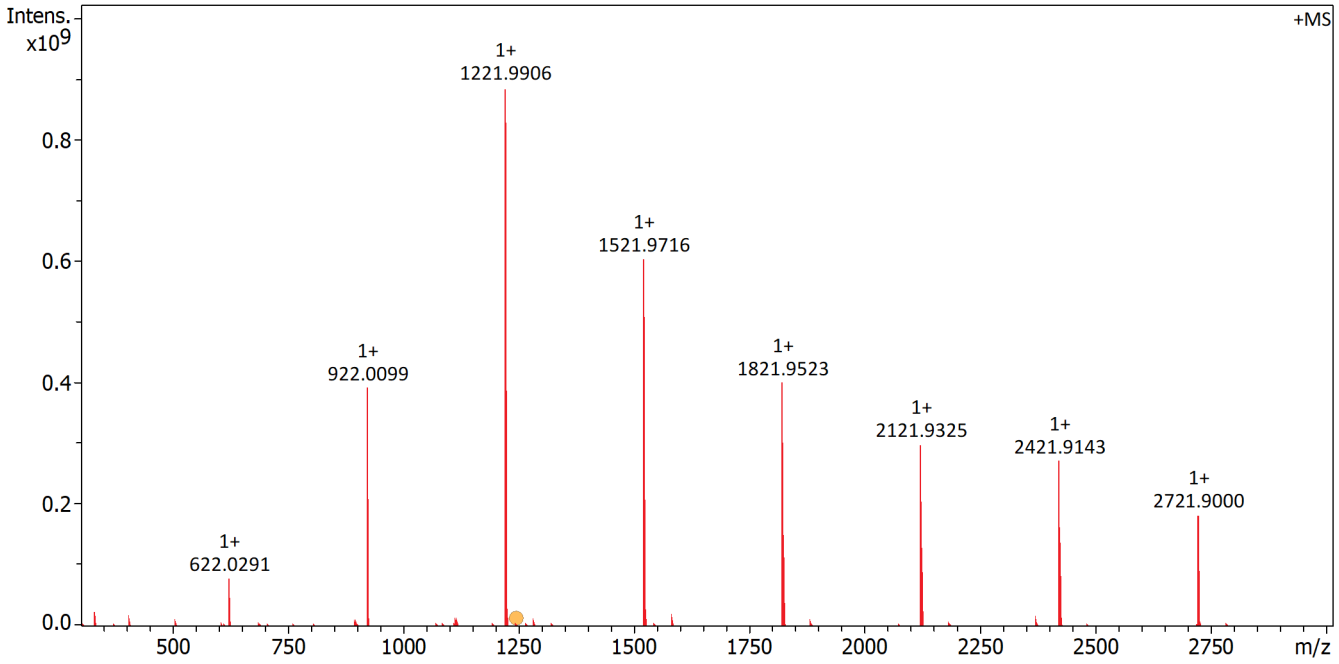
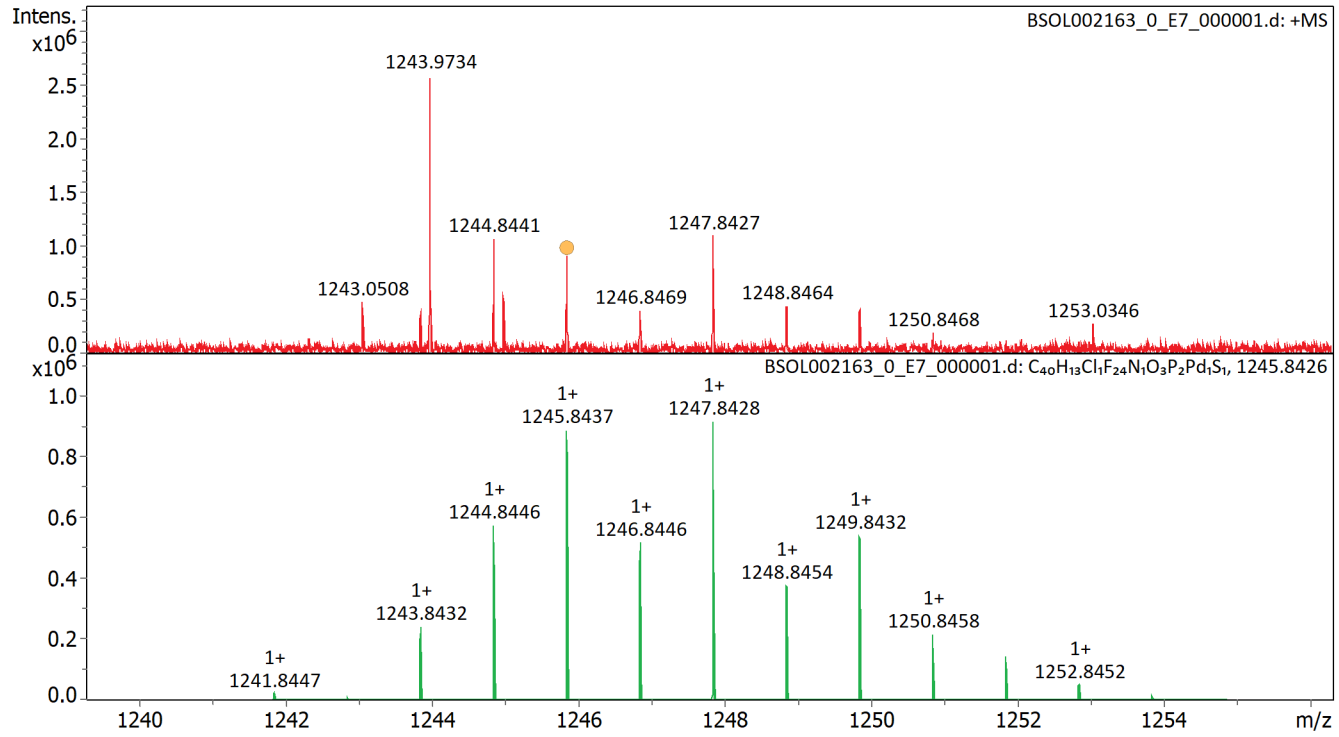
BSOL002163 Michael Bogdos/Morandi - G10-Fdppe - DCM - DCTB 1:10

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Acquisition Parameter

Method:	MALDI_MS_POS_300-3000_2M_16AvScans			Acquisition Date:	12/5/2023 10:59:09 AM
File Name:	D:\Data\ETH Data\BSOL0021xx\BSOL002163_0_E7_000001.d			Operator:	Daniel Wirz
Source	Dual (MALDI/ESI)	Polarity	Positive	Nebulizer Gas	1.0 bar
Broadband Low Mass	303.1 m/z			Drying Gas Flow Rate	4.0 L/min
Broadband High Mass	3000.0 m/z	Laser Power	23.6 lp	Capillary	4500.0 V
No. of Cell Fills	1			Drying Gas Temperature	200.0 °C
Apodization	Full-Sine	Time of Flight to Detector	0.002 sec		





Evaluation Spectra / Validation Formula:

#	Ion Formula	Adduct	m/z	z	Meas. m/z	mSigma	N-Rule	err [mDa]	err [ppm]
1	C40H13ClF24NO3P2PdS	M+H	1245.8426	1+	1245.8419	137.1	ok	1.8	1.5

Calibration Info:

Internal calibration

Date:	12/5/2023 11:00:29 AM
Polarity:	Positive
Calibration spectrum:	+MS: Scan
Reference mass list:	MALDI: DCTB Matrix + HP-Mix (pos)
Calibration mode:	Quadratic
Standard deviation:	0.175 ppm

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
250.1464			
251.1543			
273.1362			
322.0481	322.0481	1123996	0.062
332.2009	332.2009	24418436	-0.051
500.2934	500.2934	196517	-0.165
501.3013			
523.2832			
622.0290	622.0291	80006024	0.180
750.4404			
751.4483			
773.4302			
922.0098	922.0099	392775456	0.084
1000.5874			
1001.5953			
1023.5772			
1221.9906	1221.9906	887723648	-0.033
1521.9715	1521.9716	604840256	0.070
1821.9523	1821.9523	401386944	-0.016
2121.9332	2121.9325	300134432	-0.329
2421.9140	2421.9143	273037600	0.128
2721.8948			

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	332.2009	572660	2058.8	2.8	0.0006
2	407.3399	563248	919.7	1.3	0.0007
3	622.0291	220045	5472.0	9.0	0.0028
4	623.0325	210231	665.6	1.1	0.0030
5	894.8409	167384	389.4	0.8	0.0053
6	895.8394	169968	466.0	0.9	0.0053
7	897.8399	170356	486.0	0.9	0.0053
8	922.0042	242094	1618.6	3.2	0.0038
9	922.0099	170427	22652.3	44.2	0.0054
10	923.0137	153384	3694.1	7.2	0.0060
11	1113.9956	156781	343.7	0.7	0.0071
12	1115.9967	137991	370.2	0.8	0.0081
13	1221.9191	129182	492.5	1.1	0.0095
14	1221.9548	166264	1179.1	2.7	0.0073
15	1221.9810	201405	3184.9	7.2	0.0061
16	1221.9906	135852	44381.6	100.0	0.0090
17	1222.9945	135354	10938.9	24.7	0.0090
18	1223.9983	135415	1555.6	3.5	0.0090
19	1283.0449	107540	399.1	0.9	0.0119
20	1521.8608	103516	346.9	0.8	0.0147
21	1521.9716	105518	28580.1	68.1	0.0144
22	1522.9753	102023	8721.0	20.8	0.0149
23	1523.9802	99022	1497.0	3.6	0.0154
24	1583.0264	91546	514.6	1.2	0.0173
25	1821.9523	92970	17317.6	45.2	0.0196
26	1822.9563	95057	6484.2	16.9	0.0192
27	1823.9608	90725	1228.9	3.2	0.0201
28	1824.9653	87143	737.1	1.9	0.0209
29	1883.0069	85325	294.5	0.7	0.0221
30	2121.9325	84691	11798.4	33.8	0.0251
31	2122.9370	85257	5128.8	14.7	0.0249
32	2123.9410	81980	1135.2	3.3	0.0259
33	2371.9200	69797	403.9	1.2	0.0340
34	2421.7703	84101	246.0	0.8	0.0288
35	2421.9143	71348	10072.4	30.8	0.0339
36	2422.9192	72984	5085.8	15.5	0.0332
37	2423.9244	68221	1215.8	3.7	0.0355
38	2721.9000	56880	7096.0	20.8	0.0479
39	2722.9040	54475	3957.2	11.6	0.0500
40	2723.9064	51665	1145.3	3.4	0.0527

#	m/z	Res.	S/N	I %	FWHM
1	1241.8447	124157		2.3	0.0100
2	1242.8480	124257		1.0	0.0100
3	1243.8432	124357		26.5	0.0100
4	1244.8446	124457		62.7	0.0100
5	1245.8437	124557		97.1	0.0100
6	1246.8446	124657		56.3	0.0100
7	1247.8428	124756		100.0	0.0100
8	1248.8454	124857		41.2	0.0100
9	1249.8432	124956		59.0	0.0100
10	1250.8458	125057		23.6	0.0100
11	1251.8434	125156		15.9	0.0100
12	1252.8452	125257		5.6	0.0100
13	1253.8452	125357		1.6	0.0100
14	1254.8457	125457		0.4	0.0100