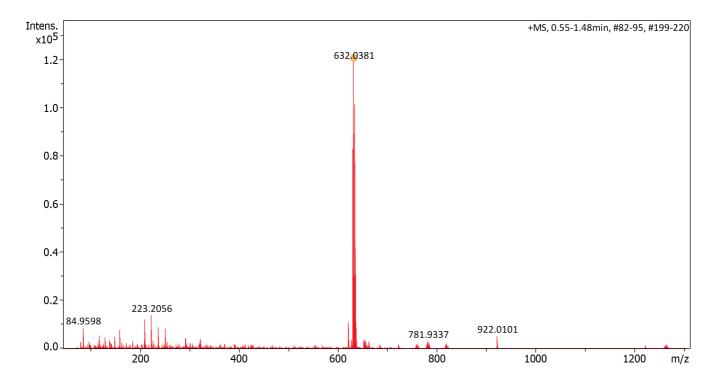
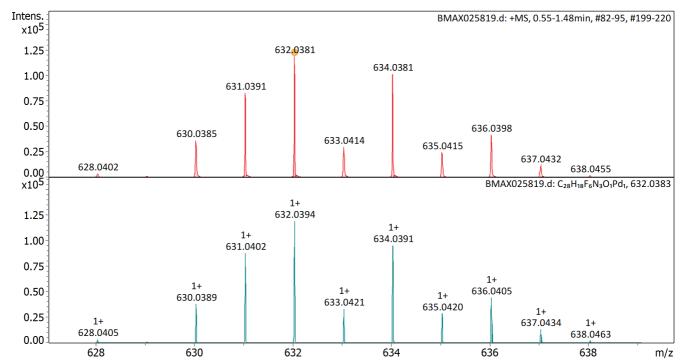
## **Acquisition Parameter**

Method: ETH\_HyStar\_HPLC\_QTOF\_POS\_LowMass\_Loop-AS.m Acquisition Date: 26.10.2023 12:05:46
File Name: D:\Data\bmax0258xx\BMAX025819.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 Set End Plate Offset -500 V Scan Begin 50 m/z 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:**

Adduct mSigma N-Rule err [mDa] err [ppm] Ion Formula m/z Meas. m/z Z C28H18F6N3OPd 28.7 M+H 632.0383 632.0381 ok 1.3

Calibration Info:			Mass List:					
Internal calibration			#	m/z	Res.	S/N	۱%	FWHM
Date: 26.1	0.2023 12:10:09	9	<b>"</b>	80.0498	15002	124.0	2.3	0.0053
Polarity: Pos			2	84.9598	15246	375.6	7.3	0.0056
•		#82-95, #199-220:	3	97.0039	15610	111.7	2.3	0.0062
Sca			4	115.0145	19012	88.7	1.9	0.0060
	" ,	ESI-TOF Spezial	5	118.0863	18001	220.7	4.6	0.0066
Calibration mode: Enhanced Quadratic			6	130.1590	15489	183.7	3.9	0.0084
Standard deviation: 0.724 ppm			7	139.0728	15906	147.5	3.1	0.0087
Defended by Decelling	- /- Lata 10	E []	8	141.0024	16048	102.7	2.2	0.0088
Reference m/z Resulting r		Error [ppm]	9	149.0232	16172	191.3	4.0	0.0092
118.0863 118.08		-0.036	10	159.0130	16718	317.1	6.6	0.0095
322.0481 322.04		0.222	11	163.1254	9277	105.4	2.2	0.0176
622.0290 622.02 922.0098 922.01		-0.155	12	172.8831	16356	94.0	1.9	0.0106
		0.289 -0.552	13	185.1147	17129	128.8	2.6	0.0108
1221.9906 1221.99 1521.9715	00 665	-0.552	14	209.1899	20039	540.3	10.3	0.0104
1821.9523			15	223.2056	20616	645.0	11.8	0.0108
2121.9332			16	227.2368	18668	149.8	2.7	0.0122
2421.9140			17	237.2213	18330	422.0	7.4	0.0129
2721.8948			18	251.2369	19190	418.9	7.0	0.0131
2721.0040			19	255.2678	17122	149.2	2.5	0.0149
			20	293.1749	17180	252.5	3.7	0.0171
			21	301.2844	17385	128.7	1.8	0.0173
			22	322.0482	18156	246.5	3.3	0.0177
			23	622.0289	20323	776.4	9.4	0.0306
			24	628.0402	17953	244.5	3.0	0.0350
			25	630.0385	30619	2516.8	30.4	0.0206
			26	631.0391	37651	5783.0	69.8	0.0168
			27	632.0381	40052	8276.1	100.0	0.0158
			28	633.0414	27947	2072.6	25.0	0.0227
			29	634.0381	42050	7068.2	85.4	0.0151
			30	635.0415	25128	1693.0	20.5	0.0253
			31 32	636.0398 637.0432	32597 19616	2889.9 792.1	35.0 9.6	0.0195 0.0325
			33	653.0216	17635	212.9	2.6	0.0325
			34	654.0208	17506	272.7	3.3	0.0374
			35	656.0206	18204	230.8	2.8	0.0360
			36	663.4536	17197	205.5	2.5	0.0386
			37	780.9345	16645	172.1	2.0	0.0469
			38	781.9337	16615	227.2	2.6	0.0471
			39	783.9331	16093	179.1	2.1	0.0487
			40	922.0101	17262	446.2	4.4	0.0534
			#			S/N	1.0/	
				<b>m/z</b>	Res.	3/N	I %	FWHM 0.0158
			1 2	628.0405 629.0436	39798 39862		2.9 0.9	0.0158 0.0158
			3	630.0389	39925		32.0	0.0158
			3 4	631.0402	39925 39988		32.0 74.0	0.0158
			5	632.0394	40052		100.0	0.0158
			6	633.0421	40032		28.1	0.0158
			7	634.0391	40178		80.0	0.0158
			8	635.0420	40242		24.4	0.0158
			U	000.0720	10272		→	3.0.00

## BMAX025819 Michael Bogdos/Morandi - MB-CF3-NAc-Ph-phen - DCM/MeOH - --



Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

#	m/z	Res.	S/N	I %	FWHM
9	636.0405	40305		37.4	0.0158
10	637.0434	40369		11.0	0.0158
11	638.0463	40432		1.7	0.0158
12	639.0493	40496		0.2	0.0158