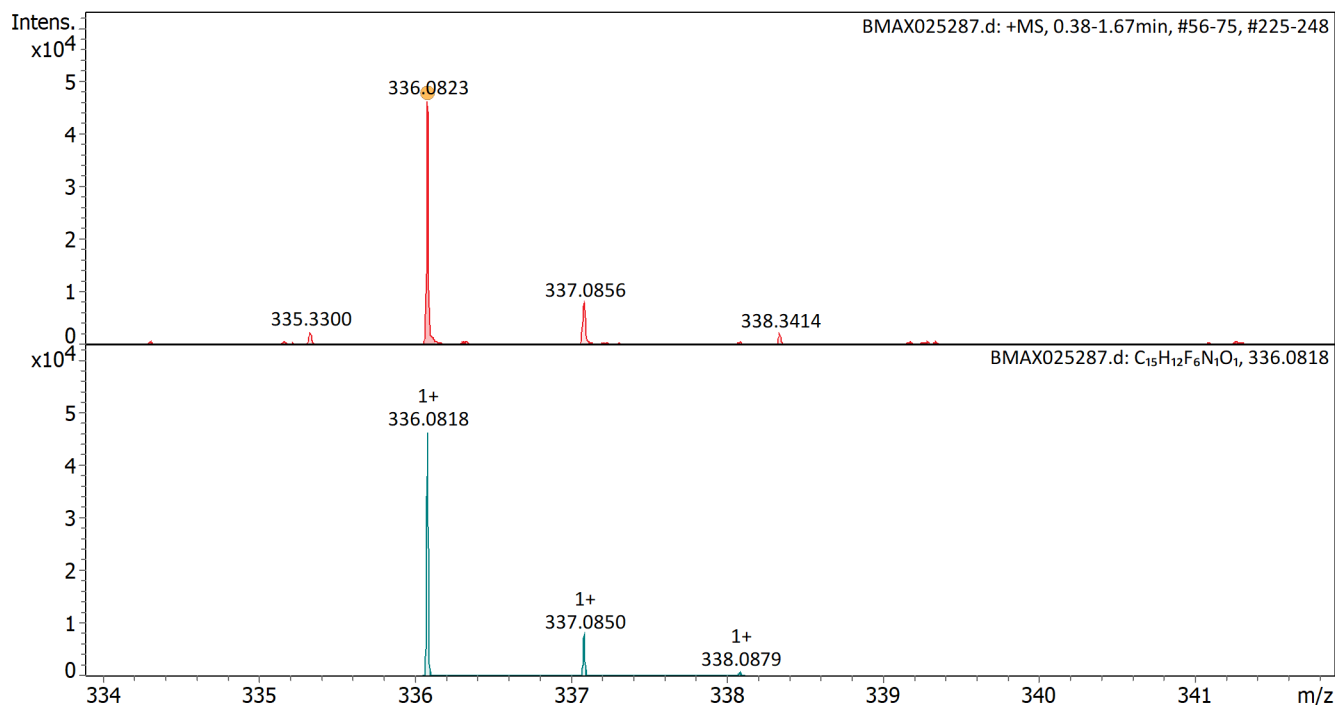
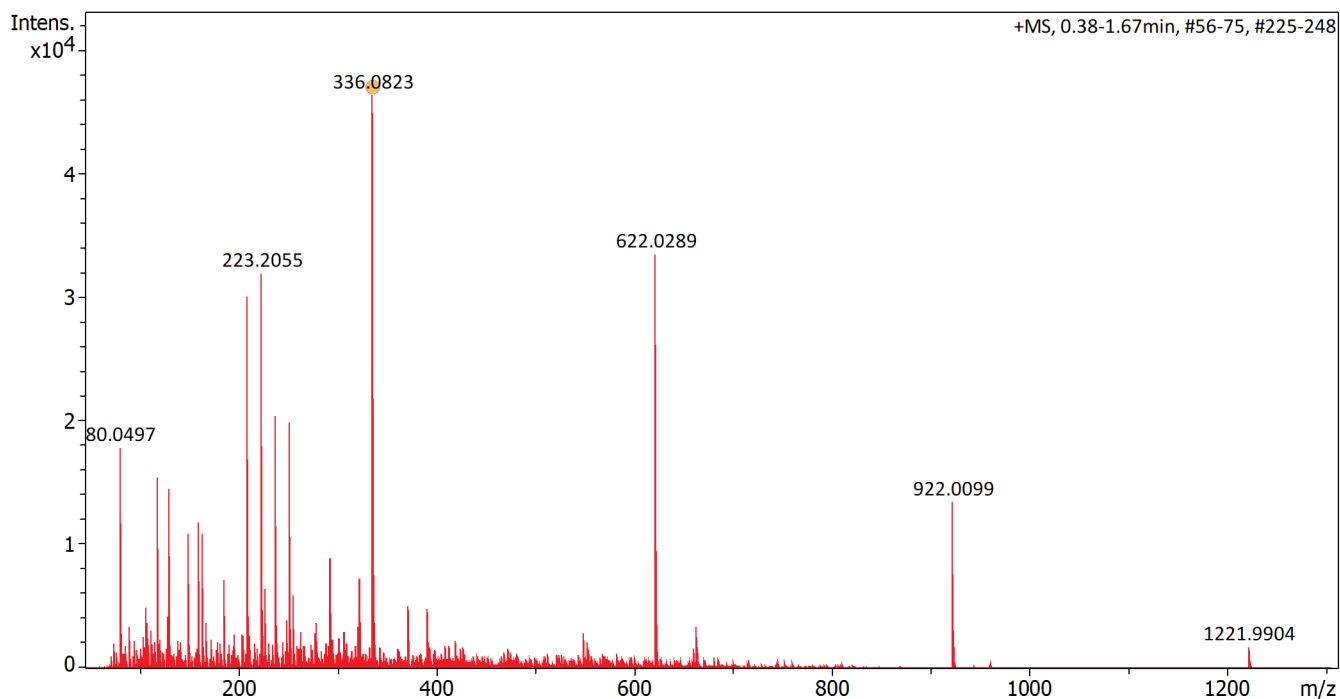


Acquisition Parameter

Method: ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m
File Name: D:\Data\bmax0252xx\BMAX025287.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: 19.09.2023 05:17:43
Operator: Michael Meier
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	C15H12F6NO	M+H	336.0818	1+	336.0823	0.7	ok	-0.5	-1.6

Calibration Info:

Internal calibration

Date: 19.09.2023 05:20:29
 Polarity: Positive
 Calibration spectrum: +MS, 0.38-1.67min, #56-75, #225-248:
 Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 0.286 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	15423	-0.010
322.0481	322.0482	7316	0.097
622.0290	622.0289	33494	-0.041
922.0098	922.0099	13485	0.091
1221.9906	1221.9904	1723	-0.229
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	80.0497	17682	1128.0	38.5	0.0045
2	89.0597	17608	208.2	7.3	0.0051
3	107.0703	16259	293.4	10.7	0.0066
4	107.9667	17003	215.0	7.8	0.0063
5	111.0204	17736	181.1	6.6	0.0063
6	118.0863	17620	903.3	33.3	0.0067
7	129.0536	18189	242.2	9.0	0.0071
8	130.1589	16910	845.9	31.4	0.0077
9	149.0232	18413	634.2	23.6	0.0081
10	158.9638	17214	182.0	6.8	0.0092
11	159.0132	18667	688.5	25.6	0.0085
12	163.1306	13248	638.0	23.6	0.0123
13	167.0778	14700	214.7	7.9	0.0114
14	185.1148	18153	424.7	15.4	0.0102
15	209.1899	23848	1840.1	64.8	0.0088
16	210.1931	17006	255.5	9.0	0.0124
17	223.2055	24294	1987.5	68.9	0.0092
18	224.2086	17322	295.4	10.2	0.0129
19	227.2366	18930	406.1	14.0	0.0120
20	237.1499	13898	250.0	8.5	0.0171
21	237.2213	21236	1294.3	44.1	0.0112
22	238.2243	16979	222.5	7.6	0.0140
23	249.2203	16913	248.9	8.3	0.0147
24	251.2368	22388	1293.9	43.0	0.0112
25	252.2399	15963	205.4	6.8	0.0158
26	255.2679	17449	391.9	12.9	0.0146
27	279.1590	17270	248.1	7.9	0.0162
28	293.1748	19434	612.0	19.4	0.0151
29	293.2835	17224	277.2	8.8	0.0170
30	321.3146	16141	232.6	7.3	0.0199
31	322.0482	18667	502.5	15.8	0.0173
32	336.0823	27327	3235.7	100.0	0.0123
33	337.0856	18185	545.5	16.9	0.0185
34	371.3161	16200	350.5	10.9	0.0229
35	391.2842	17126	322.8	10.4	0.0228
36	622.0289	30271	2169.8	72.3	0.0205
37	623.0323	17539	293.0	9.8	0.0355
38	663.4535	15603	233.1	7.3	0.0425
39	922.0099	21705	1335.2	29.1	0.0425
40	923.0133	17014	301.8	6.6	0.0542
#	m/z	Res.	S/N	I %	FWHM
1	336.0818	27326		100.0	0.0123
2	337.0850	27408		16.8	0.0123
3	338.0879	27490		1.5	0.0123