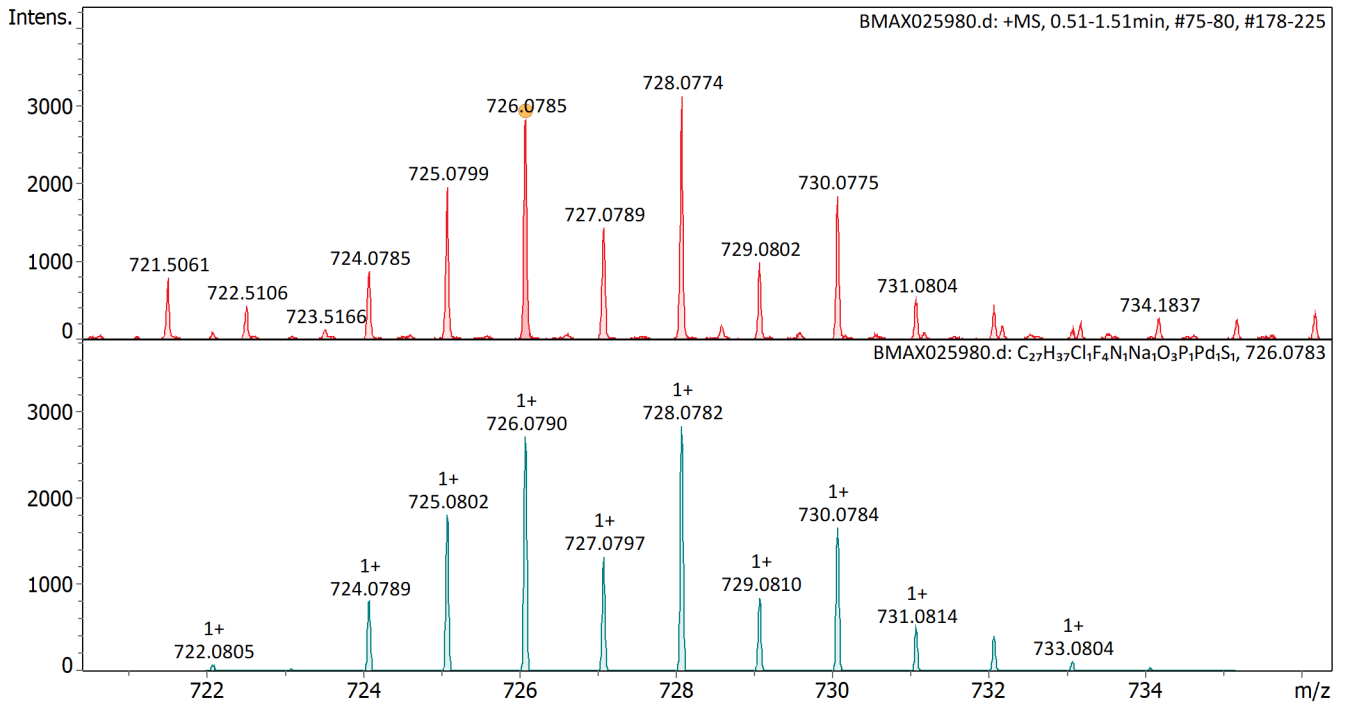
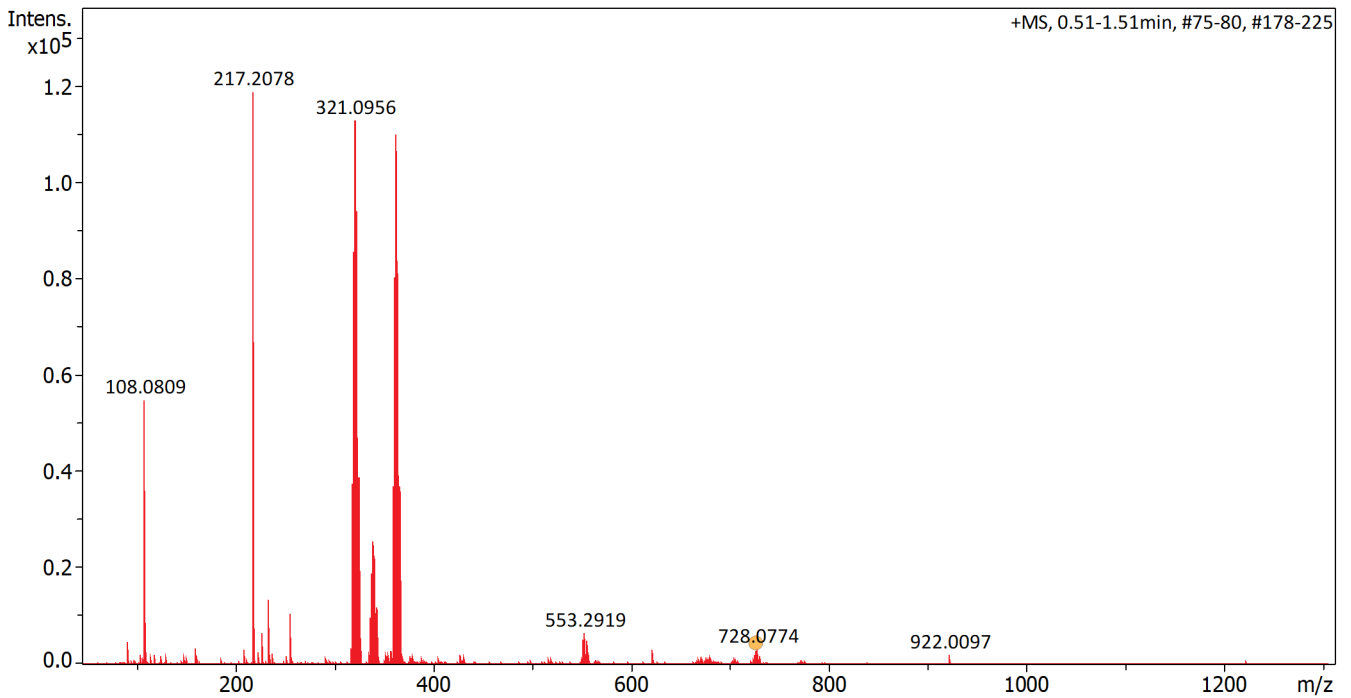


Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m	Acquisition Date:	10.11.2023 05:11:05
File Name:	D:\Data\bmax0259xx\BMAX025980.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	C27H37ClF4NNaO3PPdS	M+Na	726.0783	1+	726.0785	15.4	ok	0.6	0.8

Calibration Info:

Internal calibration

Date: 10.11.2023 05:13:59
 Polarity: Positive
 Calibration spectrum: +MS, 0.51-1.51min, #75-80, #178-225:
 Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Quadratic
 Standard deviation: 0.107 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	1879	-0.015
322.0481			
622.0290	622.0290	2958	0.057
922.0098	922.0097	1974	-0.074
1221.9906	1221.9907	771	0.028
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	90.9766	15291	272.5	3.8	0.0059
2	108.0809	19645	3135.1	46.2	0.0055
3	109.0840	16036	221.8	3.3	0.0068
4	158.9639	18772	171.9	2.8	0.0085
5	209.1901	20214	146.7	2.5	0.0103
6	217.2078	25417	5698.6	100.0	0.0085
7	218.2114	20872	795.3	14.0	0.0105
8	226.9515	21485	295.3	5.4	0.0106
9	233.2027	18904	600.2	11.2	0.0123
10	255.1847	21105	433.9	8.8	0.0121
11	317.0975	19039	122.3	2.7	0.0167
12	319.0961	27290	1396.4	31.6	0.0117
13	320.0971	32838	3179.6	72.1	0.0097
14	321.0956	36004	4181.1	94.9	0.0089
15	322.0994	20596	458.5	10.4	0.0156
16	323.0958	31865	3475.4	79.2	0.0101
17	324.0997	22362	463.3	10.6	0.0145
18	325.0974	27126	1428.1	32.7	0.0120
19	326.1009	20051	195.3	4.5	0.0163
20	337.1049	18657	348.3	8.1	0.0181
21	338.1080	22452	679.8	15.9	0.0151
22	339.1063	22956	914.7	21.4	0.0148
23	340.1093	17666	120.0	2.8	0.0193
24	341.1066	23249	809.2	19.0	0.0147
25	342.1098	17284	105.8	2.5	0.0198
26	343.1075	19814	424.0	9.9	0.0173
27	358.1240	17132	103.6	2.4	0.0209
28	360.1227	28011	1329.1	31.2	0.0129
29	361.1236	31189	2874.0	67.5	0.0116
30	362.1220	34311	3942.9	92.5	0.0106
31	363.1258	21338	530.7	12.5	0.0170
32	364.1222	29788	3004.8	70.5	0.0122
33	365.1259	22393	519.6	12.2	0.0163
34	366.1240	26322	1327.7	31.1	0.0139
35	367.1269	18642	221.7	5.2	0.0197
36	552.2930	19371	264.5	4.1	0.0285
37	553.2919	20149	353.9	5.4	0.0275
38	555.2917	19143	273.1	4.2	0.0290
39	622.0290	21914	188.9	2.5	0.0284
40	728.0774	19554	242.7	2.6	0.0372
#	m/z	Res.	S/N	I %	FWHM
1	722.0805	17963		2.5	0.0402
2	723.0837	17988		0.8	0.0402
3	724.0789	18013		28.3	0.0402
4	725.0802	18038		63.3	0.0402
5	726.0790	18063		95.2	0.0402
6	727.0797	18087		46.7	0.0402
7	728.0782	18112		100.0	0.0402
8	729.0810	18137		30.0	0.0402

#	m/z	Res.	S/N	I %	FWHM
9	730.0784	18162		58.3	0.0402
10	731.0814	18187		17.0	0.0402
11	732.0780	18212		14.2	0.0402
12	733.0804	18237		3.8	0.0402
13	734.0790	18262		1.0	0.0402
14	735.0798	18286		0.2	0.0402