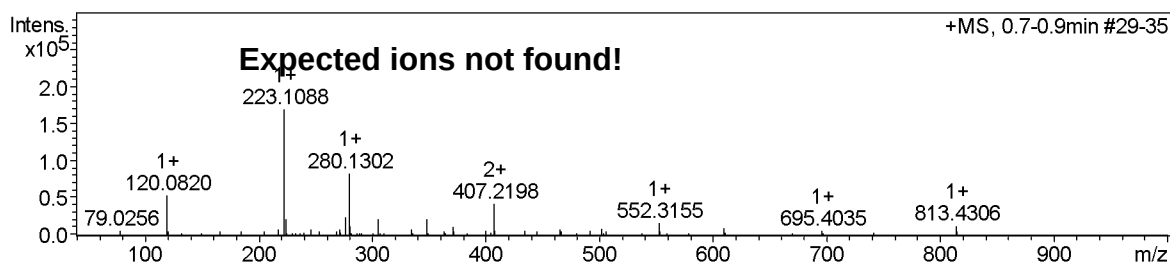




Sample-ID	bralo7_TETA-2Ac-2L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-2Ac-2L2_684414_63_01_160	Acquisition Date	4/4/2025 9:30:59 AM
Ionisation Mode	007.d ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	120.0820	31.7
2	223.1088	100.0
3	224.1120	12.9
4	246.1591	4.7
5	276.6625	14.5
6	277.1637	4.8
7	280.1302	48.8
8	281.1326	7.8
9	305.1736	12.8
10	305.6750	4.5
11	335.1948	4.3
12	348.2107	12.6
13	371.2080	6.8
14	407.2198	25.0
15	407.7202	11.4
16	465.7532	4.5
17	502.2457	5.5
18	552.3155	10.1
19	609.3381	6.0
20	813.4306	7.3

Generate Molecular Formula Parameters

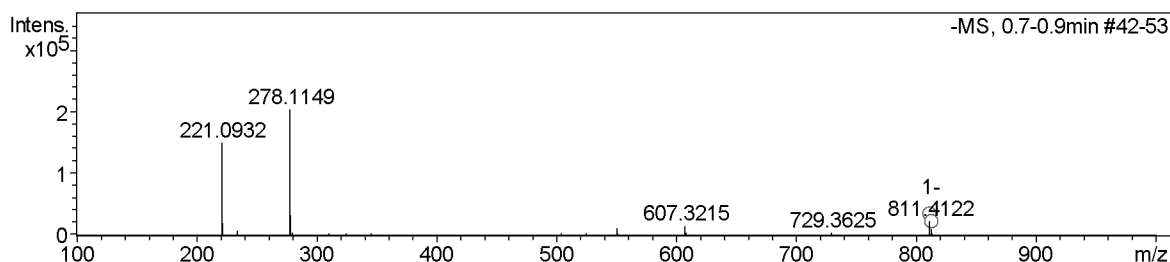
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C38 H56 N10 O10		Adduct(s):		H, Na, NH4, C3H5N2, radical	

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



Sample-ID	bralo7_TETA-2Ac-2L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-2Ac-2L2_684414_63_01_160	Acquisition Date	4/4/2025 9:38:54 AM
Ionisation Mode	ESI ⁻ Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	221.0932	73.1
2	222.0963	9.5
3	234.1243	3.4
4	278.1149	100.0
5	279.1170	15.9
6	280.1191	2.0
7	311.1680	1.5
8	325.1832	1.4
9	346.2086	1.2
10	504.2928	1.2
11	525.2701	1.3
12	550.2984	5.9
13	551.3005	1.8
14	607.3215	7.6
15	608.3213	2.6
16	729.3625	2.4
17	739.3898	1.1
18	811.4122	11.0
19	812.4142	5.1
20	813.4162	1.3

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		C38 H56 N10 O10		Adduct(s):		H, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	811.4122	811.4108	1.80	0.0127	C38H55N10O10	M- H	1.0078

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

