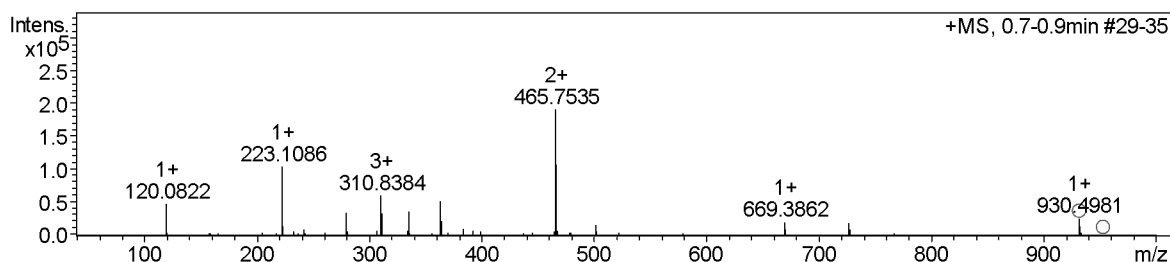




Sample-ID	bralo7_T2AEA-3L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_T2AEA-3L2_684260_15_01_15990	Acquisition Date	3/31/2025 1:58:04 PM
Ionisation Mode	5.d ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	120.0822	24.9
2	223.1086	54.3
3	224.1128	7.6
4	280.1298	18.3
5	310.8384	32.0
6	311.1728	17.2
7	311.5069	5.2
8	335.1963	19.1
9	335.6985	7.1
10	363.7085	27.1
11	364.2103	11.6
12	383.7050	5.5
13	465.7535	100.0
14	466.2544	55.6
15	466.7566	16.5
16	501.2706	8.6
17	669.3862	10.9
18	726.4060	9.7
19	930.4981	13.8
20	931.4988	7.8

Generate Molecular Formula Parameters

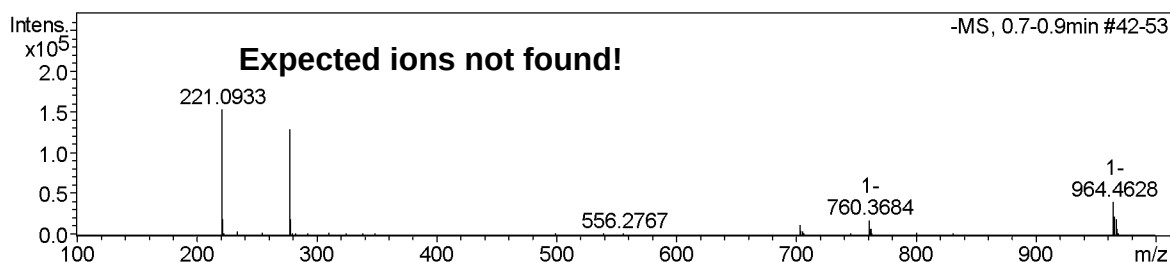
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C45 H63 N13 O9				Adduct(s):	H, Na, NH4, C3H5N2, radical
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	930.4981	930.4944	3.90	0.0125	C45H64N13O9	M+H	1.0078

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



Sample-ID	bralo7_T2AEA-3L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_T2AEA-3L2_684260_15_01_15991	Acquisition Date	3/31/2025 2:21:14 PM
Ionisation Mode	3.d ESI Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	221.0933	100.0
2	222.0961	13.2
3	234.1248	3.0
4	255.2331	2.1
5	278.1148	84.3
6	279.1167	13.1
7	311.1681	1.9
8	556.2767	1.8
9	703.3462	8.3
10	704.3469	3.5
11	705.3458	3.4
12	760.3684	12.1
13	761.3702	5.5
14	762.3646	5.3
15	763.3667	1.8
16	800.3660	2.3
17	964.4628	26.5
18	965.4637	14.8
19	966.4611	13.1
20	967.4644	5.4

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

