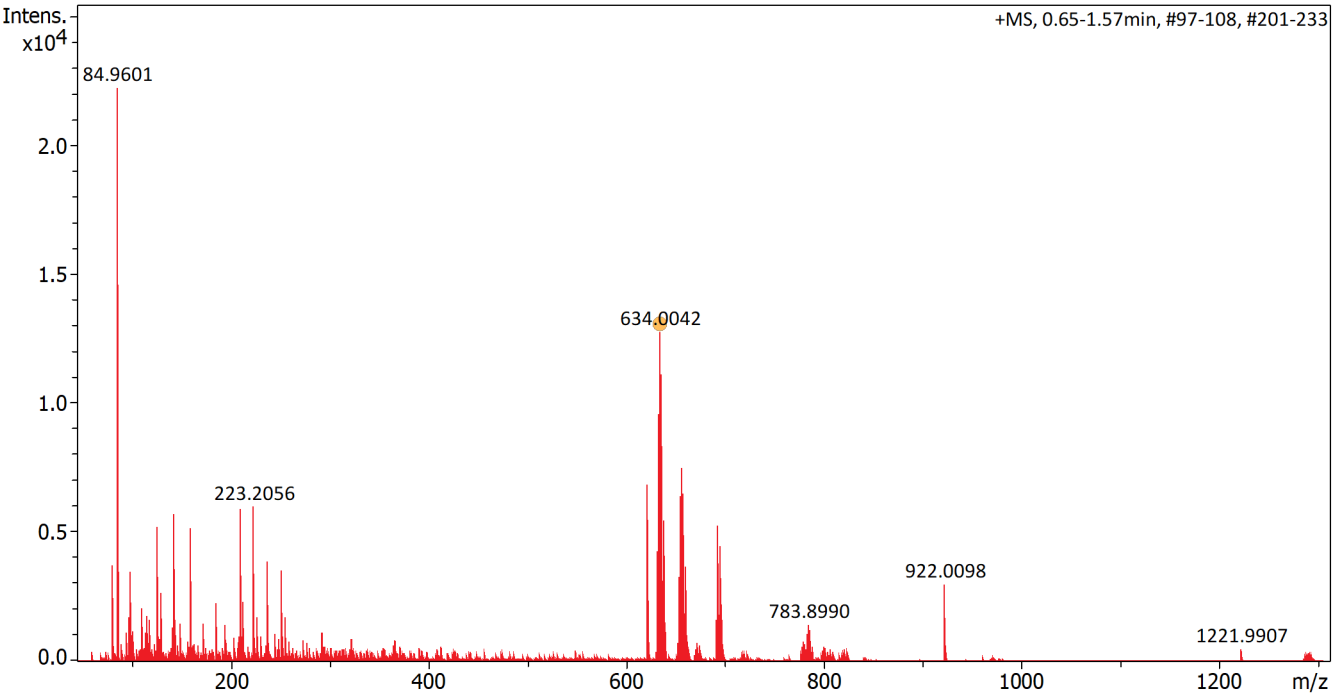
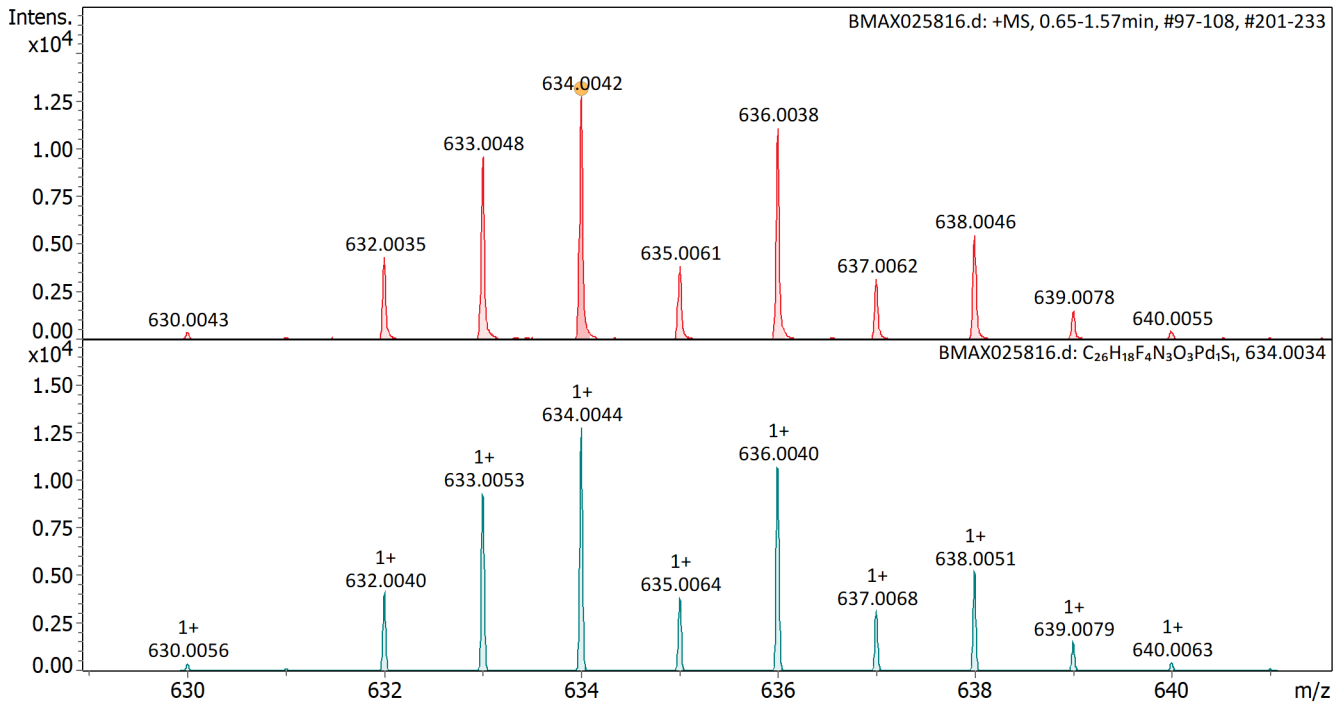
Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m			Acquisition Date:	26.10.2023 11:57:11
File Name:	D:\Data\bmax0258xx\BMAX025816.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	C26H18F4N3O3PdS	M+H	634.0034	1+	634.0042	14.5	ok	0.2	0.3

Calibration Info:

Internal calibration

Date:	26.10.2023 12:06:08
Polarity:	Positive
Calibration spectrum:	+MS, 0.65-1.57min, #97-108, #201-233: Scan
Reference mass list:	ESI: Tunemix (pos) ESI-TOF Spezial
Calibration mode:	Enhanced Quadratic
Standard deviation:	0.057 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	1616	0.005
322.0481	322.0481	854	-0.037
622.0290	622.0290	6875	0.009
922.0098	922.0098	3023	-0.017
1221.9906	1221.9907	475	0.033
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	80.0499	15061	128.1	16.8	0.0053
2	84.9601	15835	742.3	100.0	0.0054
3	97.0042	14418	54.2	7.7	0.0067
4	97.9689	16345	110.2	15.7	0.0060
5	110.0087	15037	62.3	9.2	0.0073
6	115.0146	19552	53.4	8.0	0.0059
7	125.9863	15276	155.4	23.6	0.0082
8	130.1591	15238	78.2	11.9	0.0085
9	141.9588	17588	166.9	25.6	0.0081
10	159.0132	16470	151.0	23.2	0.0097
11	185.1147	17277	67.3	10.1	0.0107
12	209.1899	19473	185.3	26.7	0.0107
13	211.9842	16891	72.5	10.4	0.0126
14	223.2056	19020	194.3	27.1	0.0117
15	227.2369	17491	56.2	7.7	0.0130
16	237.2212	17208	131.2	17.6	0.0138
17	251.2369	18250	124.0	15.9	0.0138
18	255.2679	16999	60.6	7.7	0.0150
19	622.0290	19807	471.9	30.9	0.0314
20	632.0035	17441	293.6	19.3	0.0362
21	633.0048	18002	655.2	43.2	0.0352
22	634.0042	19479	870.3	57.4	0.0325
23	635.0061	16048	261.1	17.2	0.0396
24	636.0038	19137	756.3	49.9	0.0332
25	637.0062	16248	216.1	14.3	0.0392
26	638.0046	17507	373.3	24.6	0.0364
27	653.9840	17337	222.4	14.8	0.0377
28	654.9860	18329	435.7	28.9	0.0357
29	655.9855	17316	509.0	33.8	0.0379
30	656.9878	15091	149.3	9.9	0.0435
31	657.9853	18061	443.4	29.4	0.0364
32	658.9879	16390	127.5	8.4	0.0402
33	659.9859	16887	252.5	16.7	0.0391
34	691.0773	15847	113.4	7.3	0.0436
35	692.0785	16270	258.1	16.7	0.0425
36	693.0773	17309	368.8	23.8	0.0400
37	694.0793	16925	125.9	8.1	0.0410
38	695.0769	17335	311.8	20.1	0.0401
39	697.0784	16851	153.3	9.9	0.0414
40	922.0098	17197	286.8	13.6	0.0536

#	m/z	Res.	S/N	I %	FWHM
1	630.0056	19357		2.9	0.0325
2	631.0086	19387		0.9	0.0325
3	632.0040	19418		32.0	0.0325
4	633.0053	19449		73.2	0.0325
5	634.0044	19479		100.0	0.0325
6	635.0064	19510		30.2	0.0325
7	636.0040	19541		84.0	0.0325
8	637.0068	19572		24.5	0.0325

#	m/z	Res.	S/N	I %	FWHM
9	638.0051	19602		40.7	0.0325
10	639.0079	19633		11.6	0.0325
11	640.0063	19664		3.4	0.0325
12	641.0072	19695		0.7	0.0325