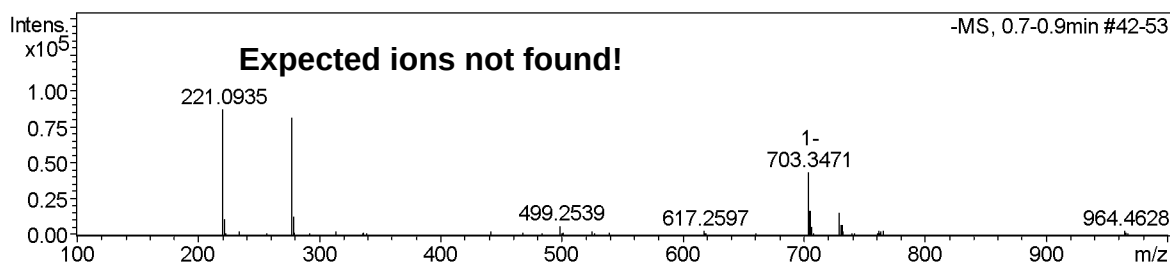




Sample-ID	bralo7_TETA-2L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-2L2_684159_71_01_159828.	Acquisition Date	3/28/2025 2:26:49 PM
Ionisation Mode	d ESI Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	221.0935	100.0
2	222.0962	13.1
3	234.1245	3.4
4	278.1150	93.6
5	279.1168	15.0
6	314.0910	3.1
7	499.2539	7.3
8	525.2696	3.3
9	617.2597	3.8
10	703.3471	50.5
11	704.3490	19.8
12	705.3451	19.7
13	706.3455	7.0
14	729.3629	18.5
15	730.3637	8.0
16	731.3593	8.6
17	732.3600	3.2
18	761.3141	3.6
19	765.3332	3.5
20	964.4628	3.5

Generate Molecular Formula Parameters

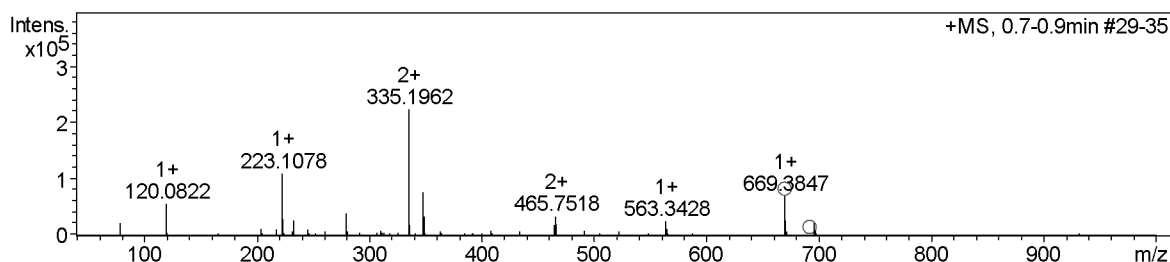
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
-1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C32 H48 N10 O6				Adduct(s):	H, radical

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



Sample-ID	bralo7_TETA-2L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-2L2_684159_71_01_159831.	Acquisition Date	3/28/2025 2:37:26 PM
Ionisation Mode	d ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	79.0258	9.7
2	120.0822	25.1
3	204.6397	5.5
4	223.1078	49.5
5	223.7997	13.1
6	224.1220	9.4
7	233.1503	12.0
8	280.1293	17.6
9	335.1962	100.0
10	335.6973	38.9
11	336.1984	8.6
12	348.2035	33.9
13	348.7051	14.8
14	465.2924	8.0
15	465.7518	15.0
16	466.2596	8.8
17	563.3428	11.3
18	669.3847	31.3
19	670.3872	12.0
20	695.4003	9.6

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		C32 H48 N10 O6		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	669.3847	669.3831	2.40	0.0035	C32H49N10O6	M+H	1.0078
1	691.3637	691.3651	1.90	0.0103	C32H48N10NaO6	M+Na	22.9898

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

