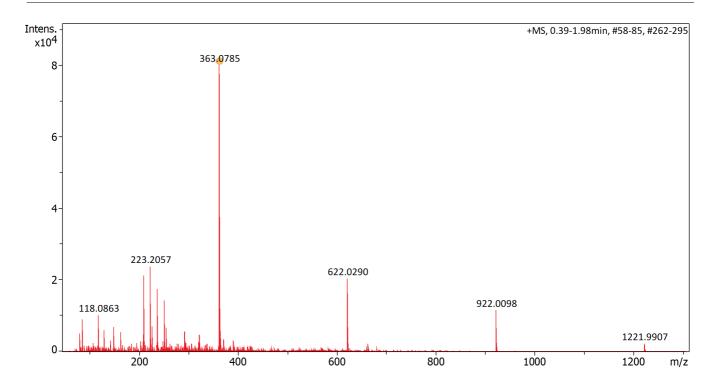
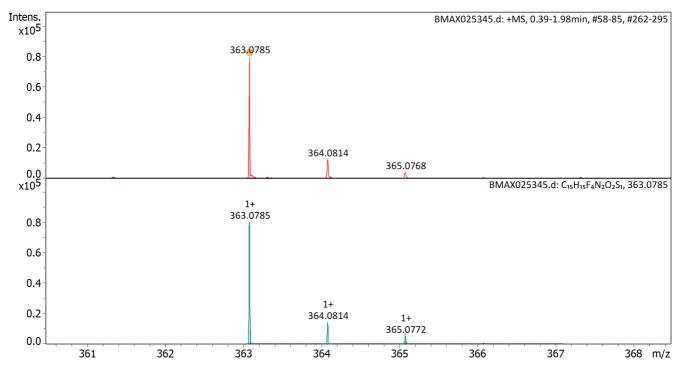
## **Acquisition Parameter**

Method: ETH\_HyStar\_HPLC\_QTOF\_POS\_LowMass\_Loop-AS.m Acquisition Date: 21.09.2023 05:43:36 File Name: D:\Data\bmax0253xx\BMAX025345.d Operator: Michael Meier

Set Nebulizer Set Dry Heater Source Type ESI Ion Polarity Positive 1.6 Bar 4500 V 230 °C 10.0 l/min Active Set Capillary Focus -500 V Scan Begin 50 m/z Set End Plate Offset Set Dry Gas Scan End 1300 m/z Set Collision Cell RF 200.0 Vpp Set Divert Valve Source







## **Evaluation Spectra / Validation Formula:**

mSigma Adduct N-Rule err [mDa] err [ppm] Ion Formula m/z Meas. m/z Z C15H15F4N2O2S M+H 363.0785 363.0785 15.2 -0.0 -0.0

Calibration Info:	Mass	Mass List:				
Internal calibration	#	m/z	Res.	S/N	1%	FWHM
Date: 21.09.2023 05:47:15	1	80.0495	18806	194.4	6.3	0.0043
Polarity: Positive	2	84.9596	18640	340.4	11.3	0.0046
Calibration spectrum: +MS, 0.39-1.98min, #58-85, #262-295:	3	107.0702	15614	88.6	3.1	0.0040
Scan	4	118.0863	17132	370.7	12.8	0.0069
Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial	5	130.1588	18733	220.5	7.5	0.0069
Calibration mode: Enhanced Quadratic	6	141.9582	18572	115.3	3.8	0.0076
Standard deviation: 0.122 ppm	7	149.0233	17048	260.6	8.5	0.0087
	8	163.1305	13868	222.3	6.9	0.0118
Reference m/z Resulting m/z Intensity Error [ppm]	9	195.1740	17655	113.6	3.0	0.0111
118.0863 118.0863 10277 0.007	10	203.1427	17796	141.7	3.6	0.0114
322.0481 322.0481 4789 -0.066	11	209.1900	21488	1086.3	26.6	0.0097
622.0290 622.0290 20502 0.030	12	210.1932	16199	159.4	3.9	0.0130
922.0098 922.0098 11656 -0.047	13	211.2049	17023	151.5	3.6	0.0124
1221.9906 1221.9907 2291 0.076	14	223.2057	22836	1323.4	29.9	0.0098
1521.9715	15	224.2088	17907	207.7	4.6	0.0125
1821.9523	16	227.2367	19002	402.0	8.8	0.0120
2121.9332	17	237.2213	21641	1069.0	22.0	0.0110
2421.9140	18	238.2246	17023	166.8	3.4	0.0140
2721.8948	19	249.2204	17311	196.9	3.8	0.0144
	20	251.2369	19687	946.5	17.9	0.0128
	21	252.2400	16438	167.6	3.2	0.0153
	22	255.2680	17443	448.3	8.3	0.0146
	23	263.2367	17743	158.8	2.8	0.0148
	24	279.1592	16711	175.5	2.9	0.0167
	25	293.1750	18528	440.6	7.0	0.0158
	26	293.2837	16214	230.7	3.7	0.0181
	27	295.2990	17059	190.7	3.0	0.0173
	28	307.2991	18349	187.3	2.8	0.0167
	29	321.3149	17924	235.4	3.5	0.0179
	30	322.0481	17707	398.2	6.0	0.0182
	31	363.0785	35206	6913.6	100.0	0.0103
	32	364.0814	20792	1062.3	15.4	0.0175
	33	365.0768	15670	336.0	4.9	0.0233
	34	371.3168	15950	302.6	4.4	0.0233
	35	391.2840	17476	263.4	3.9	0.0224
	36	622.0290	25022	1835.1	25.6	0.0249
	37	623.0319	17116	257.1	3.6	0.0364
	38	922.0098	21057	1219.0	14.6	0.0438
	39	923.0135	17284	257.0	3.1	0.0534
	40	1221.9907	17723	264.5	2.9	0.0689
	#	m/z	Res.	S/N	I %	FWHM
	1	363.0785	35206		100.0	0.0103
	2	364.0814	35303		18.0	0.0103
	3	365.0772	35400		6.4	0.0103
	4	366.0789	35497		0.9	0.0103
	5	367.0802	35594		0.1	0.0103