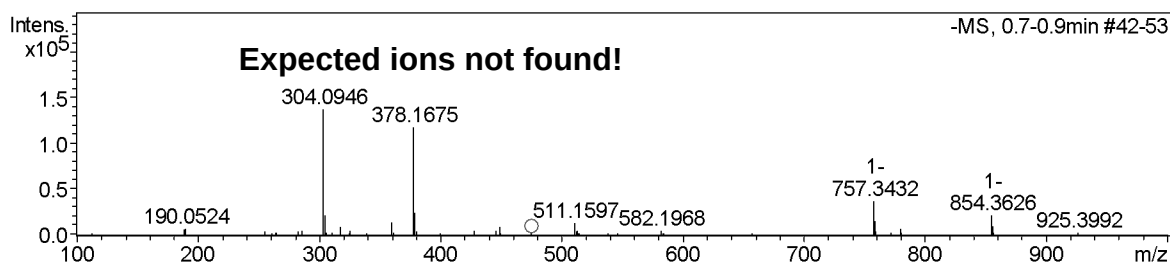




Sample-ID	bralo7_Boc-PGG-OSu	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_Boc-PGG-OSu_684157_73_01_159	Acquisition Date	3/28/2025 2:31:45 PM
Ionisation Mode	830.d ESI ⁻ Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	189.0666	4.3
2	190.0524	5.4
3	286.0833	3.6
4	304.0946	100.0
5	305.0966	16.0
6	318.1090	6.6
7	326.0765	3.5
8	360.1558	10.7
9	378.1675	85.7
10	379.1697	18.5
11	446.1537	4.1
12	449.2031	6.8
13	511.1597	9.7
14	513.1575	3.6
15	582.1968	3.8
16	757.3432	27.2
17	758.3473	11.1
18	779.3249	5.0
19	854.3626	15.9
20	855.3646	7.4

Generate Molecular Formula Parameters

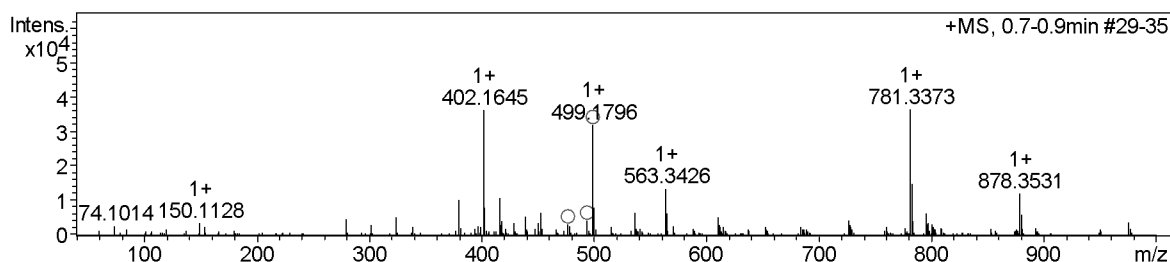
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
-1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C22 H28 N4 O8		Adduct(s):		H, radical	

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



Sample-ID	bralo7_Boc-PGG-OSu	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_Boc-PGG-OSu_684157_73_01_159	Acquisition Date	3/28/2025 2:42:24 PM
Ionisation Mode	833.d ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	280.1299	13.2
2	324.1171	14.0
3	380.1813	27.7
4	402.1645	98.8
5	403.1655	21.8
6	416.1792	29.7
7	439.2553	15.0
8	453.2698	18.3
9	494.2246	12.3
10	499.1796	87.5
11	500.1824	22.1
12	536.2596	18.3
13	563.3426	37.3
14	564.3451	17.3
15	610.1831	14.3
16	781.3373	100.0
17	782.3397	40.5
18	795.3542	17.6
19	878.3531	33.1
20	879.3545	16.7

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		C22 H28 N4 O8		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	477.1980	477.1980	0.00	0.0275	C22H29N4O8	M+H	1.0078
1	499.1796	499.1799	0.70	0.0039	C22H28N4NaO8	M+Na	22.9898
1	494.2246	494.2245	0.00	0.0314	C22H32N5O8	M+H4N	18.0344

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

