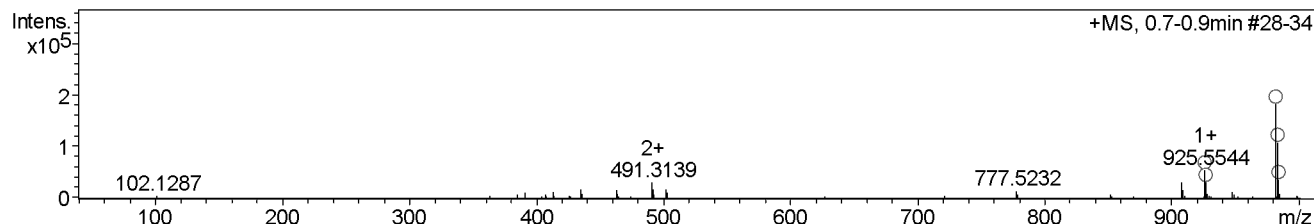




Sample-ID	pazrjk_TETA_15	Lab	C13
Submitter	Rafal Kopiasz (pazrjk)	Supervisor	Cameron Alexander (pczca1)
Analysis Name	pazrjk_TETA_15_654466_2_01_135016.d	Acquisition Date	9/7/2023 1:54:59 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #28-34



#	m/z	I %
1	391.2625	5.7
2	413.2578	7.0
3	435.2526	10.2
4	435.7536	5.2
5	463.2824	9.5
6	463.7844	5.1
7	491.3139	17.1
8	491.8158	10.5
9	502.3047	10.4
10	502.8057	6.3
11	777.5232	7.6
12	907.5442	16.8
13	908.5428	9.6
14	925.5544	29.9
15	926.5537	17.4
16	927.5582	5.4
17	947.5348	7.3
18	981.6161	100.0
19	982.6160	60.0
20	983.6203	19.8

Generate Molecular Formula Parameters

No of Most Intense MS Peaks Analysed 5

Charge	Tolerance	sigma_limit	Calibration
+1	6 ppm	0.08	TRUE

Formula Min C 45 H 75 N 5 O 5

Formula Max

C55 H85 N15 O15 H Na NH4 C3H5N2

#	meas. m/z	theo. m/z	[Err][ppm]	Sigma	Formula
1	981.6161	981.6145	1.60	0.0031	C 52 H 83 N 7 O 11
		981.6134	2.70	0.0046	C 51 H 80 N 11 Na 1 O 7
		981.6132	3.00	0.0065	C 50 H 81 N 10 O 10
		981.6132	3.00	0.0069	C 49 H 75 N 17 O 5
		981.6145	1.60	0.0076	C 51 H 77 N 14 O 6
3	925.5544	925.5535	0.90	0.0043	C 51 H 76 N 5 Na 1 O 9
		925.5519	2.70	0.0130	C 48 H 75 N 7 O 11

Analysis Name pazrjk_TETA_15_654466_2_01_135016.d

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Bruker Compass DataAnalysis 4.2

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#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula
		925.5559	1.70	0.0244	C 53 H 75 N 5 O 9
		925.5495	5.30	0.0250	C 46 H 76 N 7 Na 1 O 11
		925.5492	5.60	0.0311	C 45 H 77 N 6 O 14

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