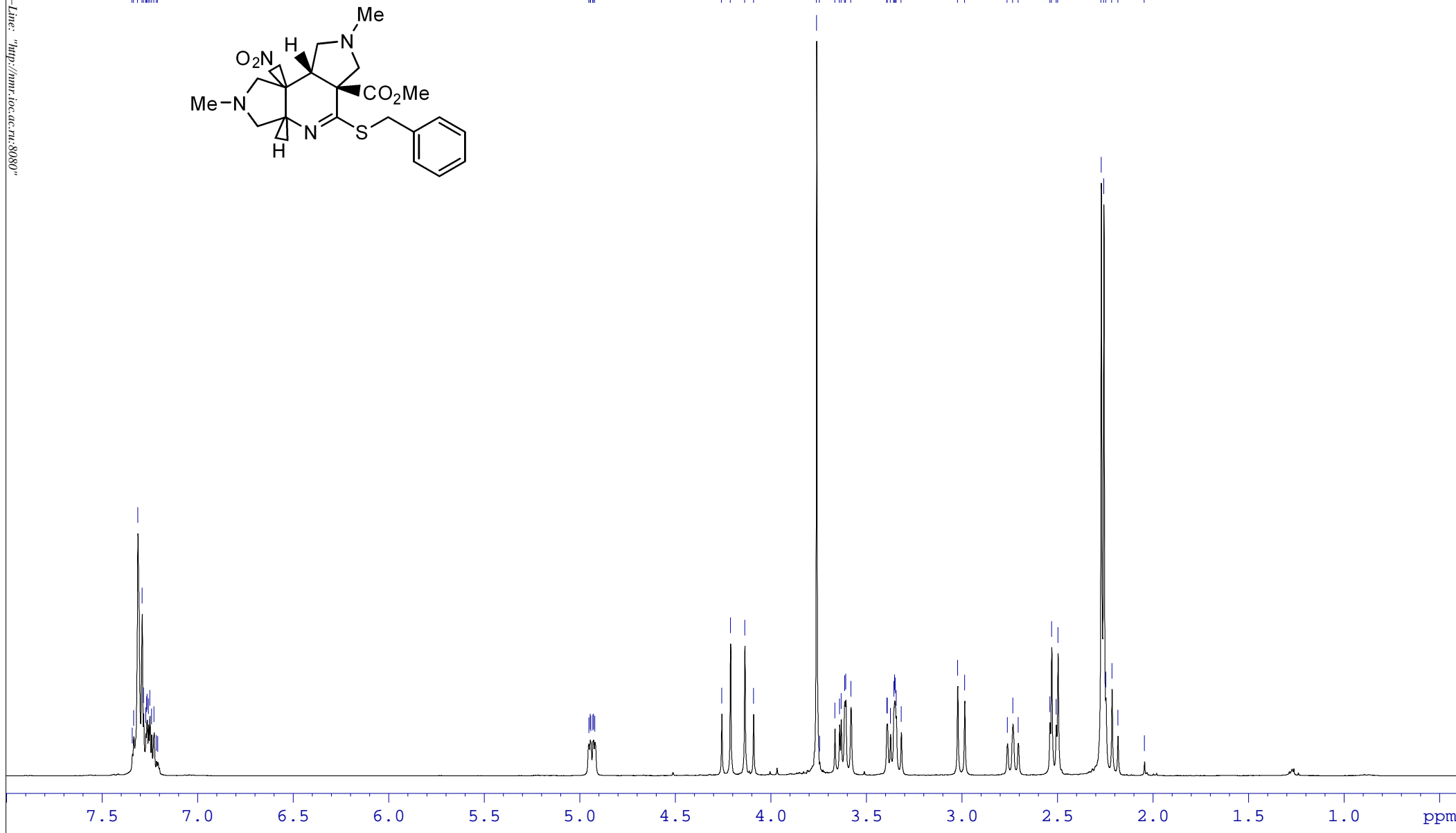
/LPIK AF-432.1.1 Kokorekin-20259



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7.216
7.209

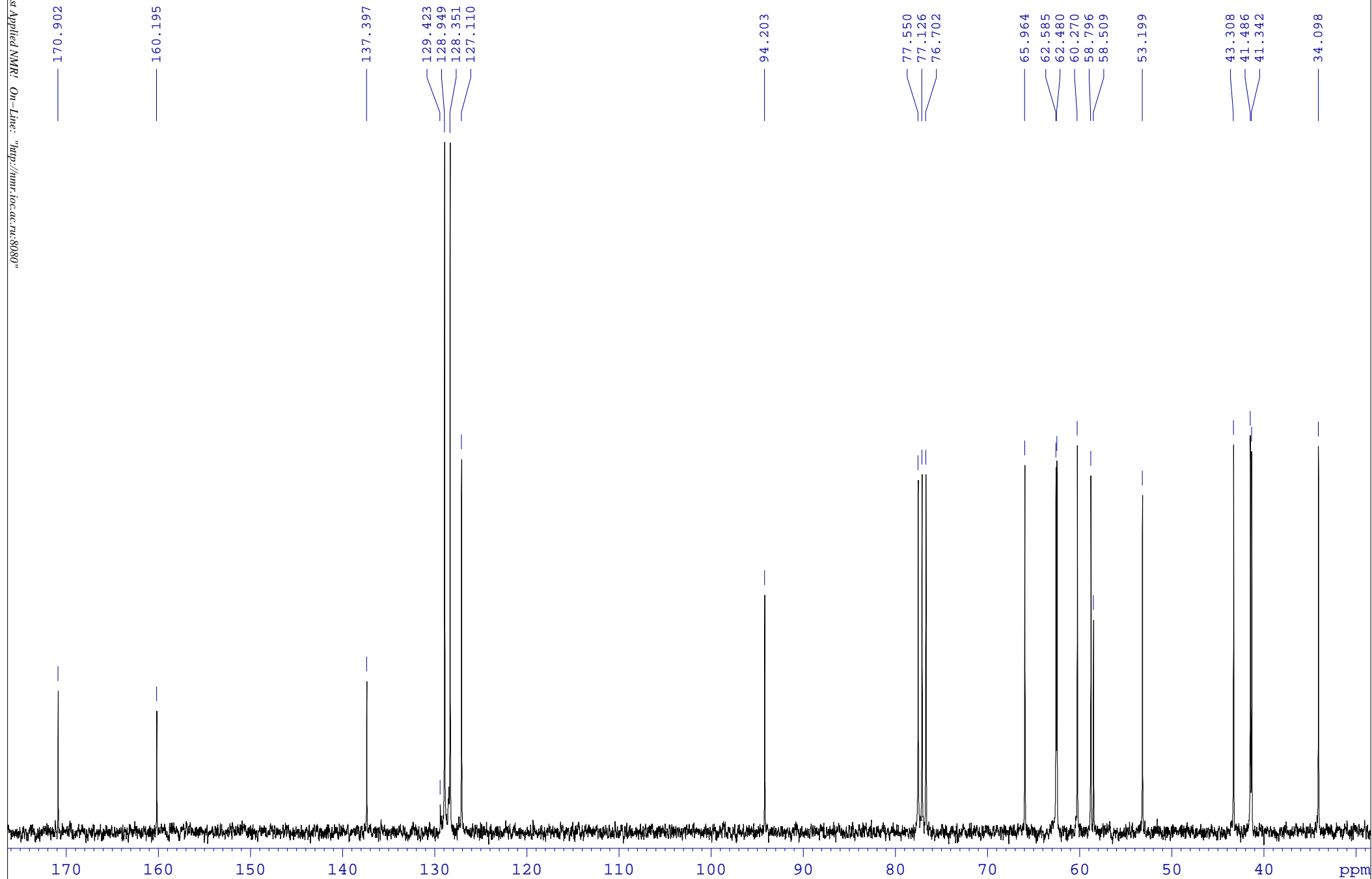
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2.045





/LPIK AF-432.1 Kokorekin-20259



Display Report

Analysis Info

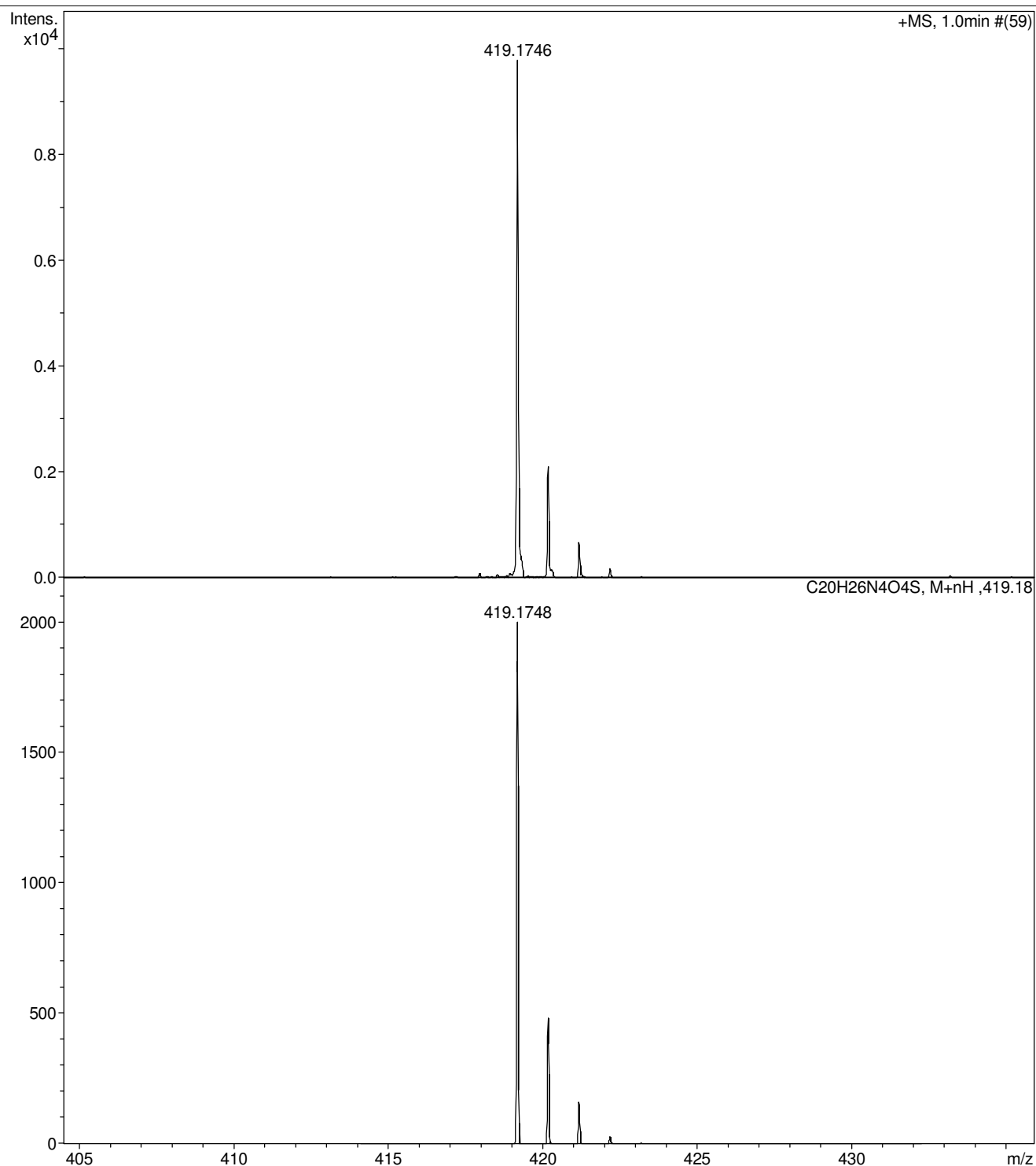
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Method tune_50-1600.m
Sample Name /LPIK AF-432.1
Comment C20H26N4O4S mH 419.1747 clb added CH3OH

Acquisition Date 29.04.2021 18:12:20

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

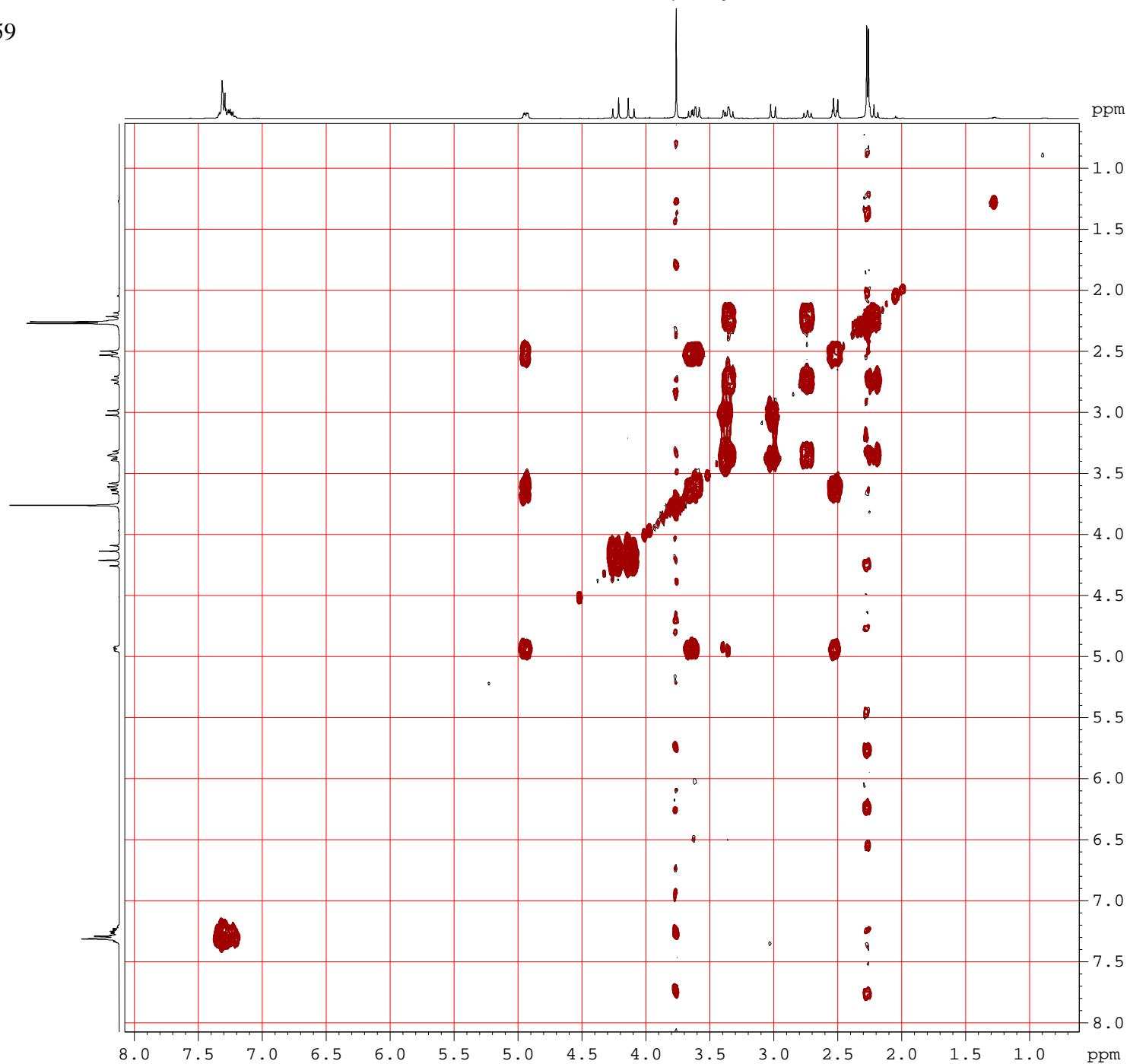
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Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





/LPIK AF-432.1.1 Kokorekin-20259

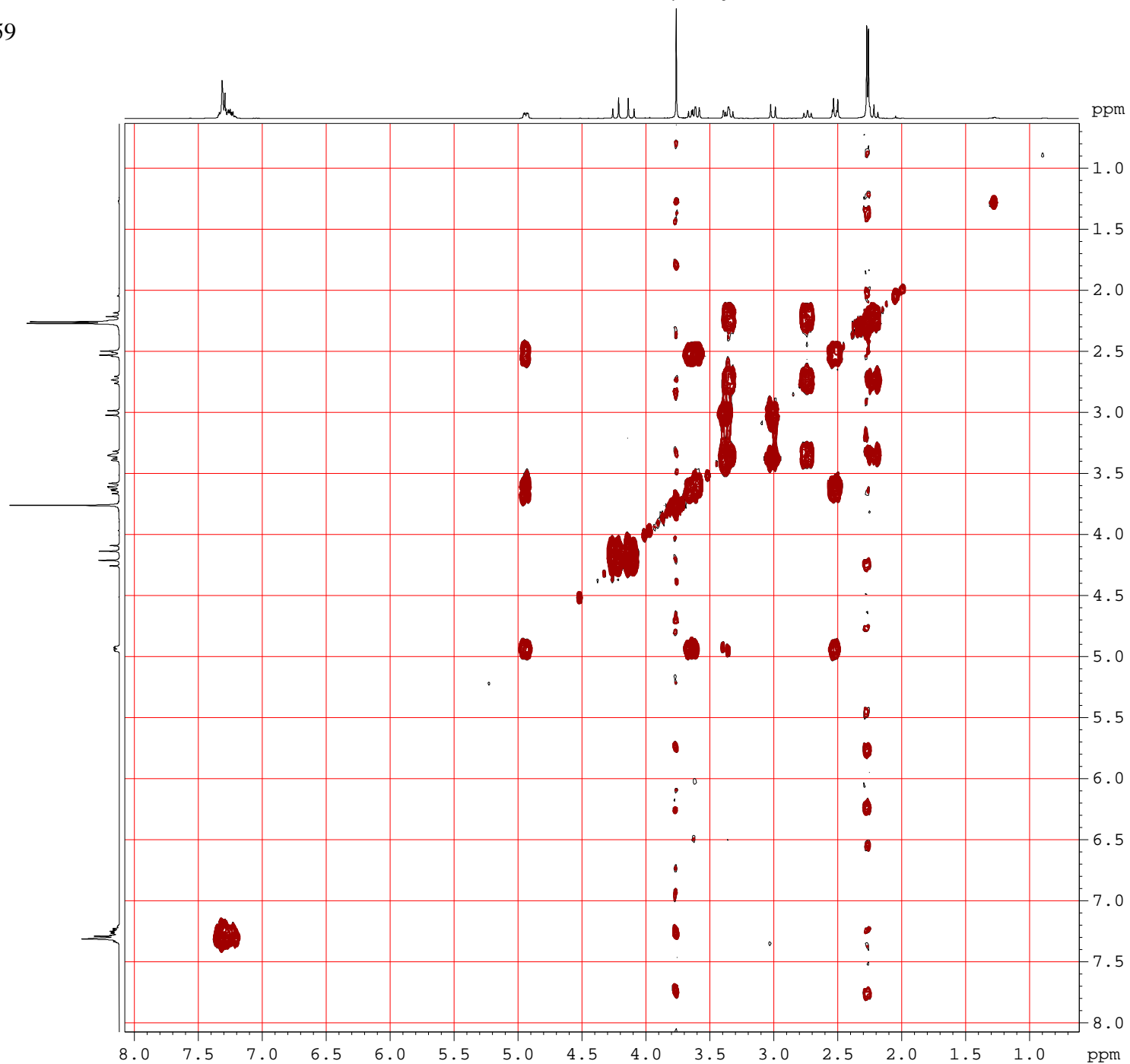
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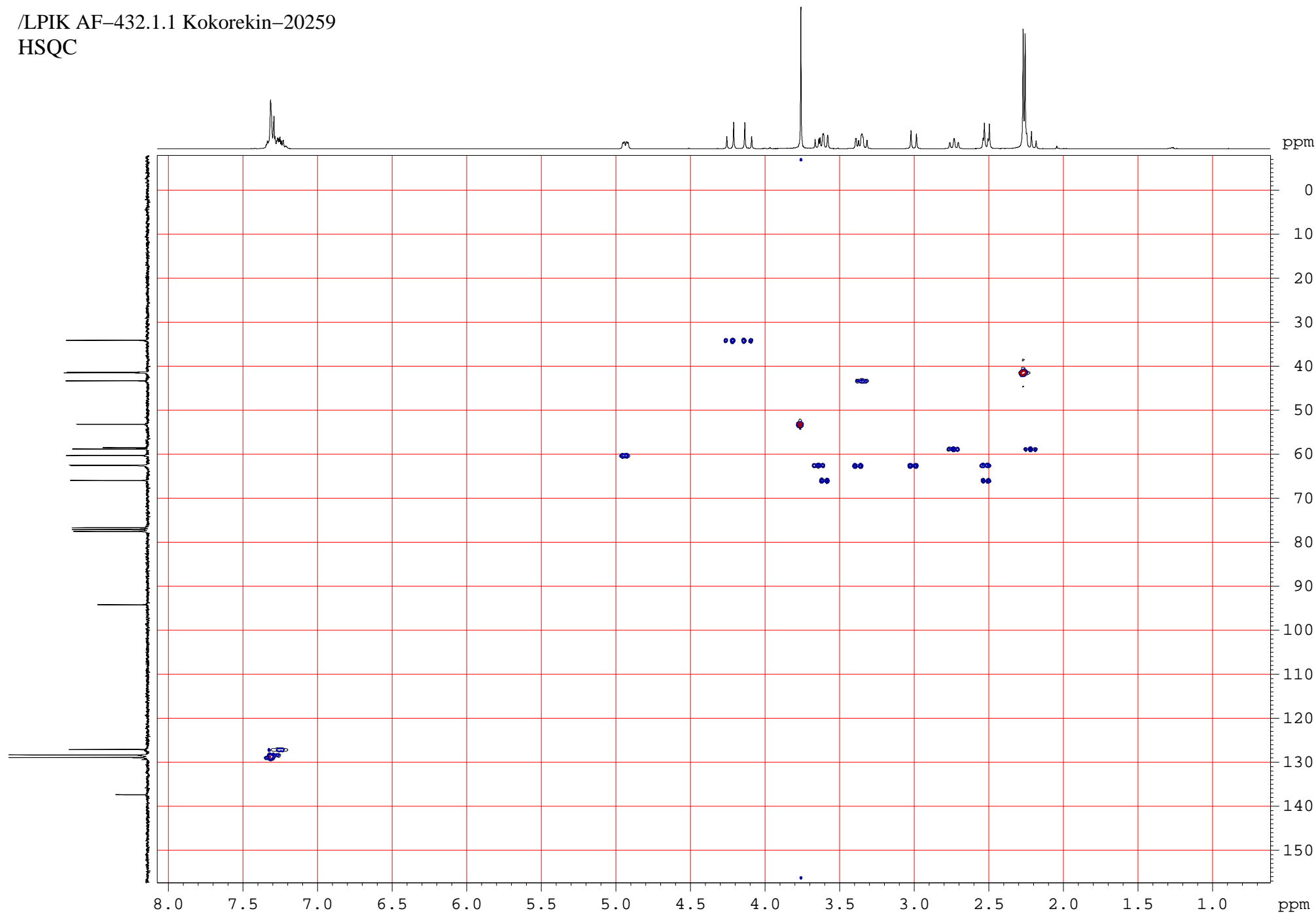
/LPIK AF-432.1.1 Kokorekin-20259

COSY





/LPIK AF-432.1.1 Kokorekin-20259
HSQC





/LPIK AF-432.1.NOESY Kokorekin-20259
NOESY

