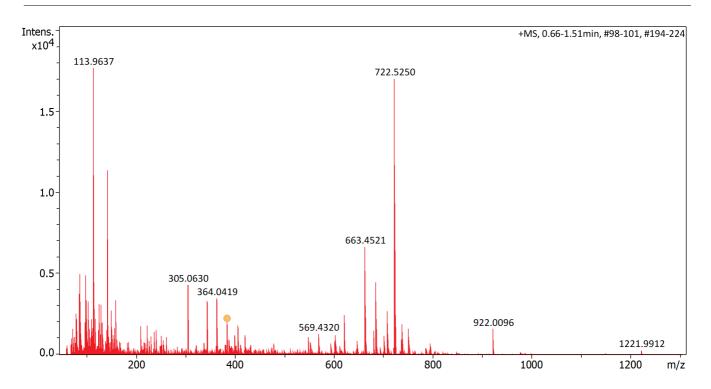
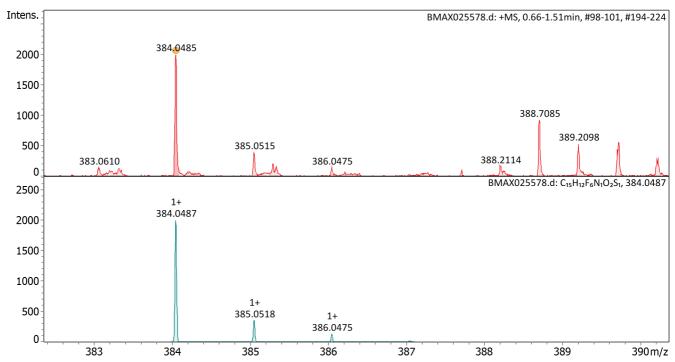
Acquisition Parameter

Method: ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.m Acquisition Date: 09.10.2023 05:23:58

File Name: D:\Data\bmax0255xx\BMAX025578.d Operator: Michael Meier

Source Type ESI Ion Polarity Positive Set Nebulizer 1.6 Bar 4500 V Set Dry Heater Active Set Capillary 230 °C Focus -500 V Scan Begin 50 m/z Set End Plate Offset 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 C15H12F6NO2S M+H 384.0487 1+ 384.0485 10.4 ok 0.2 0.5

Calibration Info:				Mass List:					
Internal calibration				#	m/z	Res.	S/N	۱%	FWHM
Date:	09.10	2023 05:26:5	4	# 1	79.0180	17167	107.9	14.5	
Polarity:	Positiv	re		2	80.0496	13878	92.2	12.4	0.0046 0.0058
Calibration spectrum: +MS, 0.66-1.51min, #98-101,			3	84.9596	13981	156.0	21.4	0.0056	
#194-224: Scan				4	87.0041	15708	204.5	28.2	0.0055
Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial				5	88.0047	14232	82.3	11.4	0.0062
Calibration mode: Enhanced Quadratic			6	88.0225	14232	67.3	9.3	0.0063	
Standard deviation: 0.731 ppm			7	97.0086	13060	78.7	11.2	0.0074	
				8	97.9686	15265	144.9	20.6	0.0064
Reference m/z	Resulting m/		Error [ppm]	9	98.5121	16200	194.4	27.7	0.0061
118.0863	118.086		0.023	10	99.5124	19384	133.0	19.1	0.0051
322.0481	322.048		-0.405	11	103.9554	15408	128.4	18.7	0.0067
622.0290	622.029		0.181	12	110.0088	18075	83.0	12.4	0.0061
922.0098	922.009		-0.251	13	113.9637	17360	664.4	100.0	0.0066
1221.9906	1221.991	2 275	0.461	14	115.9633	16848	166.9	25.3	0.0069
1521.9715				15	118.0863	15245	82.1	12.5	0.0077
1821.9523				16	125.9862	19260	114.1	17.7	0.0065
2121.9332				17	130.1591	18368	111.8	17.7	0.0003
2421.9140				18	131.9741	17883	71.6	11.3	0.0074
2721.8948				19	141.9587	18637	401.5	64.5	0.0074
				20	143.9590	15683	63.7	10.3	0.0070
				21	149.9525	15791	95.4	15.5	0.0095
				22	159.0133	15151	114.7	18.8	0.0105
									0.0103
				23 24	159.9692 209.1898	15821 17233	116.1 60.3	19.1 9.9	0.0121
				25	223.2055	17465	63.1	10.2	0.0121
				26	305.0630	16798	184.1	24.4	0.0128
				26 27	344.0361	17251	158.5	18.8	0.0182
				28	364.0419	18012	174.7	19.7	0.0202
				29	384.0485	16407	103.3	11.3	0.0234
				30	406.0298	16926	95.8	10.2	0.0234
				31	622.0291	17964	169.2	14.0	0.0346
				32	663.4521	18410	485.6	37.6	0.0340
				33	664.4553	16939	222.6	17.2	0.0392
				34	685.4339	18380	337.9	25.4	0.0392
				35	686.4376	18044	163.9	12.3	0.0373
				36		17739	209.0	15.2	
				37	708.5093 722.5250	24748	1345.9	96.4	0.0399 0.0292
				38			737.0		
					723.5287	21710		52.8	0.0333
				39	724.5314	17284	195.5	14.0	0.0419
				40	738.5208	16013	153.0	10.7	0.0461
				#	m/z	Res.	S/N	I%	FWHM
				1	384.0487	16407		100.0	0.0234
				2	385.0518	16450		17.6	0.0234
				3	386.0475	16493		6.3	0.0234
				4	387.0493	16536		0.9	0.0234