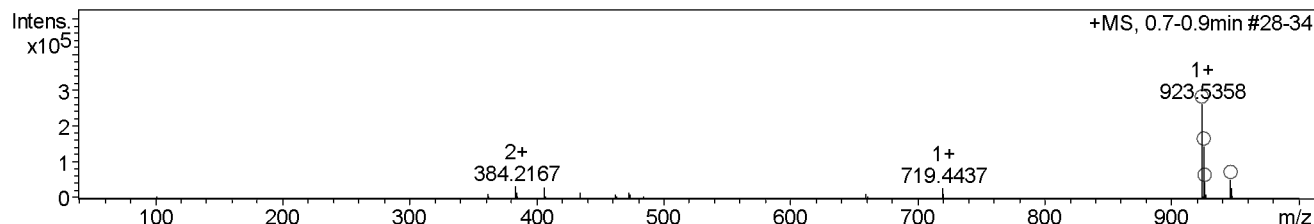




Sample-ID	pazrjk_B3APP_01	Lab	C13
Submitter	Rafal Kopiasz (pazrjk)	Supervisor	Cameron Alexander (pczca1)
Analysis Name	pazrjk_B3APP_01_654465_3_01_135017.d	Acquisition Date	9/7/2023 1:57:31 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #28-34



#	m/z	I %
1	362.2208	5.2
2	384.2167	13.6
3	384.7187	6.4
4	406.2112	11.8
5	406.7142	5.6
6	434.2436	6.5
7	434.7430	3.5
8	462.2750	3.7
9	473.2647	6.5
10	473.7675	3.7
11	659.3869	4.7
12	719.4437	11.4
13	720.4454	4.8
14	923.5358	100.0
15	924.5380	55.6
16	925.5404	17.2
17	926.5403	4.2
18	945.5168	20.0
19	946.5211	10.9
20	947.5216	3.5

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 40 H 60 N 5 O 5

Formula Max

C50 H80 N15 O15 H Na NH4 C3H5N2

#	meas. m/z	theo. m/z	[Err][ppm]	Sigma	Formula
1	923.5358	923.5363	0.50	0.0022	C 48 H 73 N 7 O 11
		923.5352	0.60	0.0042	C 47 H 70 N 11 Na 1 O 7
		923.5349	0.90	0.0061	C 46 H 71 N 10 O 10
		923.5349	0.90	0.0063	C 45 H 65 N 17 O 5
		923.5363	0.50	0.0074	C 47 H 67 N 14 O 6
3	945.5168	945.5182	1.40	0.0058	C 48 H 72 N 7 Na 1 O 11
		945.5179	1.20	0.0062	C 47 H 73 N 6 O 14

Analysis Name pazrjk_B3APP_01_654465_3_01_135017.d

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#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula
		945.5179	1.10	0.0070	C 46 H 67 N 13 O 9
		945.5169	0.00	0.0071	C 46 H 70 N 10 Na 1 O 10
		945.5166	0.30	0.0096	C 44 H 65 N 16 O 8

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