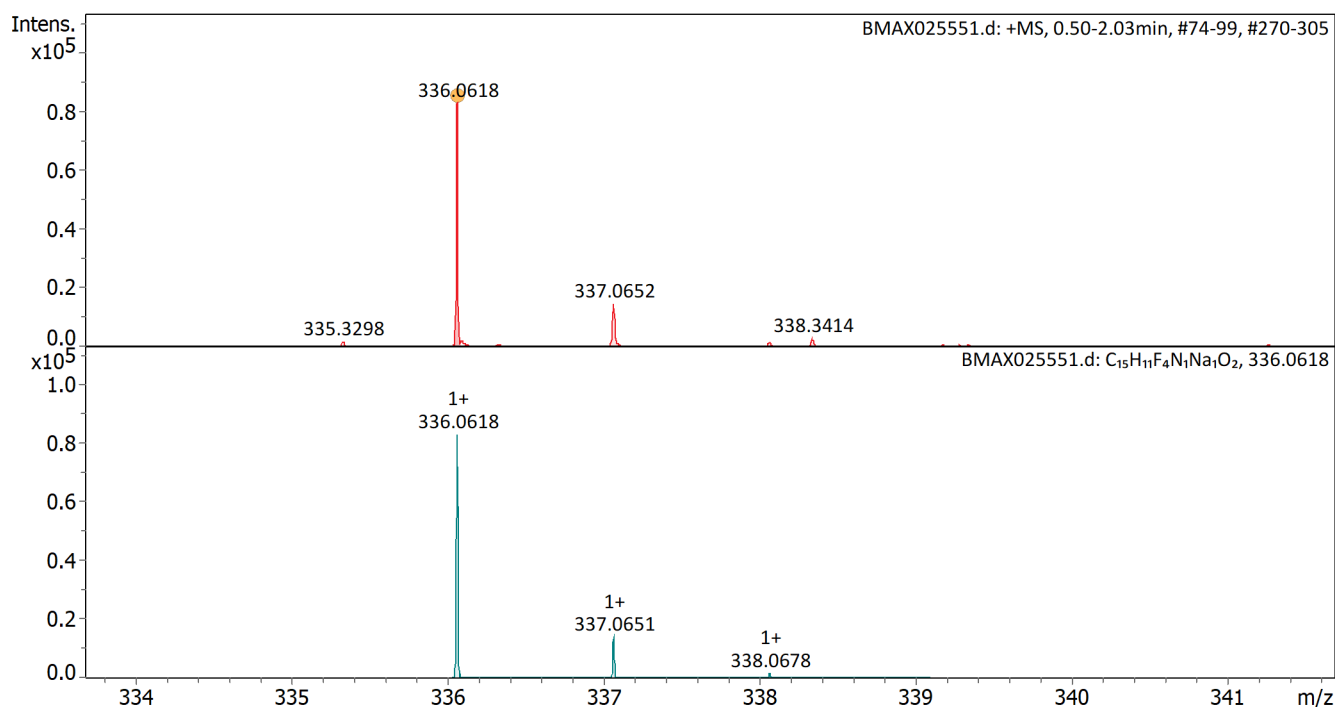
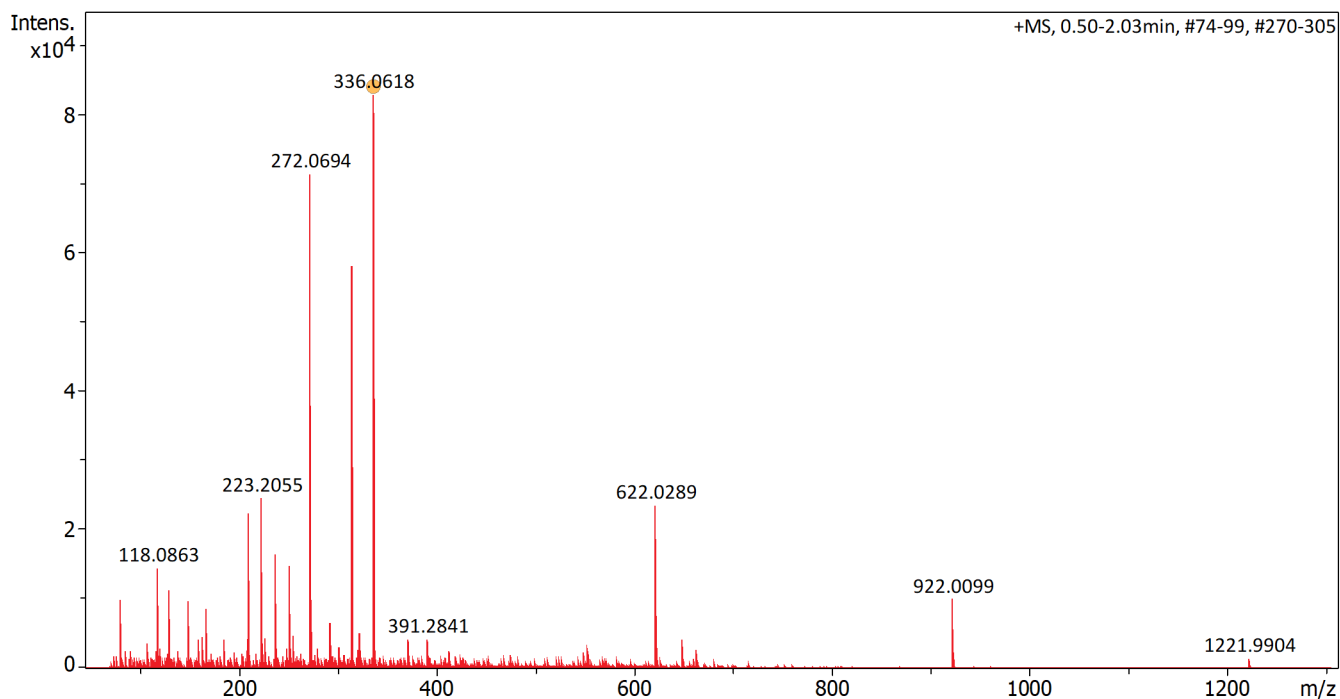


Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m			Acquisition Date:	05.10.2023 05:22:43
File Name:	D:\Data\bmax0255xx\BMAX025551.d			Operator:	Michael Meier
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	230 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	10.0 l/min
Scan End	1300 m/z	Set Collision Cell RF	200.0 Vpp	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	C15H11F4NNaO2	M+Na	336.0618	1+	336.0618	3.4	ok	0.0	0.0

Calibration Info:

Internal calibration

Date: 05.10.2023 05:25:22
 Polarity: Positive
 Calibration spectrum: +MS, 0.50-2.03min, #74-99, #270-305:
 Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 0.287 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	14558	-0.009
322.0481	322.0482	5165	0.110
622.0290	622.0289	23569	-0.047
922.0098	922.0099	10043	0.099
1221.9906	1221.9904	1445	-0.221
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	80.0498	13852	576.0	11.9	0.0058
2	107.9665	15655	208.4	4.4	0.0069
3	118.0863	18026	842.4	17.6	0.0066
4	121.0393	17011	166.5	3.5	0.0071
5	129.0534	15074	187.7	3.9	0.0086
6	130.1588	16936	659.2	13.7	0.0077
7	149.0232	17954	572.7	11.8	0.0083
8	158.9637	17970	247.9	5.1	0.0088
9	159.0128	17196	189.2	3.9	0.0092
10	163.1278	8248	263.6	5.4	0.0198
11	167.0784	16076	515.3	10.5	0.0104
12	185.1146	14982	245.1	4.9	0.0124
13	209.1897	21824	1388.0	27.1	0.0096
14	210.1929	17676	217.3	4.2	0.0119
15	223.2055	22884	1548.4	29.7	0.0098
16	224.2087	16999	231.8	4.4	0.0132
17	227.2364	16877	274.9	5.2	0.0135
18	237.1537	12551	282.6	5.4	0.0189
19	237.2211	20708	1050.5	19.9	0.0115
20	249.2199	16088	180.3	3.4	0.0155
21	251.2366	20977	965.7	18.0	0.0120
22	252.2400	16936	180.1	3.4	0.0149
23	255.2677	18483	310.0	5.8	0.0138
24	272.0694	26619	4729.8	86.3	0.0102
25	273.0726	19263	651.7	11.9	0.0142
26	279.1591	16774	198.4	3.6	0.0166
27	293.1747	17956	432.0	7.8	0.0163
28	293.2833	17033	207.8	3.8	0.0172
29	301.2846	17463	197.6	3.6	0.0173
30	314.0798	27350	3850.3	70.0	0.0115
31	315.0833	18515	654.9	12.0	0.0170
32	322.0482	18109	341.1	6.2	0.0178
33	336.0618	28897	5515.9	100.0	0.0116
34	337.0652	20322	957.5	17.4	0.0166
35	371.3162	15924	267.4	4.9	0.0233
36	391.2841	17915	267.9	5.1	0.0218
37	622.0289	27607	1553.6	28.5	0.0225
38	623.0321	17870	252.5	4.6	0.0349
39	649.1346	18579	294.7	5.1	0.0349
40	922.0099	19165	1102.8	12.1	0.0481
#	m/z	Res.	S/N	I %	FWHM
1	336.0618	28897		100.0	0.0116
2	337.0651	28983		16.8	0.0116
3	338.0678	29069		1.7	0.0116
4	339.0704	29156		0.1	0.0116