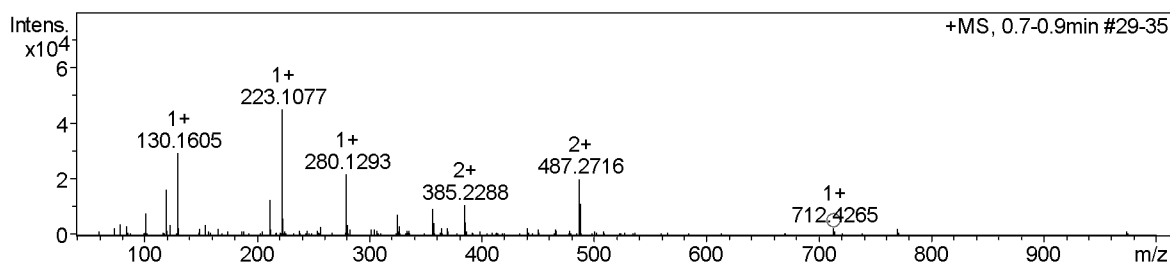




Sample-ID	bralo7_TEPA-2L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TEPA-2L2_684258_13_01_159903.	Acquisition Date	3/31/2025 1:53:05 PM
Ionisation Mode	d ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	79.0268	9.2
2	102.1314	17.8
3	120.0825	36.7
4	123.0930	8.5
5	130.1605	65.1
6	155.1309	8.6
7	212.1186	28.3
8	223.1077	100.0
9	224.1117	13.7
10	280.1293	48.6
11	281.1334	8.3
12	325.1849	16.8
13	325.5205	8.9
14	356.7167	21.4
15	357.2187	9.5
16	385.2288	24.0
17	385.7288	10.8
18	487.2716	44.6
19	487.7739	25.3
20	488.2751	8.7

Generate Molecular Formula Parameters

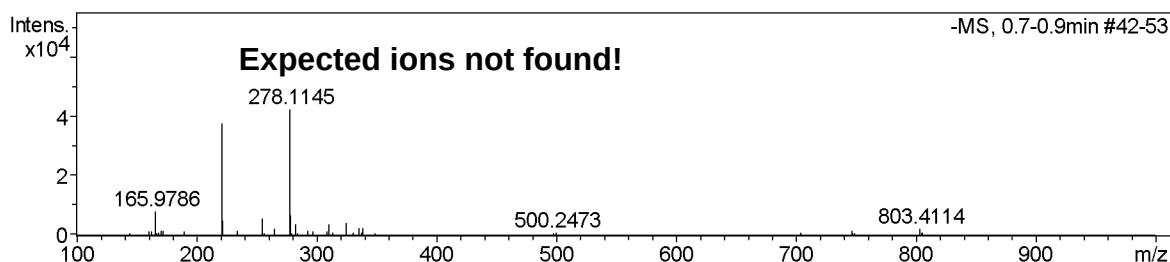
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C34 H53 N11 O6		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	712.4265	712.4253	1.70	0.0483	C34H54N11O6	M+H	1.0078

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



Sample-ID	bralo7_TEPA-2L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TEPA-2L2_684258_13_01_159911.	Acquisition Date	3/31/2025 2:16:19 PM
Ionisation Mode	d ESI Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	165.9786	18.8
2	170.8332	3.9
3	172.8310	3.4
4	190.0515	3.2
5	221.0931	88.6
6	222.0961	12.1
7	234.1247	3.9
8	255.2334	13.3
9	265.1466	5.2
10	278.1145	100.0
11	279.1144	15.8
12	283.2642	9.0
13	293.1766	4.1
14	309.1709	3.4
15	311.1687	9.1
16	325.1837	9.5
17	336.0731	6.3
18	339.1993	6.4
19	746.3854	3.7
20	803.4114	5.3

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		C34 H53 N11 O6				Adduct(s):	H, radical

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

