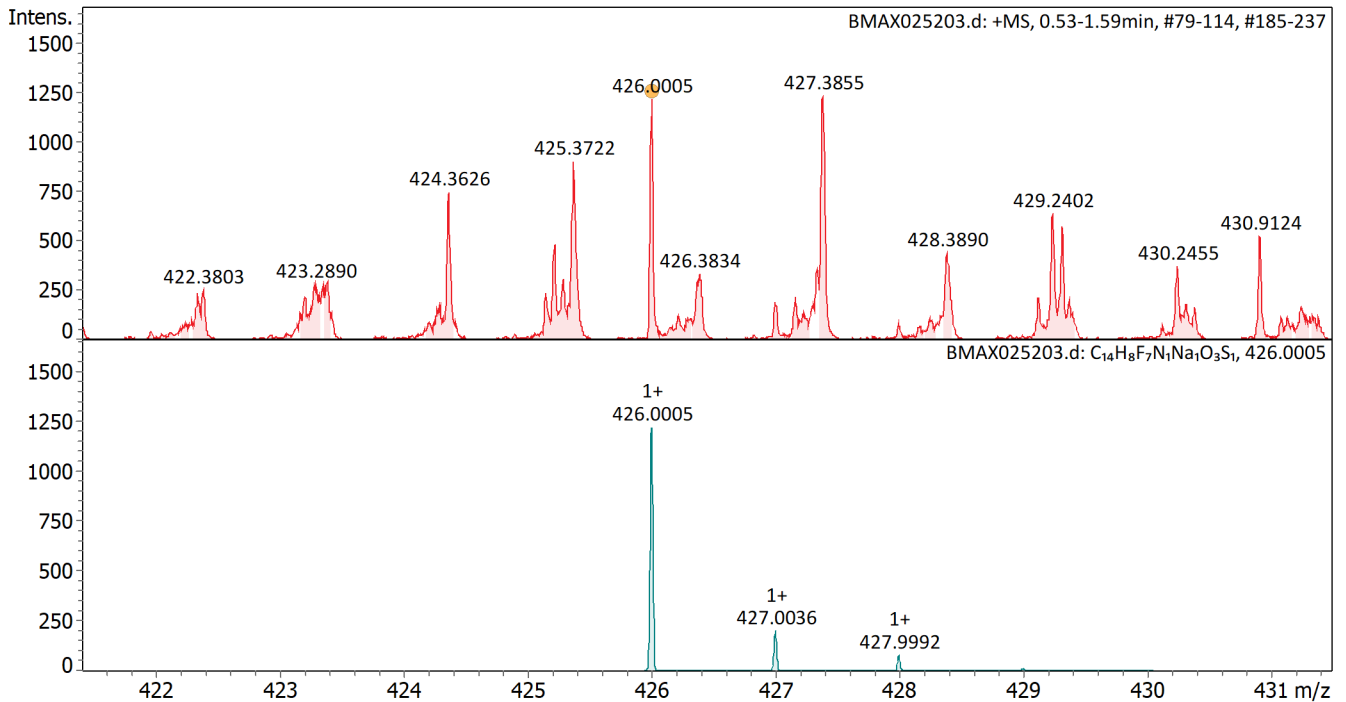
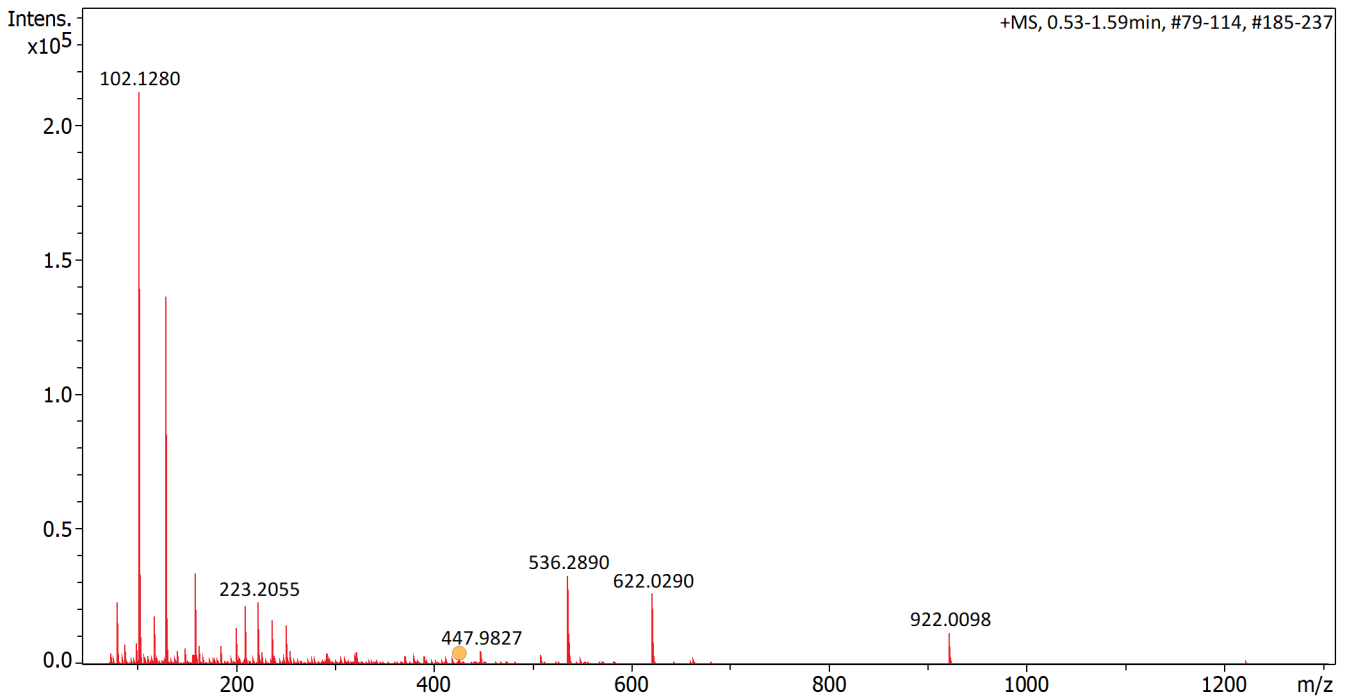


Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m	Acquisition Date:	13.09.2023 10:13:17
File Name:	D:\Data\bmax0252xx\BMAX025203.d	Operator:	Daniel Wirz
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	C14H8F7NNaO3S	M+Na	426.0005	1+	426.0005	5.2	ok	0.0	0.1

Calibration Info:

Internal calibration

Date: 13.09.2023 11:37:14
 Polarity: Positive
 Calibration spectrum: +MS, 0.53-1.59min, #79-114,
 #185-237: Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 0.092 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	17792	0.002
322.0481	322.0481	4378	-0.038
622.0290	622.0290	26167	0.012
922.0098	922.0098	11815	-0.024
1221.9906	1221.9907	1228	0.073
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	74.0967	13721	196.3	1.9	0.0054
2	80.0497	18045	1099.6	10.7	0.0044
3	88.1120	15542	354.3	3.6	0.0057
4	100.0755	16092	349.5	3.6	0.0062
5	102.1280	19109	9704.3	100.0	0.0053
6	103.1309	18591	706.7	7.3	0.0055
7	118.0863	17709	812.7	8.4	0.0067
8	129.0299	18903	175.2	1.8	0.0068
9	130.1592	28004	6269.5	64.2	0.0046
10	131.1622	16416	409.4	4.2	0.0080
11	141.0024	16136	232.4	2.3	0.0087
12	149.0233	16321	285.9	2.9	0.0091
13	157.0173	15688	163.0	1.6	0.0100
14	158.0169	15327	160.0	1.6	0.0103
15	158.9637	15343	178.2	1.7	0.0104
16	159.0131	19345	1621.1	15.9	0.0082
17	160.0140	16545	176.5	1.7	0.0097
18	163.1299	11327	334.8	3.2	0.0144
19	185.1147	17686	340.8	3.1	0.0105
20	201.1597	19062	718.3	6.3	0.0106
21	209.1900	21501	1179.1	10.2	0.0097
22	210.1930	17684	182.6	1.6	0.0119
23	223.1416	20730	1204.3	10.2	0.0108
24	223.2055	22378	1281.9	10.8	0.0100
25	224.2088	16827	199.9	1.7	0.0133
26	227.2366	17247	254.2	2.1	0.0132
27	237.1517	11941	221.1	1.8	0.0199
28	237.2213	20759	933.1	7.6	0.0114
29	251.2368	21645	862.6	6.8	0.0116
30	255.2680	18051	308.8	2.4	0.0141
31	293.1749	17277	267.1	2.0	0.0170
32	322.0481	18985	282.5	2.1	0.0170
33	391.2842	18902	201.5	1.5	0.0207
34	447.9827	17296	281.6	2.3	0.0259
35	508.2582	17560	194.6	1.7	0.0289
36	536.2890	30796	1725.8	15.5	0.0174
37	537.2926	19517	507.5	4.6	0.0275
38	622.0290	28682	1647.0	12.3	0.0217
39	623.0323	17537	248.2	1.9	0.0355
40	922.0098	20952	1436.1	5.6	0.0440
#	m/z	Res.	S/N	I %	FWHM
1	426.0005	17244		100.0	0.0247
2	427.0036	17285		16.5	0.0247
3	427.9992	17325		6.4	0.0247
4	429.0012	17365		0.9	0.0247
5	430.0023	17406		0.1	0.0247