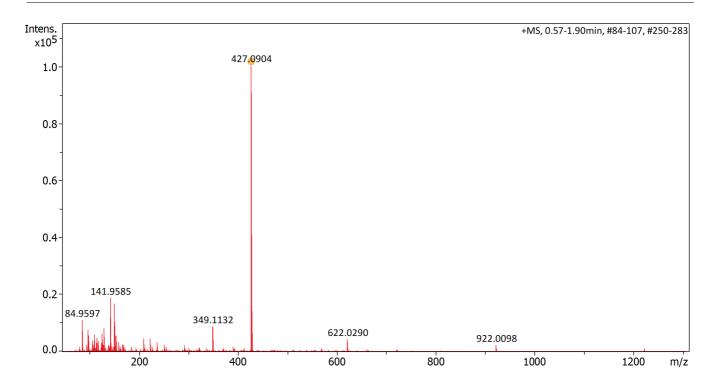
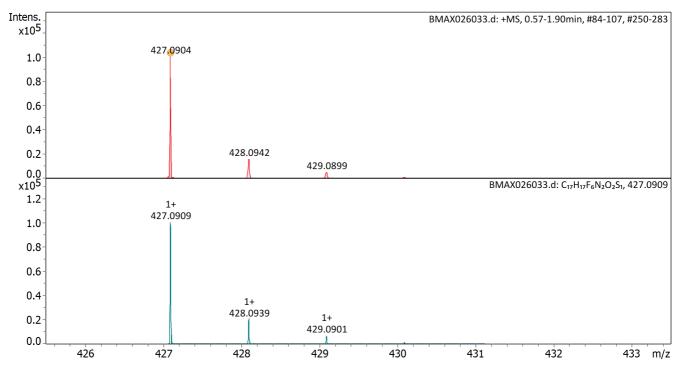
## **Acquisition Parameter**

Method: ETH\_HyStar\_HPLC\_QTOF\_POS\_LowMass\_Loop-AS.m Acquisition Date: 15.11.2023 06:15:24 Operator: Michael Meier

File Name: D:\Data\bmax0260xx\BMAX026033.d

Set Nebulizer Set Dry Heater Source Type ESI Ion Polarity Positive 1.6 Bar 4500 V 230 °C 10.0 l/min Set Capillary Active 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:**

# Ion Formula Adduct m/z z Meas. m/z mSigma N-Rule err [mDa] err [ppm]
1 C17H17F6N2O2S M+H 427.0909 1+ 427.0904 24.8 ok 0.5 1.2

Calibration Info:				Mass List:					
Internal calibration				#		Doo	S/N	1.0/	EVA/LINA
Date:	15.11.2	023 06:17:49	9		m/z	Res.		I %	FWHM
Polarity:	Polarity: Positive			1	84.9597 95.0082	18516	528.8	11.2 2.4	0.0046
Calibration spectrum: +MS, 0.57-1.90min, #84-107,			2 3		15998 20197	113.0 351.0	2.4 7.6	0.0059	
#250-283: Scan				4	97.0040 97.9685	16614	264.0	7.8 5.8	0.0048 0.0059
Reference mass list: ESI: Tunemix (pos) ESI-TOF Spezial				4 5	97.9665 105.9626		264.0 176.4		
Calibration mode: Enhanced Quadratic					16218		3.9	0.0065	
Standard deviation: 0.085 ppm			6 7	106.0042	19812	168.5	3.7 2.3	0.0054	
					107.9599	16557	104.0		0.0065
Reference m/z	Resulting m/z	Intensity	Error [ppm]	8	110.0086	15968	267.6	6.0	0.0069
118.0863	118.0863	3798	0.004	9	113.9634	17764 17903	137.5	3.1	0.0064
322.0481	322.0481	1454	-0.041	10	115.0145		212.0	4.8	0.0064
622.0290	622.0290	4301	0.027	11	118.0863	21093	166.4	3.8	0.0056
922.0098	922.0098	2255	-0.044	12	124.0147	19736	132.5	3.0	0.0063
1221.9906	1221.9907	696	0.046	13	125.9861	16858	276.1	6.4	0.0075
1521.9715				14	127.0344	20530	113.9	2.6	0.0062
1821.9523				15	128.0191	16365	97.8	2.3	0.0078
2121.9332				16	129.0300	19186	346.7	8.0	0.0067
2421.9140				17	130.1588	18129	132.6	3.1	0.0072
2721.8948				18	138.0303	16699	102.6	2.4	0.0083
				19	140.9614	16664	81.4	1.9	0.0085
				20	141.9585	20771	792.5	18.8	0.0068
				21	143.9588	16041	125.8	3.0	0.0090
				22	149.9528	19544	699.5	16.8	0.0077
				23	151.9496	18107	366.2	8.9	0.0084
				24	152.9506	17155	73.7	1.8	0.0089
				25	153.9483	16920	230.6	5.6	0.0091
				26	159.0129	16376	118.7	2.9	0.0097
				27	159.9690	17277	134.8	3.3	0.0093
				28	167.0784	18156	100.2	2.5	0.0092
				29	167.9630	18783	94.3	2.3	0.0089
				30	209.1899	18986	183.4	4.5	0.0110
				31	223.2054	18777	190.5	4.6	0.0119
				32	227.2364	19528	81.0	1.9	0.0116
				33	237.2209	18653	134.1	3.2	0.0127
				34	251.2366	17463	104.4	2.4	0.0144
				35	349.1132	20184	466.7	8.9	0.0173
				36	427.0904	39617	5455.8	100.0	0.0108
				37	428.0942	20831	856.1	15.7	0.0206
				38	429.0899	16348	260.0	4.8	0.0262
				39	622.0290	19491	390.3	4.3	0.0319
				40	922.0098	18424	222.4	2.2	0.0500
				#	m/z	Res.	S/N	I %	FWHM
				1	427.0909	39617		100.0	0.0108
				2	428.0939	39710		20.2	0.0108
				3	429.0901	39803		6.8	0.0108
				4	430.0916	39896		1.1	0.0108
				5	431.0931	39988		0.1	0.0108