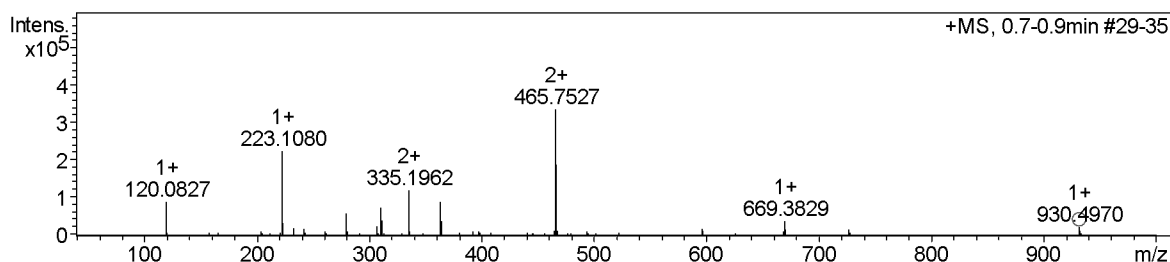




Sample-ID	bralo7_TETA-3L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-3L2_684256_11_01_159901.	Acquisition Date	3/31/2025 1:48:08 PM
Ionisation Mode	d ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	120.0827	26.6
2	223.1080	66.7
3	223.7998	5.0
4	224.1154	9.6
5	233.1505	5.9
6	242.8069	5.0
7	280.1290	17.5
8	307.1761	7.3
9	310.8372	21.9
10	311.1717	12.2
11	335.1962	35.6
12	335.6971	13.7
13	363.7074	26.1
14	364.2084	11.3
15	465.7527	100.0
16	466.2538	56.2
17	466.7553	17.0
18	596.3070	5.6
19	669.3829	11.5
20	930.4970	7.2

Generate Molecular Formula Parameters

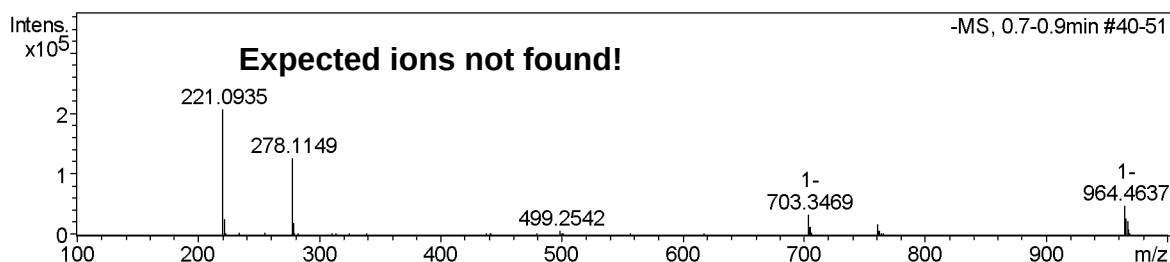
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C45 H63 N13 O9		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	930.4970	930.4944	2.80	0.0190	C45H64N13O9	M+H	1.0078

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



Sample-ID	bralo7_TETA-3L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-3L2_684256_11_01_159909.	Acquisition Date	3/31/2025 2:11:17 PM
Ionisation Mode	d ESI Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #40-51



#	m/z	I %
1	221.0935	100.0
2	222.0964	13.1
3	234.1246	2.3
4	255.2330	2.3
5	278.1149	61.7
6	279.1170	9.8
7	325.1836	1.7
8	499.2542	3.7
9	617.2590	1.7
10	703.3469	16.7
11	704.3475	6.9
12	705.3463	6.8
13	706.3450	2.5
14	760.3684	8.7
15	761.3694	4.1
16	762.3648	3.9
17	964.4637	23.1
18	965.4635	13.3
19	966.4617	11.6
20	967.4657	4.7

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		C45 H63 N13 O9		Adduct(s):		H, radical	

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

