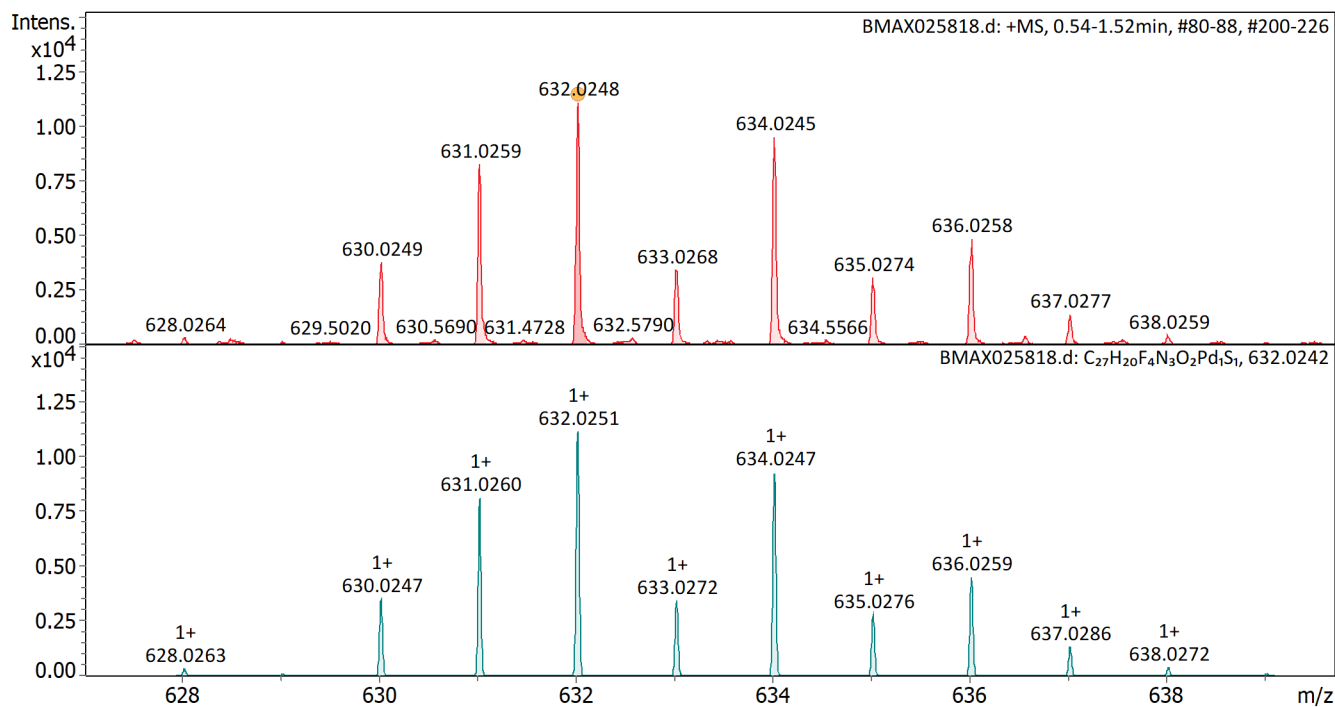
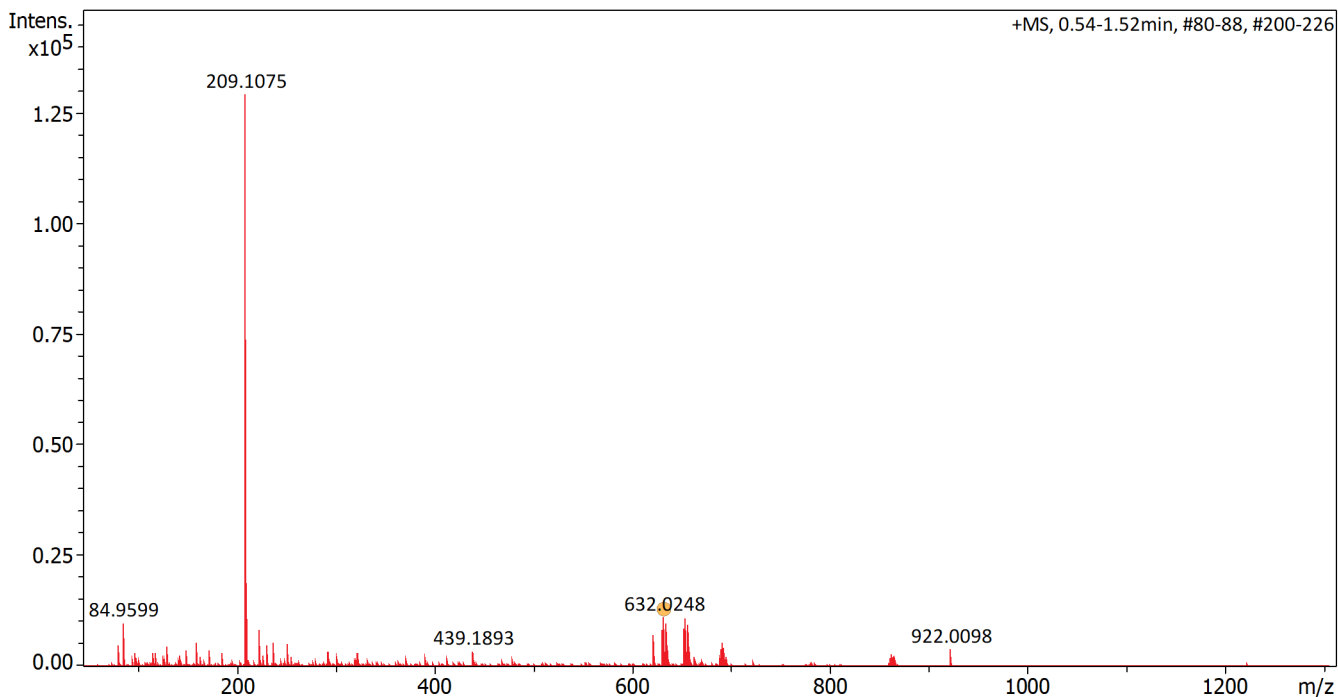


Acquisition Parameter

Method: ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m
File Name: D:\Data\bmax0258xx\BMAX025818.d
Source Type: ESI
Focus: Active
Scan Begin: 50 m/z
Scan End: 1300 m/z
Ion Polarity: Positive
Set Capillary: 4500 V
Set End Plate Offset: -500 V
Set Collision Cell RF: 200.0 Vpp

Acquisition Date: 26.10.2023 12:02:55
Operator: Michael Meier
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	C27H20F4N3O2PdS	M+H	632.0242	1+	632.0248	16.2	ok	0.4	0.6

Calibration Info:

Internal calibration

Date: 26.10.2023 12:08:48
 Polarity: Positive
 Calibration spectrum: +MS, 0.54-1.52min, #80-88, #200-226:
 Scan
 Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial
 Calibration mode: Enhanced Quadratic
 Standard deviation: 0.027 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0863	3133	-0.000
322.0481	322.0481	3169	-0.005
622.0290	622.0290	7120	0.007
922.0098	922.0098	3831	-0.013
1221.9906	1221.9907	828	0.020
1521.9715			
1821.9523			
2121.9332			
2421.9140			
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	80.0499	14276	196.8	3.6	0.0056
2	84.9599	15178	398.6	7.5	0.0056
3	97.0042	15152	112.5	2.3	0.0064
4	115.0145	17448	111.9	2.4	0.0066
5	118.0863	18607	113.6	2.4	0.0063
6	130.1590	15896	157.0	3.4	0.0082
7	149.0233	17203	128.7	2.8	0.0087
8	159.0130	16701	190.7	4.2	0.0095
9	172.8832	16130	131.0	2.9	0.0107
10	185.1148	17371	105.3	2.3	0.0107
11	209.1075	25976	4915.5	100.0	0.0081
12	209.1898	19467	281.0	5.7	0.0107
13	210.1106	18904	721.5	14.6	0.0111
14	223.2056	19915	332.1	6.5	0.0112
15	231.0893	19858	189.7	3.6	0.0116
16	237.2212	17991	222.9	4.1	0.0132
17	251.2368	19004	221.4	3.9	0.0132
18	293.1747	16712	165.0	2.5	0.0175
19	322.0481	18753	180.5	2.5	0.0172
20	439.1893	20840	237.2	2.6	0.0211
21	622.0290	20128	523.1	5.5	0.0309
22	630.0249	17597	276.3	2.9	0.0358
23	631.0259	17233	605.4	6.4	0.0366
24	632.0248	18261	813.6	8.6	0.0346
25	633.0268	16057	249.4	2.6	0.0394
26	634.0245	17765	697.3	7.4	0.0357
27	635.0274	17244	223.4	2.4	0.0368
28	636.0258	17118	352.7	3.7	0.0372
29	652.0056	17168	281.2	3.0	0.0380
30	653.0075	18276	606.3	6.5	0.0357
31	654.0068	18775	775.6	8.4	0.0348
32	655.0084	16488	243.8	2.6	0.0397
33	656.0063	19244	678.3	7.3	0.0341
34	657.0087	17678	212.0	2.3	0.0372
35	658.0073	17707	327.6	3.5	0.0372
36	690.0992	17069	267.7	2.9	0.0404
37	691.0982	17999	381.8	4.2	0.0384
38	693.0979	17062	300.7	3.3	0.0406
39	862.1070	19832	215.3	2.1	0.0435
40	922.0098	17441	316.8	3.0	0.0529
#	m/z	Res.	S/N	I %	FWHM
1	628.0263	18146		2.9	0.0346
2	629.0293	18175		0.9	0.0346
3	630.0247	18204		31.7	0.0346
4	631.0260	18233		73.0	0.0346
5	632.0251	18261		100.0	0.0346
6	633.0272	18290		30.9	0.0346
7	634.0247	18319		83.5	0.0346
8	635.0276	18348		25.2	0.0346

#	m/z	Res.	S/N	I %	FWHM
9	636.0259	18377		40.5	0.0346
10	637.0286	18406		11.9	0.0346
11	638.0272	18435		3.4	0.0346
12	639.0278	18464		0.7	0.0346