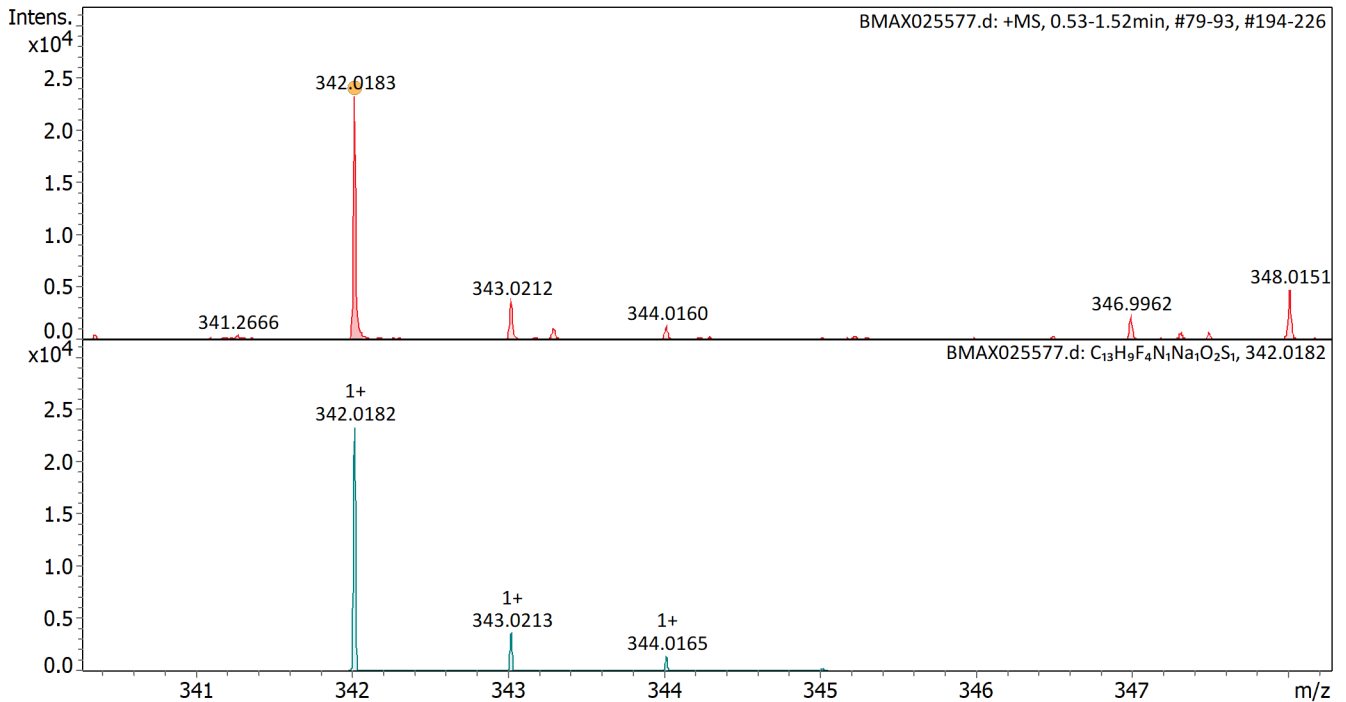
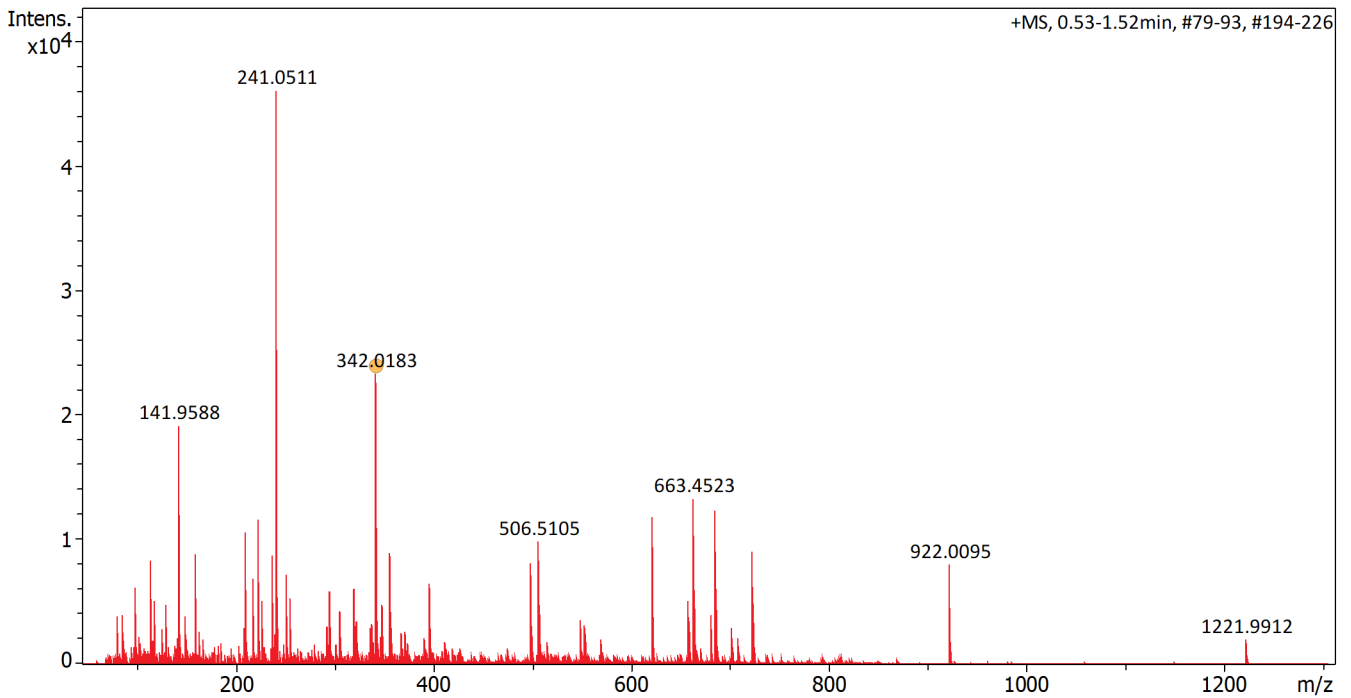


Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m	Acquisition Date:	09.10.2023 05:21:08
File Name:	D:\Data\bmax0255xx\BMAX025577.d	Operator:	Michael Meier
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	C13H9F4NNaO2S	M+Na	342.0182	1+	342.0183	2.6	ok	-0.1	-0.2

Calibration Info:

Internal calibration

Date: 09.10.2023 05:24:39
 Polarity: Positive
 Calibration spectrum: +MS, 0.53-1.52min, #79-93, #194-226:
 Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 0.899 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	5100	0.075
322.0481	322.0480	3477	-0.496
622.0290	622.0291	11867	0.285
922.0098	922.0095	8050	-0.373
1221.9906	1221.9912	1957	0.492
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	84.9593	13779	194.8	8.7	0.0062
2	97.9685	15061	298.9	13.5	0.0065
3	113.9636	16958	394.5	18.1	0.0067
4	118.0863	15377	242.3	11.1	0.0077
5	130.1592	17847	227.4	10.5	0.0073
6	141.9588	18936	900.7	41.6	0.0075
7	149.0236	15188	180.7	8.4	0.0098
8	159.0132	17214	410.6	19.2	0.0092
9	159.9694	15746	191.1	8.9	0.0102
10	209.1904	19724	513.9	23.1	0.0106
11	217.0005	18225	335.3	15.0	0.0119
12	218.0180	17312	266.0	11.9	0.0126
13	223.2061	20454	565.5	25.3	0.0109
14	227.2373	18664	247.0	11.0	0.0122
15	237.2218	19058	430.6	19.0	0.0124
16	241.0511	25802	2288.2	100.0	0.0093
17	242.0543	16758	267.2	11.7	0.0144
18	251.2373	19082	366.6	15.8	0.0132
19	255.2687	18635	268.7	11.5	0.0137
20	295.1179	18454	312.1	12.7	0.0160
21	306.0713	17486	227.9	9.2	0.0175
22	320.0363	17301	326.5	13.2	0.0185
23	342.0183	22914	1293.2	50.7	0.0149
24	348.0151	17178	262.7	10.3	0.0203
25	356.0017	19055	503.2	19.6	0.0187
26	396.0850	17847	345.9	14.1	0.0222
27	498.5241	19417	389.6	17.6	0.0257
28	506.5105	18308	471.4	21.4	0.0277
29	507.0120	18110	230.4	10.5	0.0280
30	507.5199	12320	210.5	9.6	0.0412
31	622.0291	22741	604.9	25.8	0.0274
32	658.0383	17895	267.1	10.9	0.0368
33	663.4523	20026	709.7	28.9	0.0331
34	664.4558	16900	322.2	13.1	0.0393
35	680.4788	16182	215.0	8.5	0.0421
36	685.4337	25562	689.2	26.9	0.0268
37	686.4374	21186	341.9	13.3	0.0324
38	722.5250	22639	549.2	19.8	0.0319
39	723.5288	19340	292.0	10.5	0.0374
40	922.0095	19673	741.7	17.5	0.0469
#	m/z	Res.	S/N	I %	FWHM
1	342.0182	22914		100.0	0.0149
2	343.0213	22981		15.4	0.0149
3	344.0165	23048		6.0	0.0149
4	345.0186	23115		0.8	0.0149