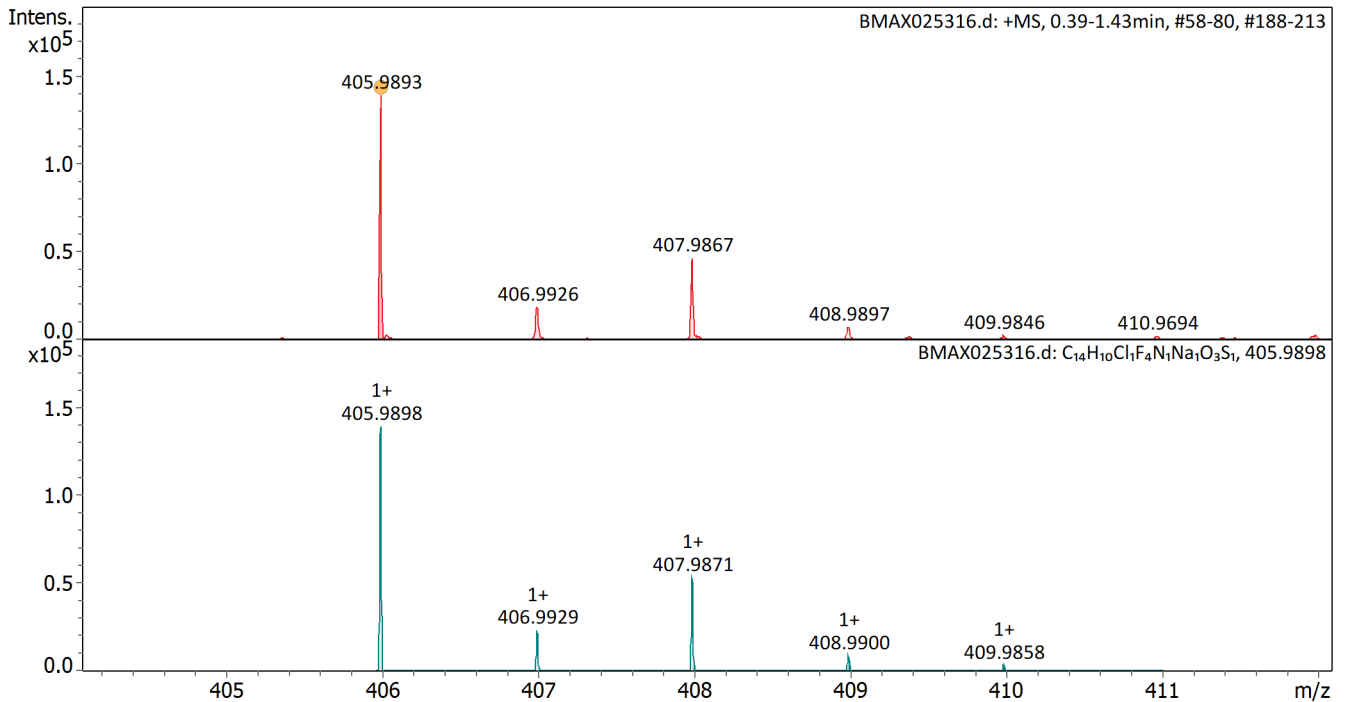
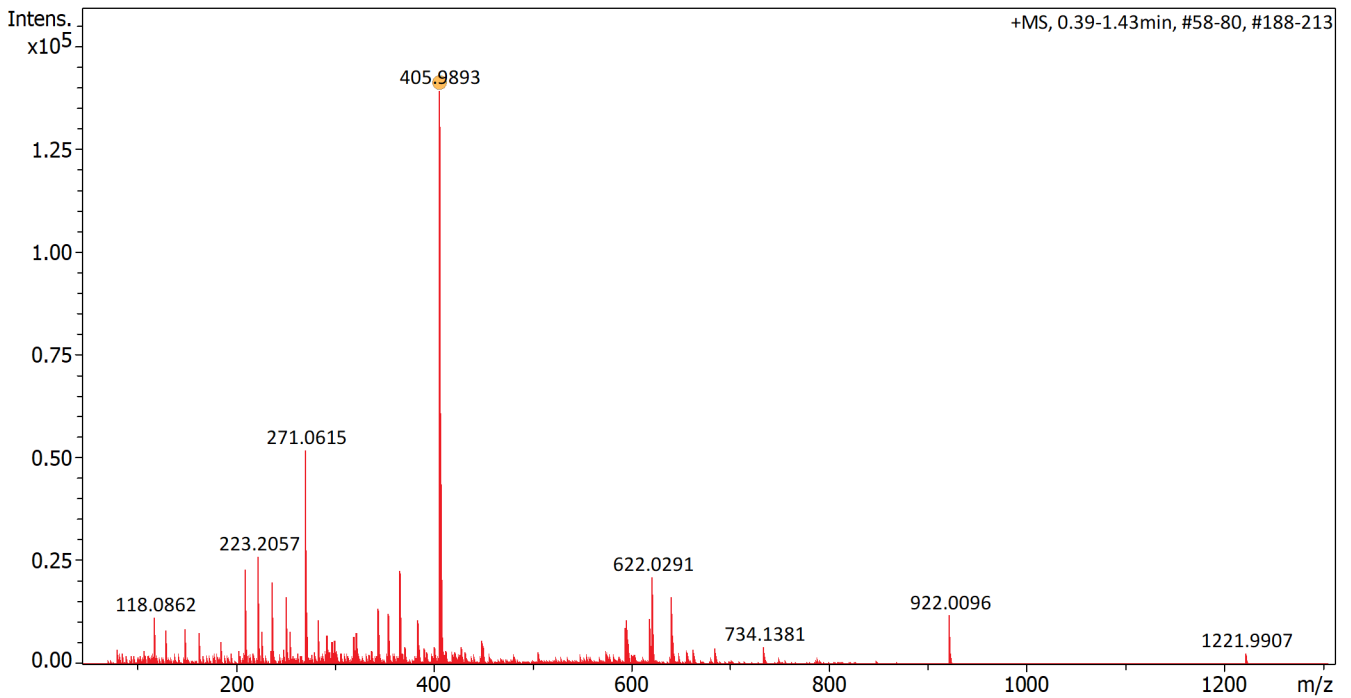


Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m	Acquisition Date:	20.09.2023 05:26:06
File Name:	D:\Data\bmax0253xx\BMAX025316.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	C14H10CIF4NNaO3S	M+Na	405.9898	1+	405.9893	27.1	ok	0.5	1.3

Calibration Info:

Internal calibration

Date: 20.09.2023 05:28:30
 Polarity: Positive
 Calibration spectrum: +MS, 0.39-1.43min, #58-80, #188-213:
 Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Quadratic
 Standard deviation: 0.319 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0862	11418	-0.045
322.0481			
622.0290	622.0291	21248	0.170
922.0098	922.0096	11855	-0.220
1221.9906	1221.9907	2511	0.084
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	118.0862	17874	634.6	8.2	0.0066
2	130.1588	17972	460.6	5.9	0.0072
3	149.0233	17436	503.6	6.2	0.0085
4	163.1306	14230	454.9	5.5	0.0115
5	185.1147	16675	335.3	3.8	0.0111
6	209.1900	21179	1526.5	16.6	0.0099
7	223.2057	22847	1772.6	18.8	0.0098
8	227.2367	18673	539.7	5.7	0.0122
9	237.2213	21621	1395.2	14.4	0.0110
10	251.2369	20155	1149.7	11.6	0.0125
11	255.2680	17864	563.8	5.7	0.0143
12	271.0615	29983	3641.4	37.3	0.0090
13	272.0668	18979	868.5	8.9	0.0143
14	284.0691	19260	735.0	7.6	0.0147
15	293.1750	18364	465.1	4.9	0.0160
16	298.0484	18441	371.2	4.0	0.0162
17	300.1004	17373	386.5	4.2	0.0173
18	320.0459	17374	408.0	4.7	0.0184
19	322.0469	16502	456.8	5.4	0.0195
20	344.0903	20066	753.5	9.6	0.0171
21	355.1426	20009	659.0	8.8	0.0177
22	366.0721	22982	1147.3	16.4	0.0159
23	384.0078	19785	494.7	7.7	0.0194
24	405.9893	37525	5672.4	100.0	0.0108
25	406.9926	21814	744.8	13.2	0.0187
26	407.9867	30155	1877.7	33.5	0.0135
27	408.9897	18357	282.1	5.0	0.0223
28	449.0052	17650	195.5	4.0	0.0254
29	450.0043	17206	155.6	3.2	0.0262
30	594.4821	18624	280.3	6.4	0.0319
31	594.9834	17604	140.9	3.2	0.0338
32	595.4811	18562	334.4	7.7	0.0321
33	595.9829	17163	163.5	3.7	0.0347
34	596.4829	14767	186.7	4.3	0.0404
35	619.0521	20111	354.2	8.0	0.0308
36	620.0549	17393	144.1	3.3	0.0357
37	622.0291	25053	675.7	15.3	0.0248
38	641.0338	21716	521.9	11.6	0.0295
39	642.0368	18965	223.5	5.0	0.0339
40	922.0096	20398	853.7	8.5	0.0452
#	m/z	Res.	S/N	I %	FWHM
1	405.9898	37525		100.0	0.0108
2	406.9929	37618		16.5	0.0108
3	407.9871	37710		38.4	0.0108
4	408.9900	37802		6.2	0.0108
5	409.9858	37894		2.1	0.0108
6	410.9878	37987		0.3	0.0108