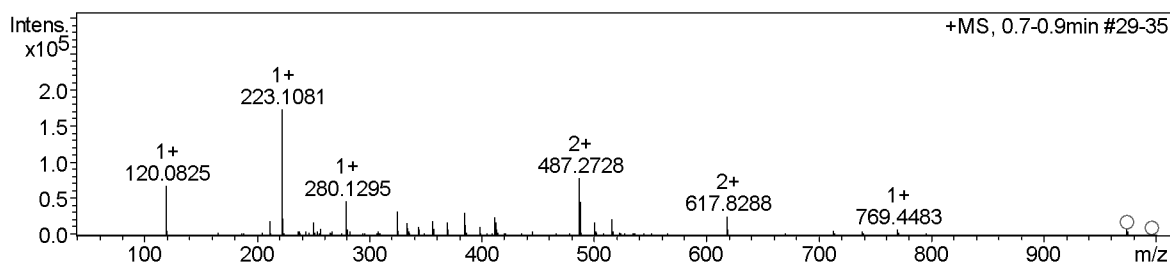




Sample-ID	bralo7_TEPA-3L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TEPA-3L2_684259_14_01_159904.	Acquisition Date	3/31/2025 1:55:34 PM
Ionisation Mode	d ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	120.0825	39.6
2	212.1182	11.2
3	223.1081	100.0
4	224.1115	13.5
5	251.1395	10.9
6	280.1295	27.1
7	325.1860	18.8
8	325.5200	10.8
9	333.8572	9.8
10	356.7166	11.7
11	369.7264	10.8
12	385.2292	18.5
13	412.2234	14.4
14	412.5574	10.4
15	487.2728	45.4
16	487.7750	26.4
17	500.2813	10.2
18	515.7840	12.7
19	617.8288	15.0
20	618.3307	11.4

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		C47 H68 N14 O9		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	973.5366	973.5366	0.10	0.0188	C47H69N14O9	M+H	1.0078

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



Sample-ID	bralo7_TEPA-3L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TEPA-3L2_684259_14_01_159912.	Acquisition Date	3/31/2025 2:18:46 PM
Ionisation Mode	d ESI Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	160.0764	1.1
2	221.0933	100.0
3	222.0962	13.0
4	223.0983	1.4
5	234.1243	2.3
6	278.1146	63.8
7	279.1162	9.9
8	280.1188	1.3
9	349.1505	1.2
10	704.3300	1.1
11	746.3844	2.6
12	747.3878	1.2
13	748.3822	1.1
14	772.4047	2.2
15	773.4047	1.1
16	774.4008	1.1
17	803.4105	4.0
18	804.4110	1.9
19	805.4071	1.9
20	829.4243	1.5

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		C47 H68 N14 O9				Adduct(s):	H, radical

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

