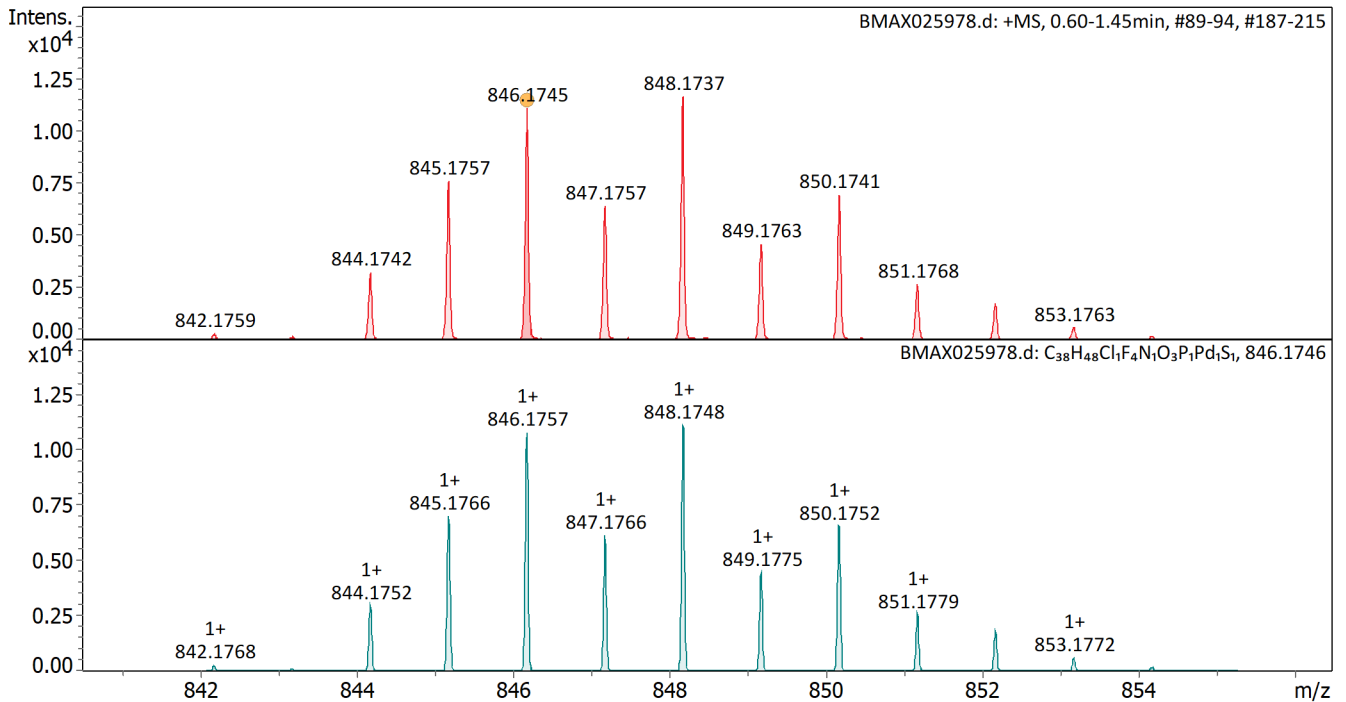
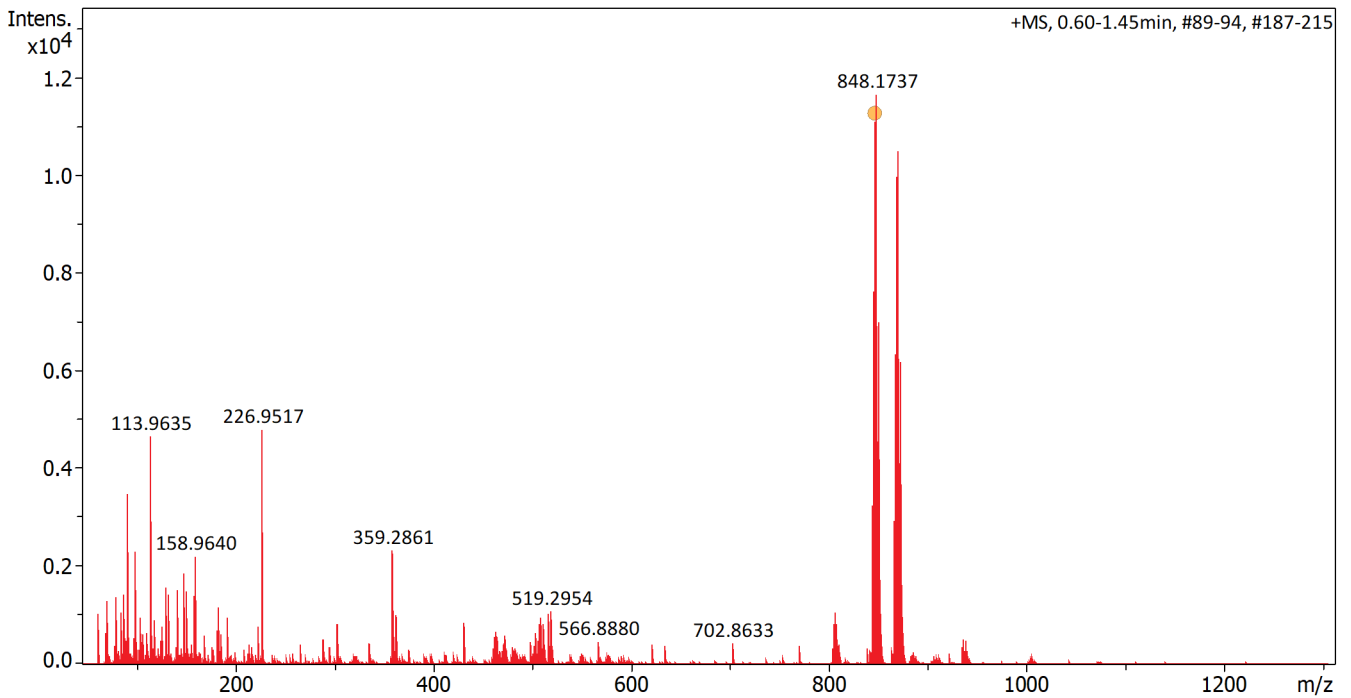


Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m	Acquisition Date:	10.11.2023 05:05:26
File Name:	D:\Data\bmax0259xx\BMAX025978.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	5.0 Bar
		Set Dry Heater	250 °C
		Set Dry Gas	12.0 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	C38H48ClF4NO3PPdS	M+H	846.1746	1+	846.1745	10.2	ok	1.2	1.4

Calibration Info:

Internal calibration

Date: 10.11.2023 05:08:08
 Polarity: Positive
 Calibration spectrum: +MS, 0.60-1.45min, #89-94, #187-215:
 Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Quadratic
 Standard deviation: 0.419 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0862	906	-0.170
322.0481	322.0482	46	0.294
622.0290	622.0288	412	-0.181
922.0098			
1221.9906	1221.9907	39	0.031
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	61.0078	19022	52.6	8.8	0.0032
2	70.0131	22113	65.6	11.1	0.0032
3	79.0182	21197	68.2	11.8	0.0037
4	84.9596	17074	52.4	9.1	0.0050
5	87.0042	21010	70.2	12.3	0.0041
6	90.9765	15323	171.2	30.0	0.0059
7	98.5123	18784	113.6	19.9	0.0052
8	113.9635	16754	230.7	39.9	0.0068
9	130.0079	17468	79.8	13.5	0.0074
10	132.0037	18853	72.1	12.1	0.0070
11	141.9586	15574	79.7	13.1	0.0091
12	147.9310	19624	98.4	16.0	0.0075
13	149.9308	16194	80.5	13.0	0.0093
14	158.0026	20018	75.3	11.9	0.0079
15	158.9640	18645	120.5	19.1	0.0085
16	183.1001	16283	67.4	10.0	0.0112
17	226.9517	20660	300.8	41.2	0.0110
18	359.2861	19659	164.5	20.0	0.0183
19	362.9264	19663	72.1	8.7	0.0185
20	517.2958	17939	89.7	8.9	0.0288
21	519.2954	18345	94.5	9.3	0.0283
22	806.2578	18283	104.1	9.1	0.0441
23	844.1742	19078	311.9	27.8	0.0442
24	845.1757	20225	731.2	65.3	0.0418
25	846.1745	20410	1066.0	95.3	0.0415
26	847.1757	19458	616.3	55.1	0.0435
27	848.1737	21096	1118.3	100.0	0.0402
28	849.1763	18696	438.4	39.2	0.0454
29	850.1741	20150	669.3	59.9	0.0422
30	851.1768	18617	253.7	22.7	0.0457
31	852.1748	17752	165.3	14.8	0.0480
32	866.1559	19145	279.4	25.3	0.0452
33	867.1573	19193	599.9	54.3	0.0452
34	868.1564	21636	945.8	85.6	0.0401
35	869.1574	19868	543.7	49.3	0.0437
36	870.1553	22314	993.3	90.0	0.0390
37	871.1589	18755	390.5	35.4	0.0465
38	872.1559	20178	586.0	53.1	0.0432
39	873.1582	18181	228.9	20.8	0.0480
40	874.1554	18033	153.4	13.9	0.0485
#	m/z	Res.	S/N	I %	FWHM
1	842.1768	20314		2.3	0.0415
2	843.1800	20338		1.0	0.0415
3	844.1752	20362		26.7	0.0415
4	845.1766	20386		62.8	0.0415
5	846.1757	20410		96.9	0.0415
6	847.1766	20434		55.1	0.0415
7	848.1748	20458		100.0	0.0415
8	849.1775	20483		39.8	0.0415

#	m/z	Res.	S/N	I %	FWHM
9	850.1752	20507		58.9	0.0415
10	851.1779	20531		22.8	0.0415
11	852.1753	20555		15.7	0.0415
12	853.1772	20579		5.3	0.0415
13	854.1771	20603		1.5	0.0415
14	855.1776	20627		0.3	0.0415