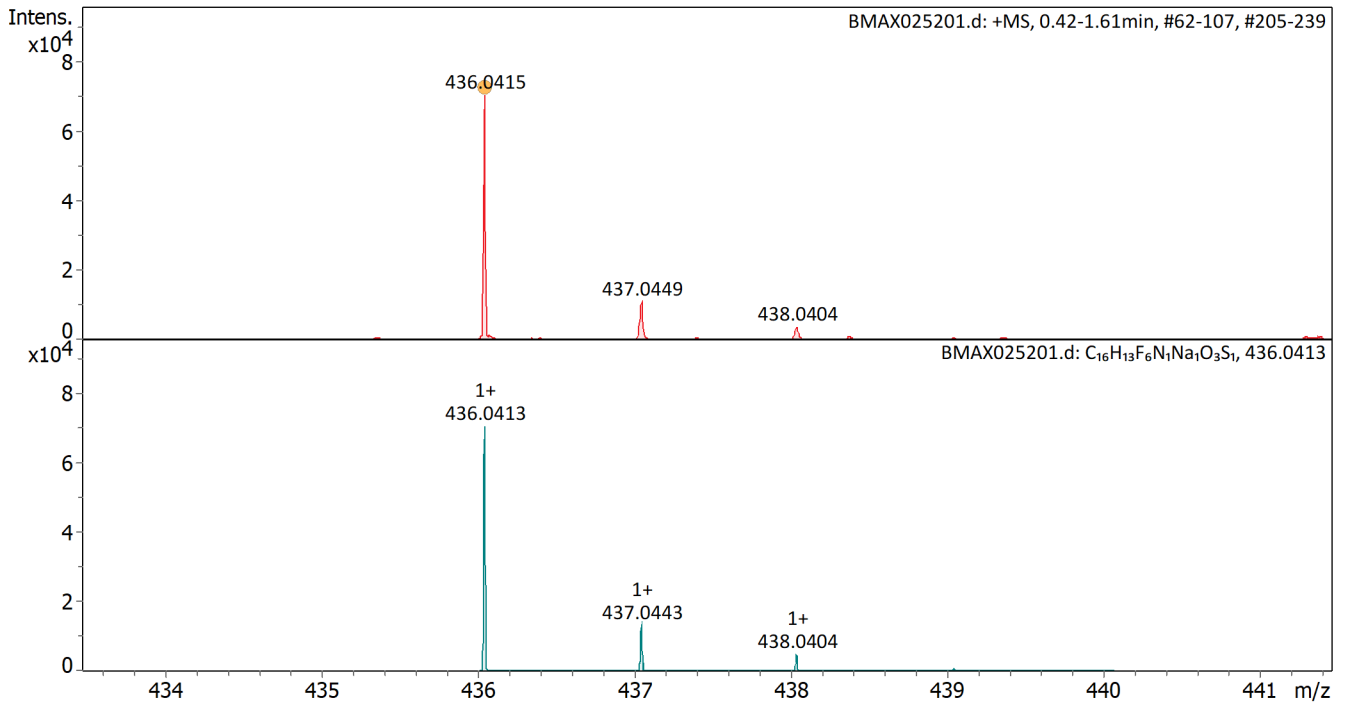
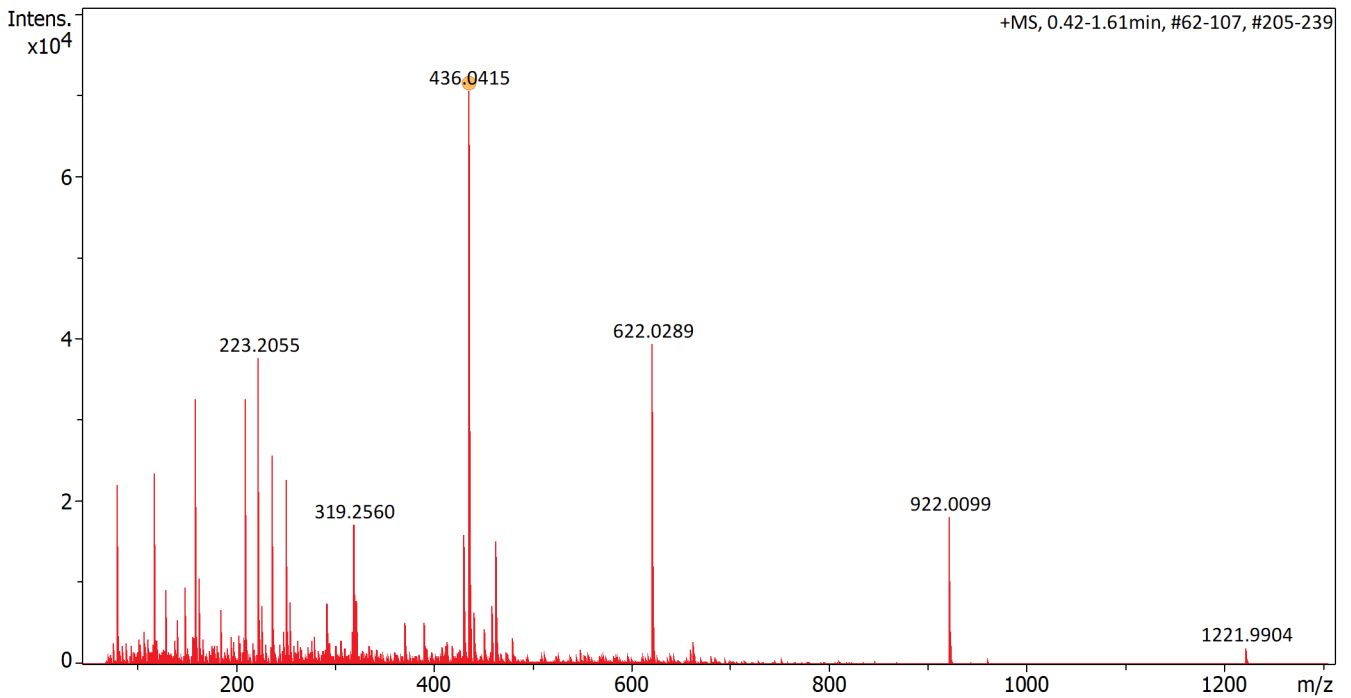


Acquisition Parameter

Method: ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m
File Name: D:\Data\bmax0251xx\BMAX025201.d
Source Type: ESI
Focus: Active
Scan Begin: 50 m/z
Scan End: 1300 m/z
Ion Polarity: Positive
Set Capillary: 4500 V
Set End Plate Offset: -500 V
Set Collision Cell RF: 200.0 Vpp

Acquisition Date: 13.09.2023 10:07:36
Operator: Daniel Wirz
Set Nebulizer: 1.6 Bar
Set Dry Heater: 230 °C
Set Dry Gas: 10.0 l/min
Set Divert Valve: Source



Evaluation Spectra / Validation Formula:

#	Ion Formula	Adduct	m/z	z	Meas. m/z	mSigma	N-Rule	err [mDa]	err [ppm]
1	C16H13F6NNaO3S	M+Na	436.0413	1+	436.0415	19.0	ok	-0.2	-0.5

Calibration Info:

Internal calibration

Date: 13.09.2023 10:18:33
 Polarity: Positive
 Calibration spectrum: +MS, 0.42-1.61min, #62-107,
 #205-239: Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 0.283 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	23507	-0.008
322.0481	322.0482	7746	0.107
622.0290	622.0289	39325	-0.041
922.0098	922.0099	18122	0.080
1221.9906	1221.9904	2035	-0.226
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	80.0497	18749	1203.6	31.4	0.0043
2	107.0703	15152	228.3	5.8	0.0071
3	118.0863	17289	1357.9	33.3	0.0068
4	130.1590	19159	552.8	13.1	0.0068
5	141.0024	16829	328.9	7.6	0.0084
6	149.0232	16670	595.6	13.5	0.0089
7	158.9638	16061	257.8	5.7	0.0099
8	159.0132	19766	2076.3	46.2	0.0080
9	163.1297	10765	688.9	15.1	0.0152
10	185.1148	17226	461.4	9.6	0.0107
11	209.1899	21632	2354.6	46.3	0.0097
12	210.1929	17705	377.1	7.4	0.0119
13	223.2055	23708	2753.1	53.3	0.0094
14	224.2088	16866	402.1	7.8	0.0133
15	227.2366	18027	534.4	10.3	0.0126
16	237.1771	17625	660.1	12.5	0.0135
17	237.2212	21994	1929.2	36.5	0.0108
18	238.2244	17781	326.7	6.2	0.0134
19	249.2200	15878	307.8	5.7	0.0157
20	251.1929	17469	349.5	6.4	0.0144
21	251.2367	21638	1758.5	32.2	0.0116
22	252.2399	16793	309.6	5.7	0.0150
23	255.2679	18624	594.3	10.9	0.0137
24	293.1750	17373	603.8	10.5	0.0169
25	293.2835	18148	378.9	6.6	0.0162
26	318.2590	18860	324.8	5.7	0.0169
27	319.2560	24884	1389.1	24.4	0.0128
28	322.0482	19357	625.5	11.0	0.0166
29	371.3162	16455	413.9	7.2	0.0226
30	391.2843	18340	400.2	7.2	0.0213
31	431.0863	23008	1144.0	22.7	0.0187
32	436.0415	38146	5040.7	100.0	0.0114
33	437.0449	20438	775.1	15.4	0.0214
34	442.0913	18358	445.8	9.0	0.0241
35	452.0159	17557	302.4	6.2	0.0257
36	459.1176	18431	491.3	10.2	0.0249
37	464.0730	25051	1035.1	21.6	0.0185
38	622.0289	31099	2901.8	55.8	0.0200
39	623.0324	18225	440.9	8.5	0.0342
40	922.0099	23614	1962.8	25.7	0.0390
#	m/z	Res.	S/N	I %	FWHM
1	436.0413	38146		100.0	0.0114
2	437.0443	38234		18.7	0.0114
3	438.0404	38321		6.7	0.0114
4	439.0422	38409		1.0	0.0114
5	440.0434	38497		0.1	0.0114