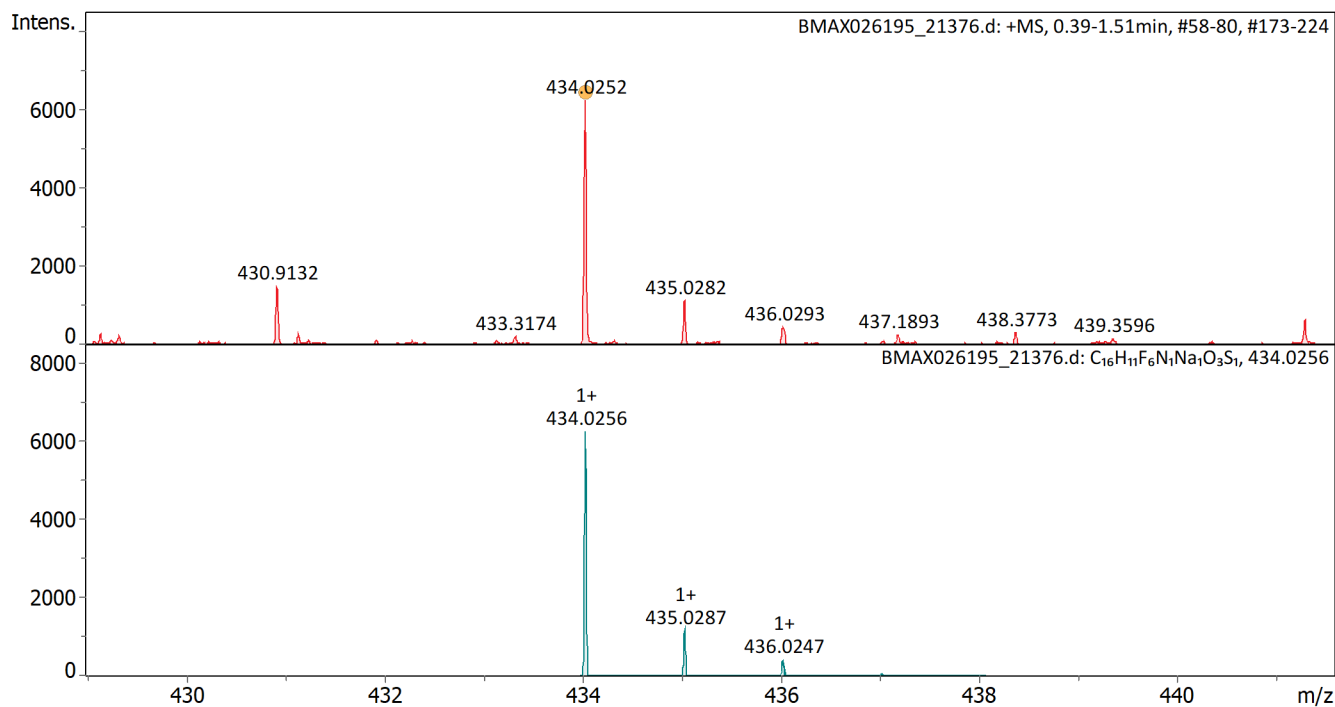
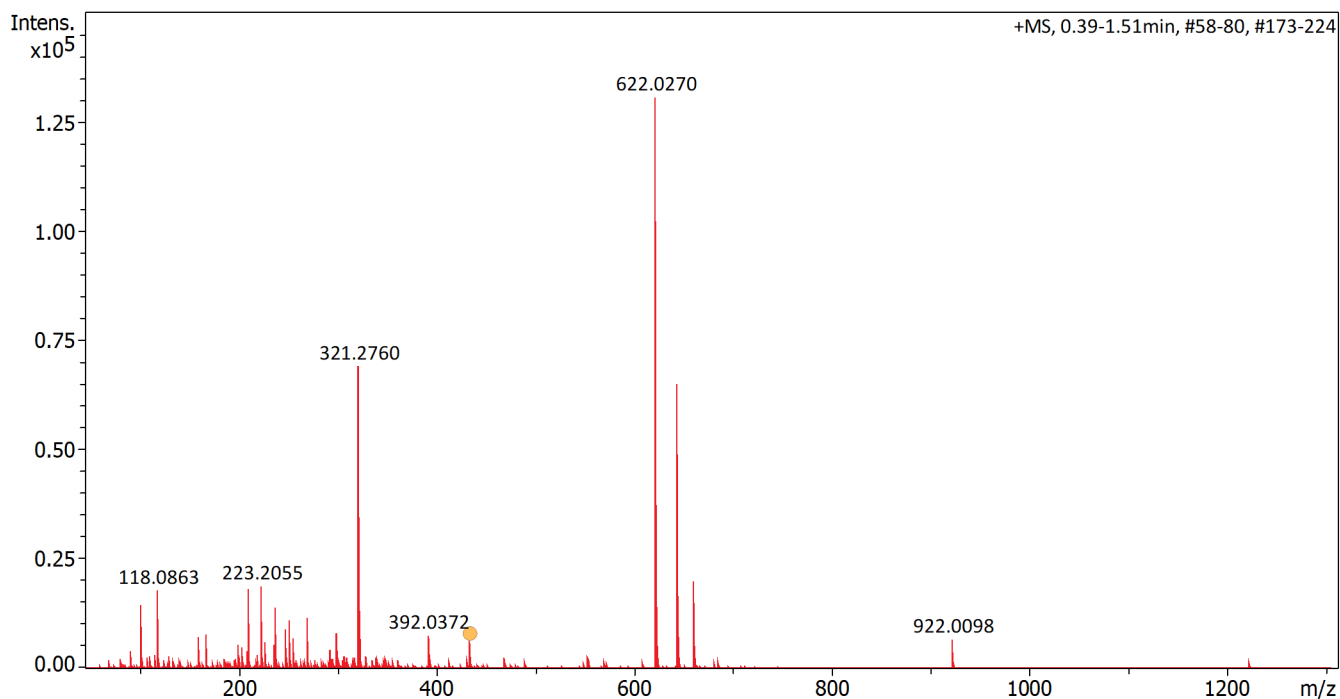


## Acquisition Parameter

Method: ETH\_HyStar\_HPLC\_QTOF\_POS\_LowMass\_Loop-AS.m  
File Name: D:\Data\bmax0261xx\BMAX026195\_21376.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: 24.11.2023 15:51:05  
Operator: Louis Bertschi  
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	C16H11F6NNaO3S	M+Na	434.0256	1+	434.0252	4.4	ok	0.5	1.0

## Calibration Info:

## Internal calibration

Date: 24.11.2023 15:54:39  
 Polarity: Positive  
 Calibration spectrum: +MS, 0.39-1.51min, #58-80, #173-224:  
 Scan  
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial  
 Calibration mode: Quadratic  
 Standard deviation: 0.045 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	17920	0.020
322.0481	322.0481	4033	-0.027
622.0290			
922.0098	922.0098	6702	0.021
1221.9906	1221.9906	1271	-0.011
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

## Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	90.9763	15803	163.9	2.9	0.0058
2	101.0083	15900	601.4	11.1	0.0064
3	115.0346	16755	119.6	2.3	0.0069
4	118.0863	22718	721.9	13.7	0.0052
5	130.1586	17071	110.6	2.1	0.0076
6	158.9637	19485	294.4	5.5	0.0082
7	167.0785	16563	313.6	5.8	0.0101
8	199.6592	19204	235.6	4.1	0.0104
9	203.1919	17665	211.5	3.7	0.0115
10	208.6645	17812	177.9	3.1	0.0117
11	209.1899	22145	808.0	14.0	0.0094
12	210.1929	20077	132.3	2.3	0.0105
13	219.0252	13961	133.6	2.3	0.0157
14	223.2055	24243	848.3	14.5	0.0092
15	226.9512	16719	128.6	2.2	0.0136
16	227.2366	18794	264.9	4.5	0.0121
17	235.1646	19475	238.9	4.1	0.0121
18	237.1544	13087	147.7	2.5	0.0181
19	237.2211	23617	621.2	10.5	0.0100
20	247.0891	20737	406.4	6.8	0.0119
21	251.2368	21505	496.9	8.3	0.0117
22	255.2680	20629	308.4	5.2	0.0124
23	269.0711	21412	522.7	8.8	0.0126
24	293.2834	19586	189.5	3.2	0.0150
25	299.2939	18770	365.9	6.2	0.0159
26	321.2760	29858	3056.2	52.9	0.0108
27	321.3127	17699	172.9	3.0	0.0182
28	322.0481	19001	178.4	3.1	0.0169
29	322.2794	20864	594.3	10.3	0.0154
30	392.0372	19447	328.5	5.8	0.0202
31	434.0252	20807	269.8	4.8	0.0209
32	553.4586	17860	147.0	2.2	0.0310
33	622.0270	36329	8326.9	100.0	0.0171
34	623.0317	20470	1141.8	13.7	0.0304
35	624.0330	17583	187.0	2.2	0.0355
36	644.0095	34482	4446.1	49.7	0.0187
37	645.0133	20020	642.6	7.2	0.0322
38	659.9845	22059	1451.9	15.4	0.0299
39	660.9873	18932	219.5	2.3	0.0349
40	922.0098	21005	809.0	5.1	0.0439
#	m/z	Res.	S/N	I %	FWHM
1	434.0256	20807		100.0	0.0209
2	435.0287	20855		18.7	0.0209
3	436.0247	20903		6.7	0.0209
4	437.0265	20951		1.0	0.0209
5	438.0278	20999		0.1	0.0209