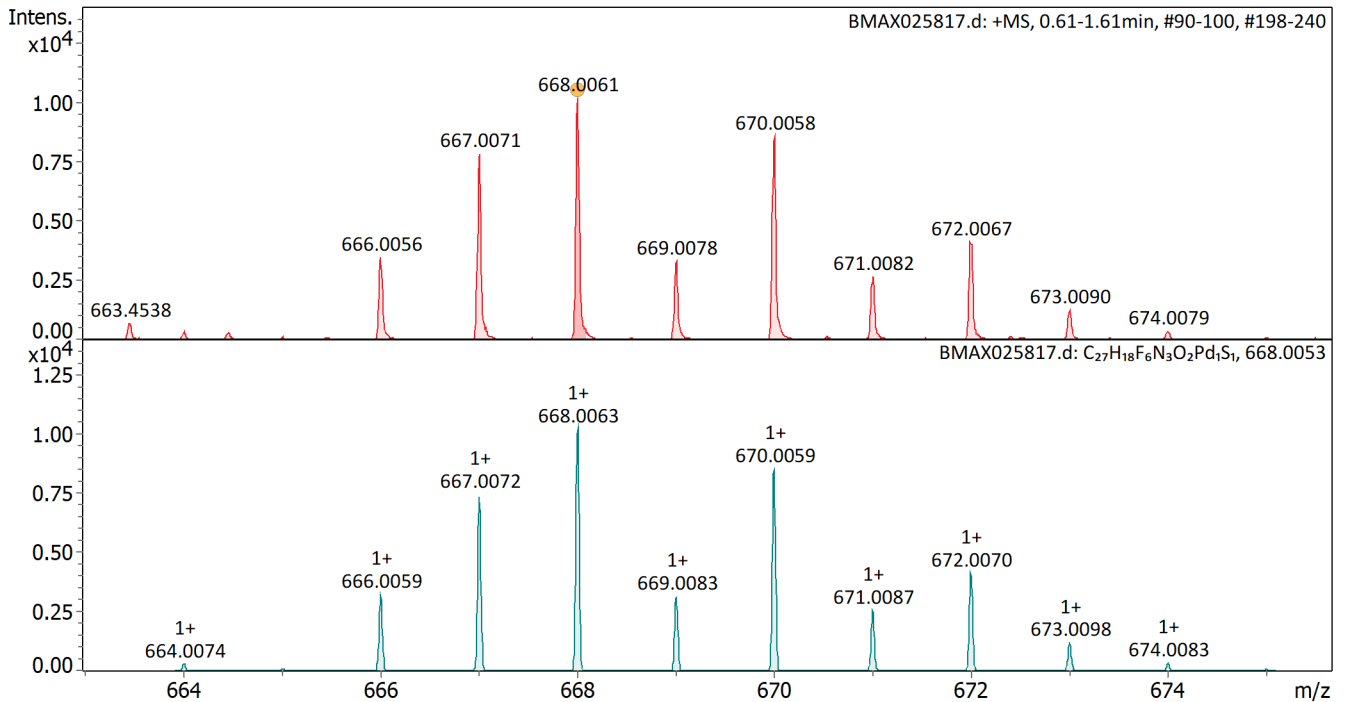
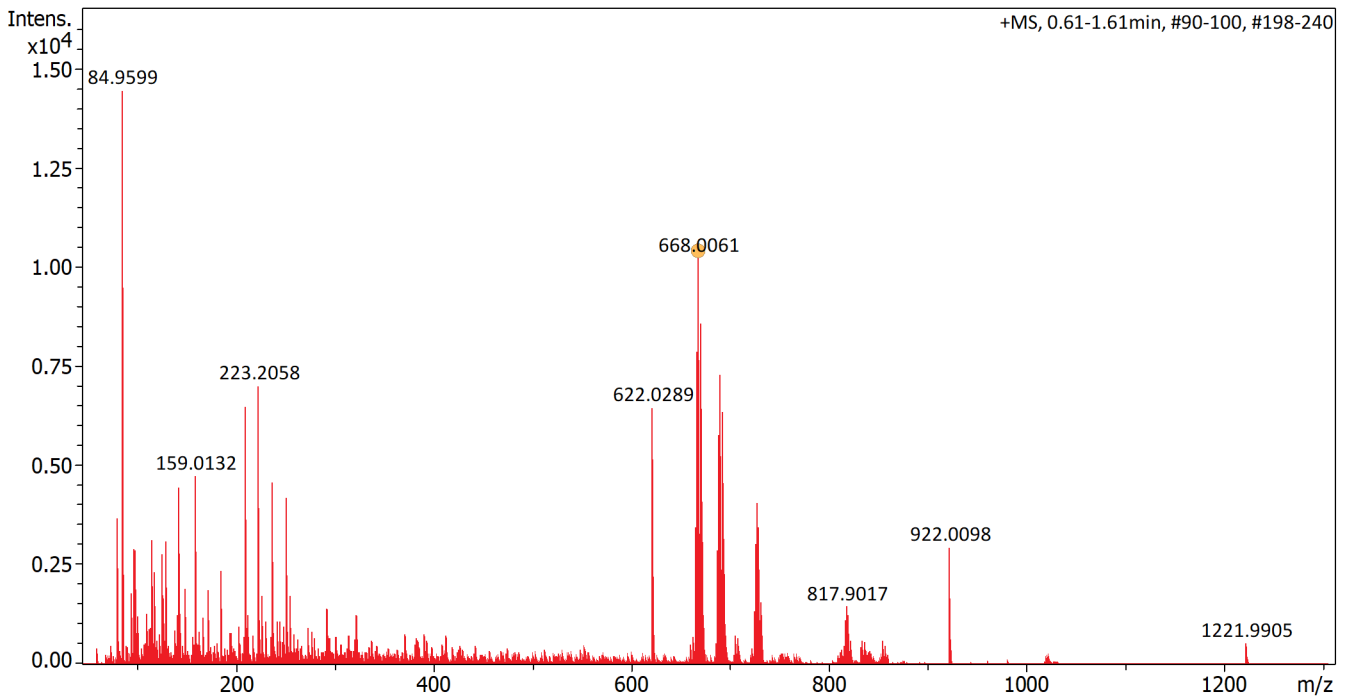


Acquisition Parameter

Method:	ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m	Acquisition Date:	26.10.2023 12:00:03
File Name:	D:\Data\bmax0258xx\BMAX025817.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	C27H18F6N3O2PdS	M+H	668.0053	1+	668.0061	15.8	ok	0.2	0.3

Calibration Info:

Internal calibration

Date: 26.10.2023 12:07:21
 Polarity: Positive
 Calibration spectrum: +MS, 0.61-1.61min, #90-100,
 #198-240: Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 0.112 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	2345	-0.006
322.0481	322.0481	1236	0.055
622.0290	622.0289	6463	-0.021
922.0098	922.0098	2947	0.042
1221.9906	1221.9905	518	-0.076
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	80.0498	14398	134.6	25.6	0.0056
2	84.9599	15321	514.6	100.0	0.0055
3	95.0083	15817	61.2	12.3	0.0060
4	97.0040	15094	99.6	20.2	0.0064
5	97.9687	16056	97.4	19.8	0.0061
6	115.0145	18296	101.5	21.6	0.0063
7	118.0863	17708	75.6	16.2	0.0067
8	125.9863	14959	89.2	19.3	0.0084
9	129.0301	15634	83.5	18.2	0.0083
10	130.1591	15469	98.7	21.5	0.0084
11	141.9587	17735	139.9	30.8	0.0080
12	149.0234	15458	59.8	13.2	0.0096
13	159.0132	16316	148.3	32.8	0.0097
14	172.8834	15867	59.7	13.1	0.0109
15	185.1150	17607	76.5	16.4	0.0105
16	209.1901	19812	220.0	44.9	0.0106
17	223.2058	19988	247.2	48.6	0.0112
18	227.2368	17171	61.8	12.0	0.0132
19	237.2214	18094	169.6	31.6	0.0131
20	251.2371	18735	165.1	29.0	0.0134
21	255.2681	17438	69.6	12.0	0.0146
22	622.0289	20418	581.3	44.7	0.0305
23	666.0056	16916	294.3	24.0	0.0394
24	667.0071	18087	667.2	54.4	0.0369
25	668.0061	17912	864.2	70.7	0.0373
26	669.0078	16565	279.8	22.9	0.0404
27	670.0058	17310	723.4	59.4	0.0387
28	671.0082	16268	224.9	18.5	0.0412
29	672.0067	15867	346.5	28.5	0.0424
30	687.9861	15712	240.0	20.0	0.0438
31	688.9881	16851	479.5	40.0	0.0409
32	689.9879	17062	604.3	50.5	0.0404
33	690.9896	15986	197.8	16.5	0.0432
34	691.9876	17430	525.1	44.0	0.0397
35	692.9895	17575	165.7	13.9	0.0394
36	693.9880	17187	261.8	21.9	0.0404
37	726.0805	16814	248.1	21.0	0.0432
38	727.0795	17076	333.3	28.2	0.0426
39	729.0786	17079	283.8	24.0	0.0427
40	922.0098	16977	284.7	20.4	0.0543
#	m/z	Res.	S/N	I %	FWHM
1	664.0074	17805		2.9	0.0373
2	665.0105	17832		0.9	0.0373
3	666.0059	17859		31.7	0.0373
4	667.0072	17886		73.0	0.0373
5	668.0063	17912		100.0	0.0373
6	669.0083	17939		30.9	0.0373
7	670.0059	17966		83.5	0.0373
8	671.0087	17993		25.1	0.0373

#	m/z	Res.	S/N	I %	FWHM
9	672.0070	18020		40.5	0.0373
10	673.0098	18047		11.9	0.0373
11	674.0083	18073		3.4	0.0373
12	675.0090	18100		0.7	0.0373