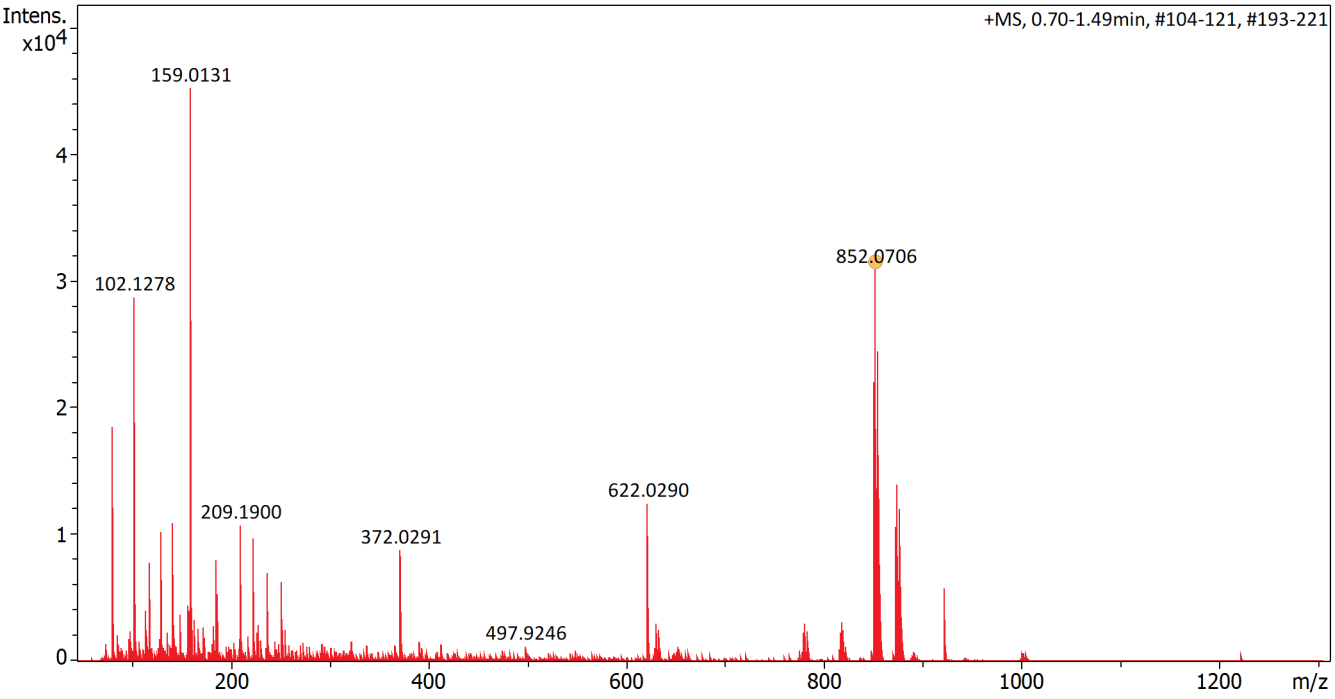
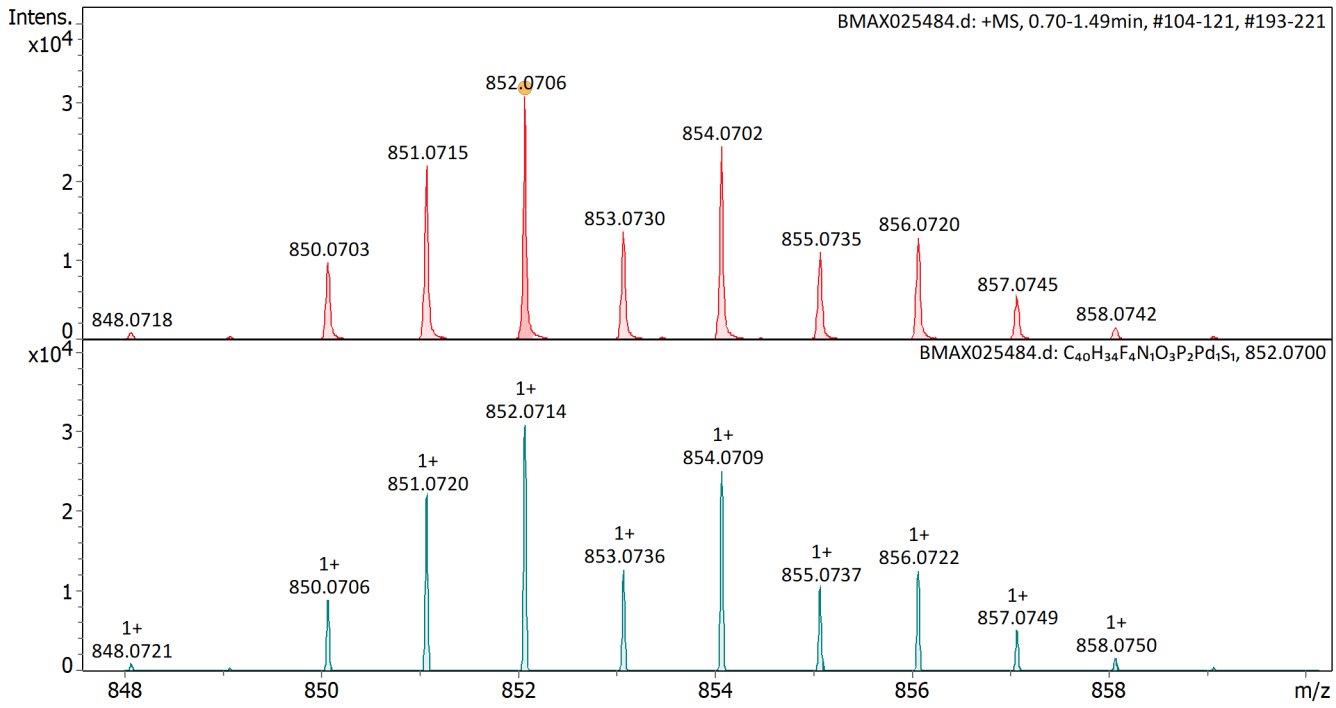
Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m			Acquisition Date:	02.10.2023 04:51:16
File Name:	D:\Data\bmax0254xx\BMAX025484.d			Operator:	Michael Meier
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	C40H34F4NO3P2PdS	M+H	852.0700	1+	852.0706	15.8	ok	0.8	0.9

Calibration Info:

Internal calibration

Date:	02.10.2023 04:54:25
Polarity:	Positive
Calibration spectrum:	+MS, 0.70-1.49min, #104-121, #193-221: Scan
Reference mass list:	ESI: Tunemix (pos) ESI-TOF Spezial
Calibration mode:	Enhanced Quadratic
Standard deviation:	0.569 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	7781	0.010
322.0481	322.0480	1613	-0.220
622.0290	622.0290	12480	0.056
922.0098	922.0097	5755	-0.107
1221.9906	1221.9912	416	0.472
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	80.0497	17808	848.1	40.9	0.0045
2	102.1278	16464	1316.4	63.5	0.0062
3	113.9636	15797	187.3	8.9	0.0072
4	118.0863	16433	365.3	17.2	0.0072
5	130.1588	16634	490.3	22.6	0.0078
6	141.0023	18550	536.5	24.2	0.0076
7	149.0233	17355	179.0	8.0	0.0086
8	157.0175	15422	218.7	9.8	0.0102
9	158.0169	15036	199.0	8.9	0.0105
10	158.1538	18556	176.8	7.9	0.0085
11	158.9636	16764	147.7	6.6	0.0095
12	159.0131	21114	2242.5	100.0	0.0075
13	160.0139	15212	208.7	9.3	0.0105
14	161.0108	14693	157.8	7.0	0.0110
15	163.1316	15319	163.5	7.2	0.0106
16	185.1147	17930	402.9	17.7	0.0103
17	186.0239	16465	266.5	11.7	0.0113
18	209.1900	19624	531.2	23.9	0.0107
19	223.2055	18808	466.8	21.5	0.0119
20	237.2212	17760	329.2	15.5	0.0134
21	251.2367	18629	287.5	13.9	0.0135
22	372.0291	19300	385.1	19.4	0.0193
23	622.0290	22287	886.9	27.6	0.0279
24	817.9294	16987	275.9	6.8	0.0481
25	850.0703	18648	898.7	21.5	0.0456
26	851.0715	25245	2039.8	48.8	0.0337
27	852.0706	29815	2858.4	68.3	0.0286
28	853.0730	20940	1262.0	30.2	0.0407
29	854.0702	26061	2262.0	54.1	0.0328
30	855.0735	19484	1020.9	24.4	0.0439
31	856.0720	19524	1193.1	28.5	0.0438
32	857.0745	17306	493.3	11.8	0.0495
33	872.0523	16903	413.5	9.9	0.0516
34	873.0535	19626	981.9	23.5	0.0445
35	874.0529	20823	1295.4	31.0	0.0420
36	875.0555	17933	589.6	14.1	0.0488
37	876.0525	20410	1112.0	26.6	0.0429
38	877.0557	18589	489.5	11.7	0.0472
39	878.0537	16773	546.6	13.1	0.0523
40	922.0097	18996	530.5	12.7	0.0485

#	m/z	Res.	S/N	I %	FWHM
1	848.0721	29675		2.6	0.0286
2	849.0754	29710		1.2	0.0286
3	850.0706	29745		28.9	0.0286
4	851.0720	29780		70.1	0.0286
5	852.0714	29815		100.0	0.0286
6	853.0736	29850		41.0	0.0286
7	854.0709	29885		80.5	0.0286
8	855.0737	29920		33.4	0.0286

#	m/z	Res.	S/N	I %	FWHM
9	856.0722	29955		40.7	0.0286
10	857.0749	29990		16.0	0.0286
11	858.0750	30025		5.0	0.0286
12	859.0757	30060		1.2	0.0286
13	860.0771	30095		0.2	0.0286