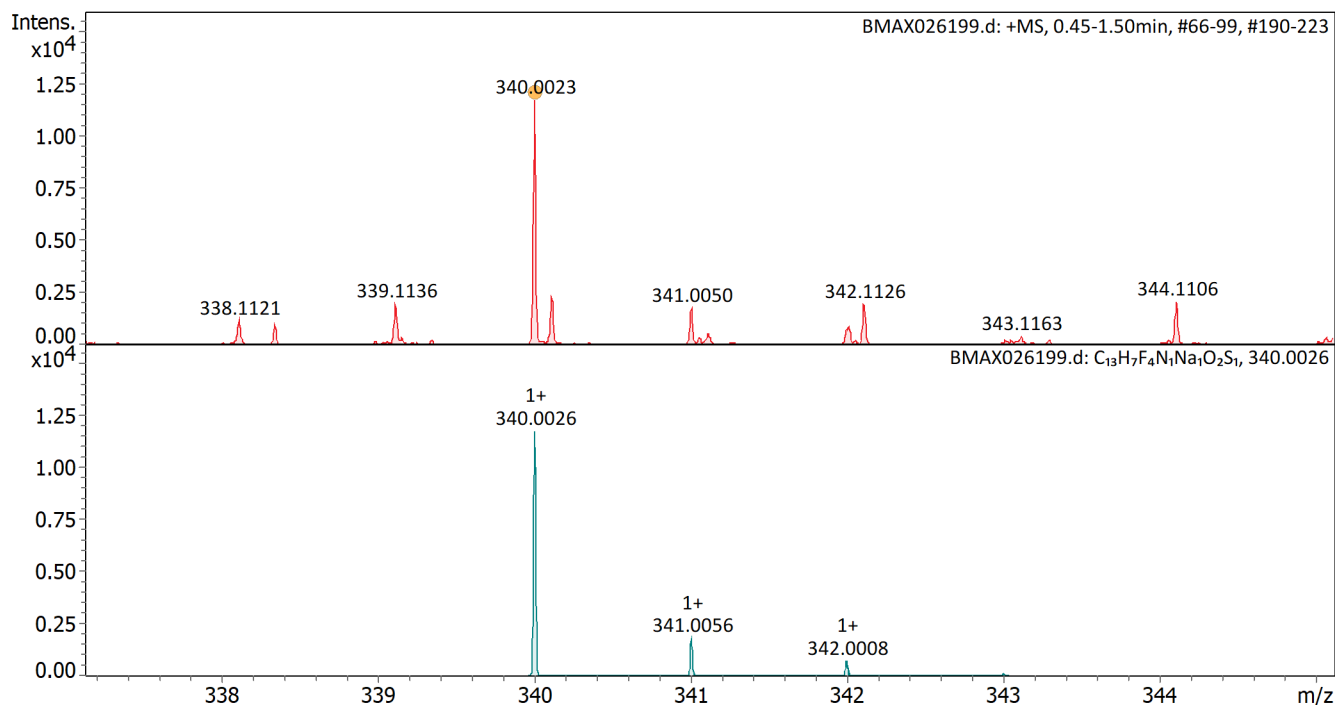
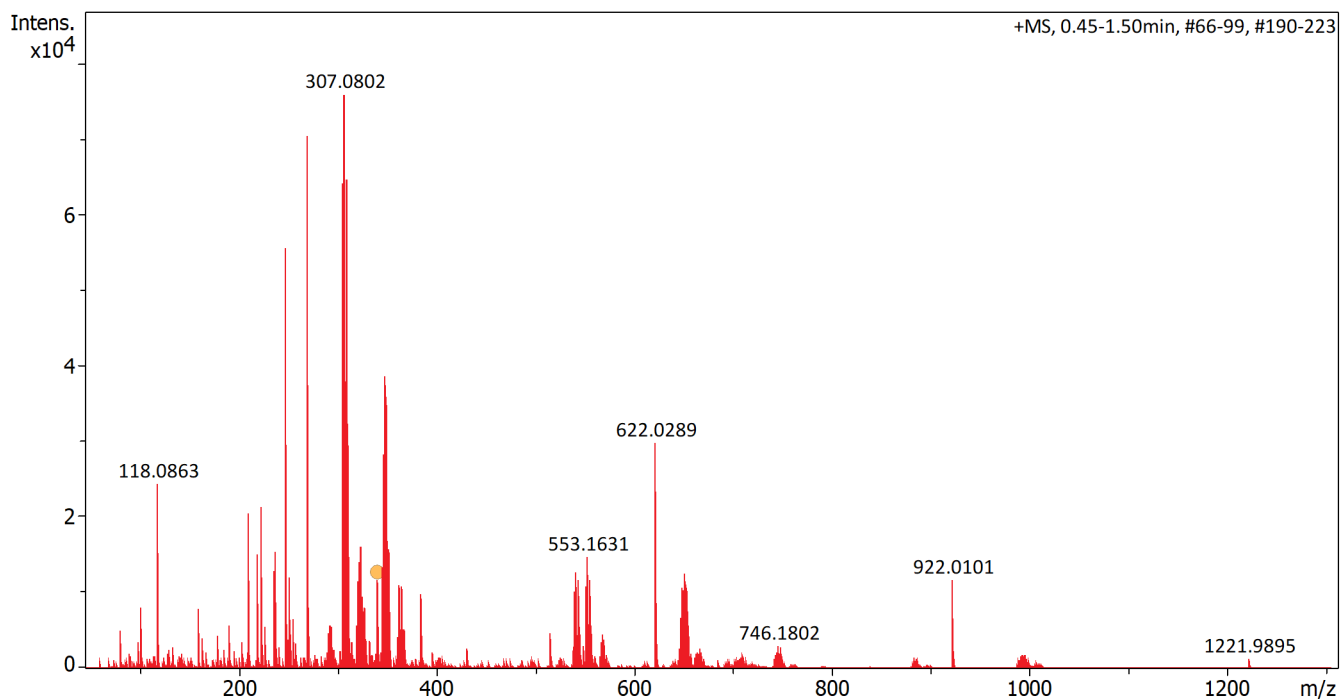


Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m	Acquisition Date:	24.11.2023 15:09:18
File Name:	D:\Data\bmax0261xx\BMAX026199.d	Operator:	Louis Bertschi
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1300 m/z	Set Collision Cell RF	200.0 Vpp
		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	C13H7F4NNaO2S	M+Na	340.0026	1+	340.0023	7.6	ok	0.3	0.9

Calibration Info:

Internal calibration

Date: 24.11.2023 15:12:17
 Polarity: Positive
 Calibration spectrum: +MS, 0.45-1.50min, #66-99, #190-223:
 Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 1.281 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	24380	-0.020
322.0481	322.0483	3476	0.633
622.0290	622.0289	29810	-0.144
922.0098	922.0101	11728	0.325
1221.9906	1221.9895	1267	-0.961
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	118.0863	21206	1168.0	32.1	0.0056
2	209.1897	20683	910.8	27.0	0.0101
3	219.0579	21613	674.3	20.0	0.0101
4	219.1866	19218	492.2	14.6	0.0114
5	223.2053	22448	950.4	28.2	0.0099
6	235.1645	20951	573.7	17.1	0.0112
7	237.2208	22517	686.2	20.4	0.0105
8	247.0890	27841	2417.2	73.1	0.0089
9	251.2366	20894	526.2	16.0	0.0120
10	269.0709	29051	3081.1	92.8	0.0093
11	305.0804	21943	1143.0	34.9	0.0139
12	306.0816	28153	2767.8	84.6	0.0109
13	307.0802	27516	3262.1	100.0	0.0112
14	309.0803	26147	2770.8	85.2	0.0118
15	311.0817	22395	1261.8	38.9	0.0139
16	321.1032	18525	483.4	15.2	0.0173
17	322.1023	18888	593.1	18.7	0.0171
18	324.0993	15806	677.0	21.3	0.0205
19	325.0924	16571	399.4	12.6	0.0196
20	340.0023	21193	477.8	15.4	0.0160
21	346.1070	19664	541.2	17.6	0.0176
22	347.1082	22239	1145.6	37.4	0.0156
23	348.1070	24234	1555.9	50.8	0.0144
24	350.1069	24566	1445.4	47.4	0.0143
25	352.1082	21116	633.9	20.9	0.0167
26	363.1287	17817	437.4	14.7	0.0204
27	365.1288	20379	429.8	14.5	0.0179
28	384.0290	19380	378.0	13.0	0.0198
29	540.2398	22729	377.8	13.5	0.0238
30	541.2386	22229	472.7	16.9	0.0243
31	543.2378	23112	435.9	15.5	0.0235
32	552.1642	20861	409.2	14.4	0.0265
33	553.1631	23193	553.6	19.4	0.0239
34	555.1630	21389	447.7	15.6	0.0260
35	622.0289	29313	1363.3	39.3	0.0212
36	649.1307	20999	529.2	14.1	0.0309
37	650.1315	21043	515.8	13.7	0.0309
38	651.1306	21785	631.6	16.7	0.0299
39	653.1307	21670	544.4	14.4	0.0301
40	922.0101	22132	1169.1	15.5	0.0417
#	m/z	Res.	S/N	I %	FWHM
1	340.0026	21193		100.0	0.0160
2	341.0056	21256		15.4	0.0160
3	342.0008	21318		6.0	0.0160
4	343.0029	21380		0.8	0.0160