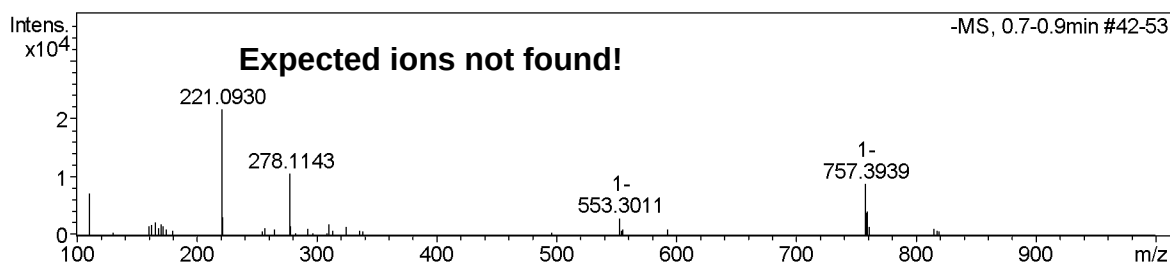




Sample-ID	bralo7_B3APP-2L2 repeat	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_B3APP-2L2	Acquisition Date	4/1/2025 10:38:57 AM
Ionisation Mode	repeat_684312_39_01_159966.d ESI - Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	110.9754	33.1
2	160.8421	7.7
3	162.8389	8.1
4	165.9789	10.4
5	168.8365	5.9
6	170.8333	9.4
7	172.8310	7.5
8	221.0930	100.0
9	222.0966	14.0
10	257.0694	5.8
11	278.1143	48.9
12	279.1017	7.8
13	293.1761	5.3
14	311.1675	8.9
15	325.1832	6.7
16	553.3011	13.7
17	757.3939	40.5
18	758.3973	18.4
19	759.3912	19.1
20	760.3940	6.6

Generate Molecular Formula Parameters

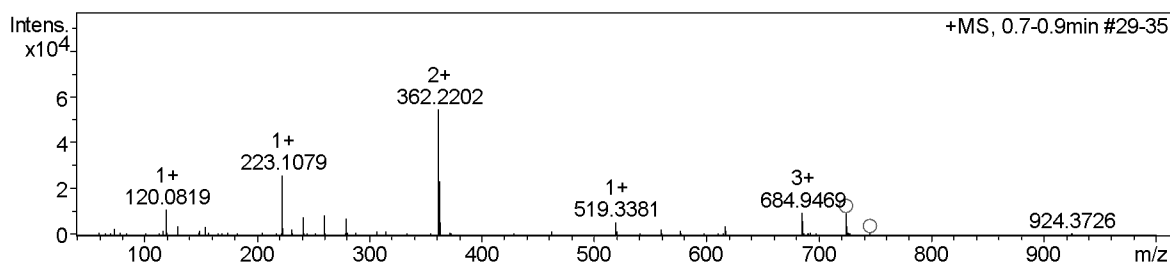
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
-1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C36 H54 N10 O6				Adduct(s):	H, radical

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



Sample-ID	bralo7_B3APP-2L2 repeat	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_B3APP-2L2	Acquisition Date	4/1/2025 10:47:11 AM
Ionisation Mode	repeat_684312_39_01_159968.d ESI - Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	120.0819	20.1
2	130.1601	7.9
3	155.1311	6.9
4	223.1079	47.7
5	224.1107	6.2
6	241.8156	14.7
7	242.1490	7.1
8	260.1746	16.2
9	280.1442	13.3
10	362.2202	100.0
11	362.7219	42.7
12	363.2233	10.8
13	519.3381	10.3
14	616.5829	7.7
15	616.9172	7.3
16	684.6109	17.2
17	684.9469	18.4
18	685.2793	11.1
19	723.4284	17.1
20	724.4328	7.3

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		C36 H54 N10 O6		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	723.4284	723.4301	2.30	0.0108	C36H55N10O6	M+H	1.0078
1	745.4103	745.4120	2.30	0.0552	C36H54N10NaO6	M+Na	22.9898

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

