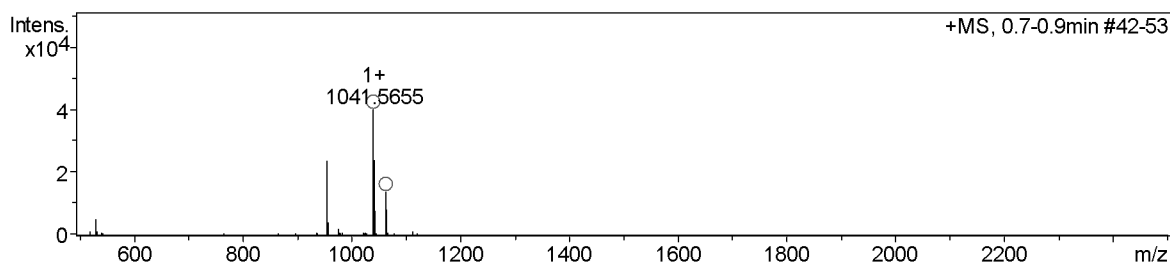




Sample-ID	pazrjk_TETA_v2	Lab	C13
Submitter	Rafal Kopiasz (pazrjk)	Supervisor	Cameron Alexander (pczca1)
Analysis Name	pazrjk_TETA_v2_658635_45_01_139022.d	Acquisition Date	11/27/2023 3:01:19 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #42-53



#	m/z	I %
1	521.2923	3.3
2	532.2790	13.2
3	532.7815	8.2
4	533.2778	3.4
5	955.5283	58.8
6	956.5312	32.3
7	957.5384	10.6
8	958.5353	2.7
9	977.5068	5.0
10	978.5155	2.6
11	1023.5567	2.5
12	1026.5580	2.3
13	1041.5655	100.0
14	1042.5708	59.6
15	1043.5684	19.3
16	1044.5723	5.6
17	1063.5422	34.9
18	1064.5492	20.4
19	1065.5427	7.2
20	1112.5986	2.7

Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C50 H76 N10 O14				Adduct(s):	H, Na, NH4, C3H5N2, radical
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	1 041.5655	1 041.5615	3.80	0.0066	C50H77N10O14	M+H	1.0078
1	1 063.5422	1 063.5435	1.20	0.0080	C50H76N10NaO14	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF