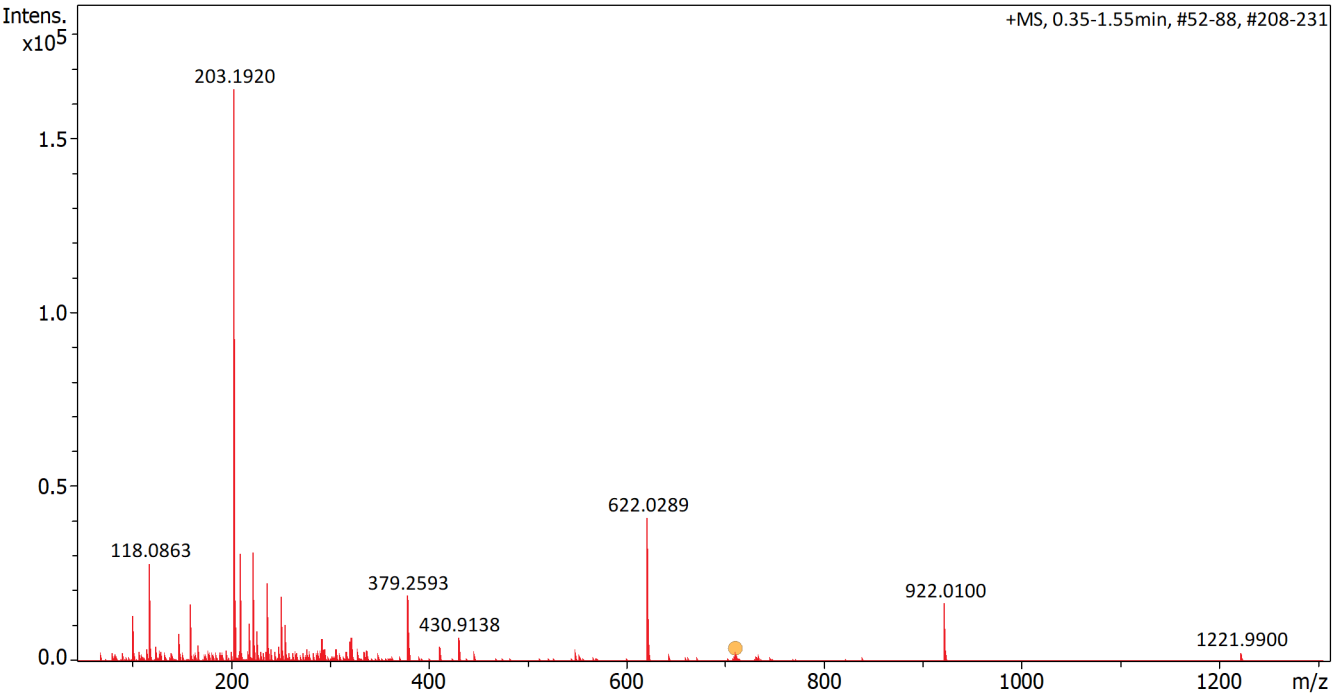
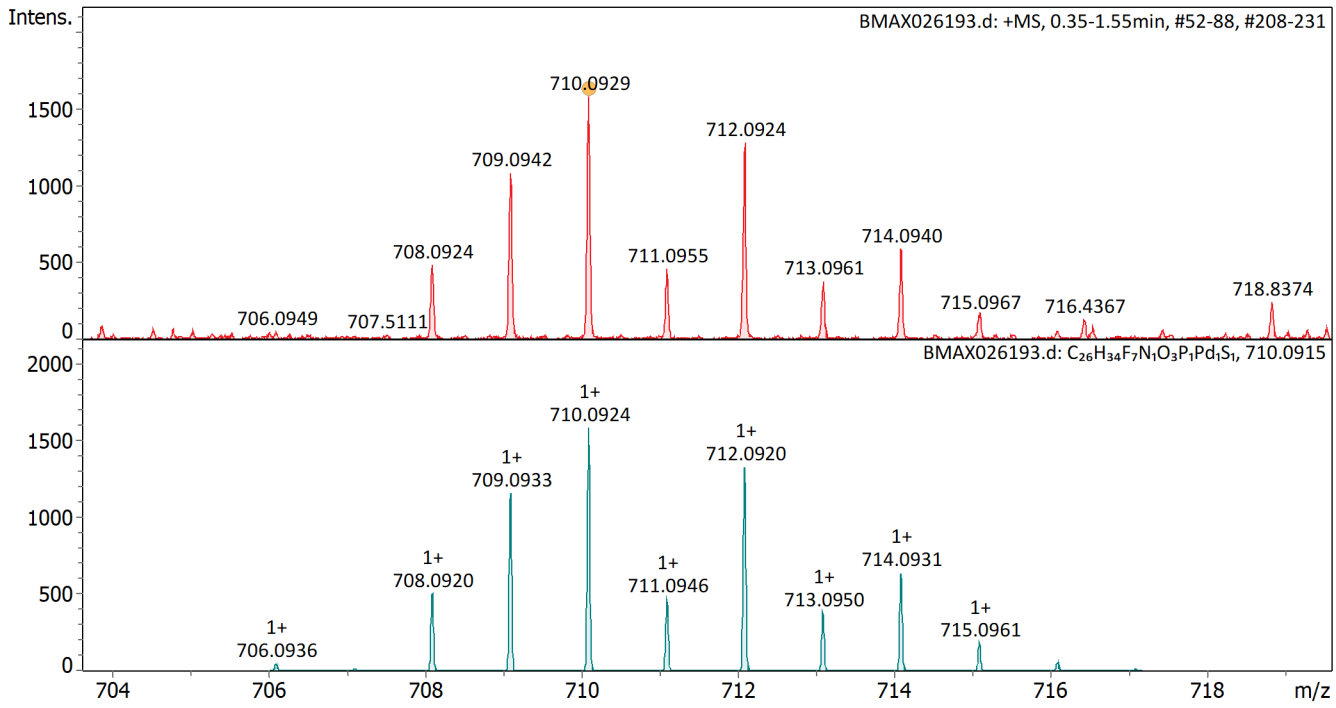
Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m			Acquisition Date:	24.11.2023 14:52:13
File Name:	D:\Data\bmax0261xx\BMAX026193.d			Operator:	Louis Bertschi
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	230 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	10.0 l/min
Scan End	1300 m/z	Set Collision Cell RF	200.0 Vpp	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	C26H34F7NO3PPdS	M+H	710.0915	1+	710.0929	21.8	ok	-0.5	-0.7

Calibration Info:

Internal calibration

Date:	24.11.2023 14:54:50
Polarity:	Positive
Calibration spectrum:	+MS, 0.35-1.55min, #52-88, #208-231: Scan
Reference mass list:	ESI: Tunemix (pos) ESI-TOF Spezial
Calibration mode:	Enhanced Quadratic
Standard deviation:	0.751 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	28138	-0.019
322.0481	322.0482	6756	0.361
622.0290	622.0289	41113	-0.117
922.0098	922.0100	16617	0.256
1221.9906	1221.9900	2543	-0.537
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	101.0085	16702	581.1	8.0	0.0060
2	115.0336	17721	146.7	2.1	0.0065
3	118.0863	20494	1185.4	17.2	0.0058
4	125.0360	16425	173.8	2.6	0.0076
5	147.1295	20998	318.9	4.9	0.0070
6	158.9638	20132	648.3	9.9	0.0079
7	167.0780	15845	178.4	2.7	0.0105
8	195.1737	17894	133.9	2.0	0.0109
9	203.1427	17046	135.4	2.0	0.0119
10	203.1920	35976	6885.5	100.0	0.0056
11	204.1958	22516	737.4	10.7	0.0091
12	209.1900	21690	1312.4	18.9	0.0096
13	210.1930	19488	212.7	3.1	0.0108
14	219.0238	16728	253.7	3.6	0.0131
15	219.1867	19664	464.1	6.6	0.0111
16	223.2055	22954	1363.8	19.2	0.0097
17	224.2088	17003	197.0	2.8	0.0132
18	227.2366	18224	374.0	5.2	0.0125
19	237.2211	22325	1007.9	13.7	0.0106
20	238.2243	18575	172.5	2.3	0.0128
21	241.1689	18089	159.6	2.2	0.0133
22	249.2202	17937	196.2	2.6	0.0139
23	251.2368	21611	840.9	11.2	0.0116
24	252.2399	18196	150.9	2.0	0.0139
25	255.2681	21042	480.8	6.4	0.0121
26	277.2513	17593	167.2	2.2	0.0158
27	293.2835	19146	304.3	4.0	0.0153
28	295.2988	17455	161.4	2.1	0.0169
29	307.2993	17356	168.1	2.2	0.0177
30	321.3148	19922	257.2	3.4	0.0161
31	322.0482	19246	313.4	4.1	0.0167
32	338.3416	18947	145.8	1.9	0.0179
33	379.2593	20393	872.0	11.5	0.0186
34	380.2623	17550	197.7	2.6	0.0217
35	411.2853	17459	192.2	2.5	0.0236
36	430.9138	18841	312.2	4.0	0.0229
37	622.0289	30425	2876.5	25.1	0.0204
38	623.0324	19139	421.3	3.7	0.0326
39	922.0100	23270	1795.1	10.1	0.0396
40	923.0129	17679	356.1	2.0	0.0522

#	m/z	Res.	S/N	I %	FWHM
1	706.0936	19335		2.9	0.0365
2	707.0968	19363		0.9	0.0365
3	708.0920	19390		32.1	0.0365
4	709.0933	19417		73.3	0.0365
5	710.0924	19445		100.0	0.0365
6	711.0946	19472		29.8	0.0365
7	712.0920	19499		84.1	0.0365
8	713.0950	19527		24.1	0.0365

#	m/z	Res.	S/N	I %	FWHM
9	714.0931	19554		40.8	0.0365
10	715.0961	19582		11.4	0.0365
11	716.0944	19609		3.3	0.0365
12	717.0954	19636		0.7	0.0365