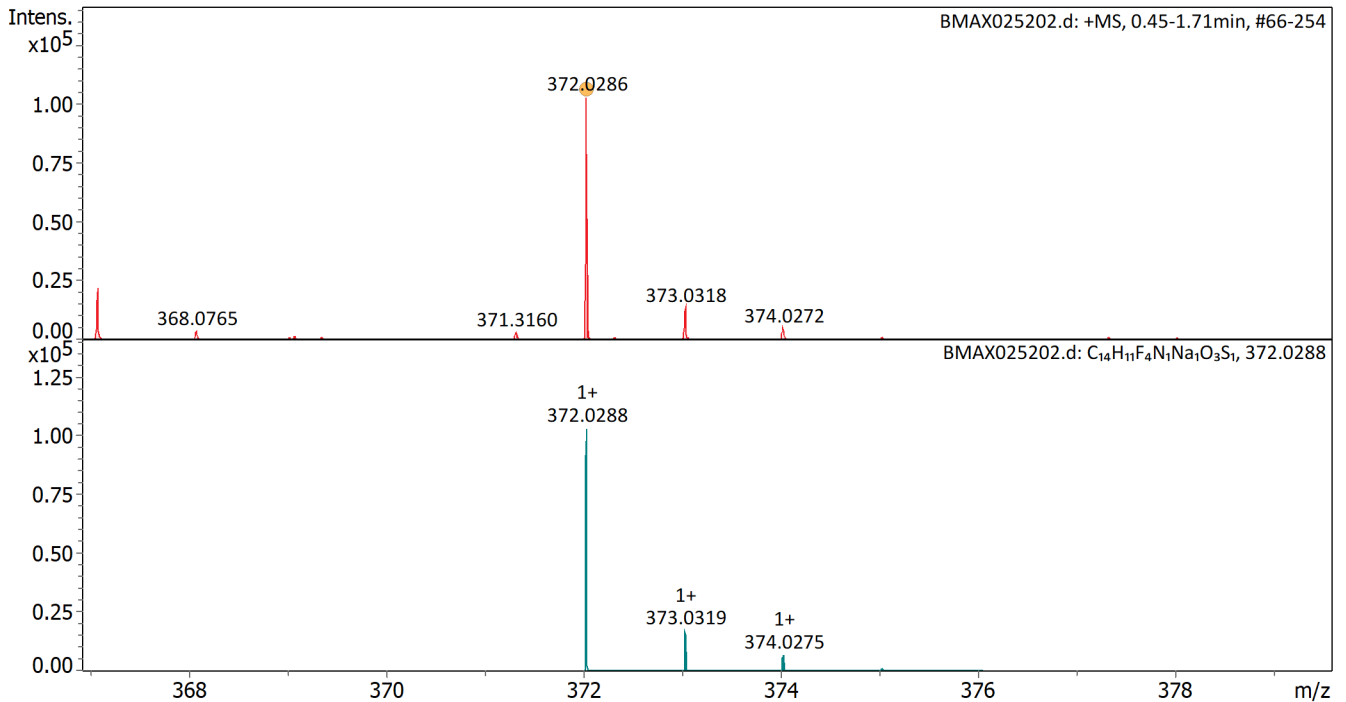
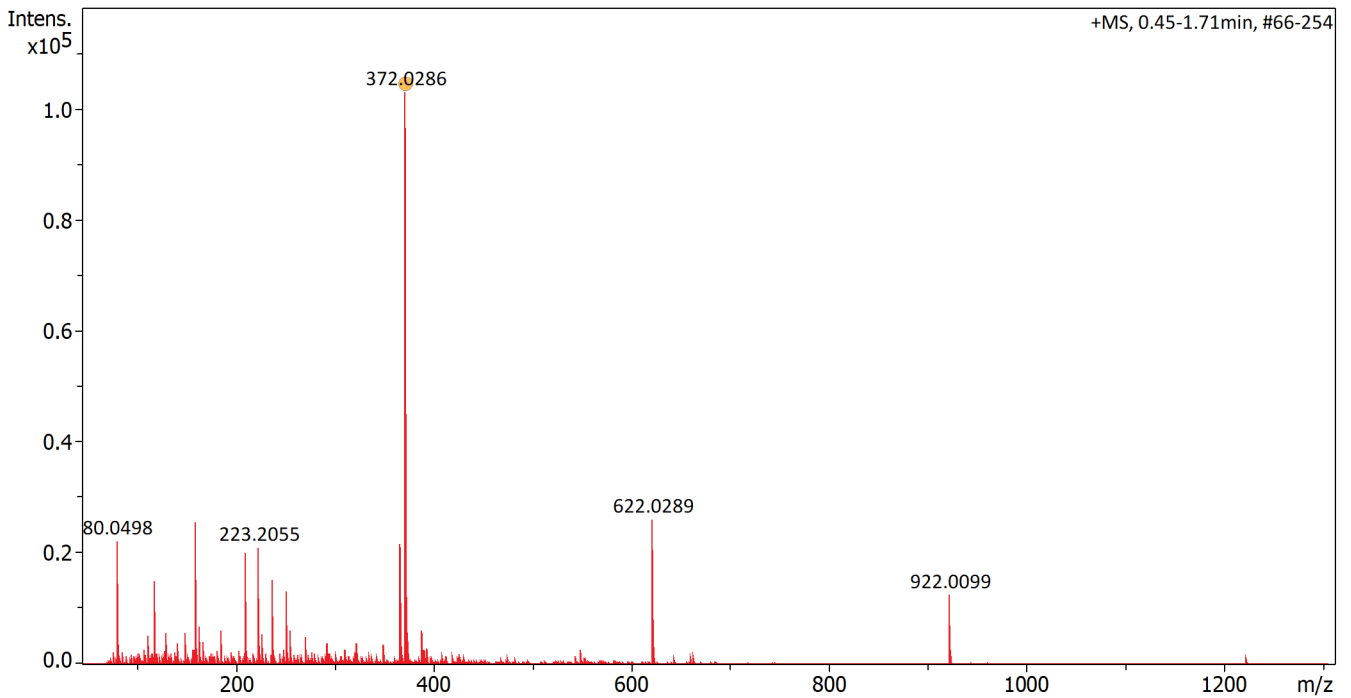


Acquisition Parameter

Method: ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m
File Name: D:\Data\bmax0251xx\BMAX025202.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: 13.09.2023 10:10:27
Operator: Daniel Wirz
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	C ₁₄ H ₁₁ F ₄ NNaO ₃ S	M+Na	372.0288	1+	372.0286	21.8	ok	0.2	0.6

Calibration Info:

Internal calibration

Date: 13.09.2023 10:23:04
 Polarity: Positive
 Calibration spectrum: +MS, 0.45-1.71min, #66-254: Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 0.353 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	15011	-0.008
322.0481	322.0482	3869	0.139
622.0290	622.0289	26214	-0.040
922.0098	922.0099	12583	0.073
1221.9906	1221.9903	1005	-0.289
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	80.0498	17909	840.7	21.6	0.0045
2	111.0204	15825	188.6	5.0	0.0070
3	118.0863	17710	547.7	14.6	0.0067
4	129.0300	18709	126.7	3.3	0.0069
5	130.1590	19436	212.0	5.5	0.0067
6	141.0026	16047	148.6	3.8	0.0088
7	149.0233	16135	221.3	5.5	0.0092
8	158.9638	16317	240.7	5.8	0.0097
9	159.0132	19024	1026.9	24.9	0.0084
10	160.0140	16793	114.6	2.8	0.0095
11	163.1302	12079	280.4	6.7	0.0135
12	167.0778	14724	170.4	4.0	0.0113
13	185.1148	17151	272.9	6.0	0.0108
14	209.1899	21100	966.7	19.4	0.0099
15	210.1930	17383	150.0	3.0	0.0121
16	223.2055	22104	1068.2	20.5	0.0101
17	224.2088	17205	169.3	3.2	0.0130
18	227.2366	17507	281.4	5.3	0.0130
19	237.1503	12922	213.0	3.9	0.0184
20	237.2212	20866	809.3	14.8	0.0114
21	251.2367	21170	740.5	12.8	0.0119
22	255.2679	18270	350.2	6.0	0.0140
23	271.0615	19568	295.4	4.8	0.0139
24	293.1749	17150	237.6	3.7	0.0171
25	322.0482	19045	255.0	3.8	0.0169
26	350.0471	17792	239.5	3.4	0.0197
27	367.0735	25693	1525.3	21.2	0.0143
28	368.0765	17653	237.6	3.3	0.0209
29	371.3160	15656	197.9	2.7	0.0237
30	372.0286	40965	7207.6	100.0	0.0091
31	373.0318	23314	914.9	12.7	0.0160
32	374.0272	16436	307.7	4.3	0.0228
33	388.0028	20444	420.2	5.9	0.0190
34	391.2843	18247	188.9	2.6	0.0214
35	394.0108	17210	194.1	2.7	0.0229
36	548.5036	16949	208.1	2.7	0.0324
37	622.0289	26674	2532.4	25.4	0.0233
38	623.0322	17782	387.3	3.9	0.0350
39	922.0099	20427	1771.1	12.2	0.0451
40	923.0132	17259	381.4	2.6	0.0535
#	m/z	Res.	S/N	I %	FWHM
1	372.0288	40965		100.0	0.0091
2	373.0319	41076		16.5	0.0091
3	374.0275	41185		6.4	0.0091
4	375.0295	41295		0.9	0.0091
5	376.0306	41406		0.1	0.0091