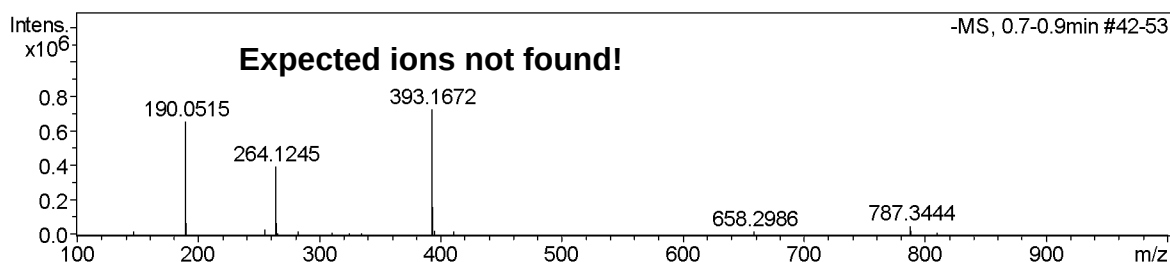




Sample-ID	bralo7_Boc-P-OSu	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_Boc-P-OSu_684158_72_01_159829	Acquisition Date	3/28/2025 2:29:17 PM
Ionisation Mode	ESI Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	147.0450	3.2
2	190.0515	90.3
3	191.0540	10.0
4	255.2330	4.2
5	264.1245	54.6
6	265.1296	9.5
7	266.1325	1.2
8	283.2639	3.1
9	311.1681	2.0
10	325.1836	1.8
11	335.1605	1.4
12	393.1672	100.0
13	394.1695	22.4
14	395.1715	3.7
15	411.1921	3.0
16	658.2986	2.7
17	680.2804	1.1
18	787.3444	7.9
19	788.3464	3.5
20	809.3241	2.3

Generate Molecular Formula Parameters

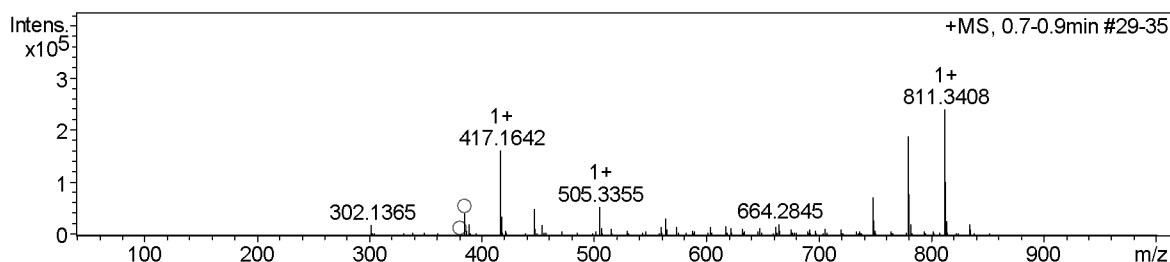
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
-1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C18 H22 N2 O6		Adduct(s):		H, radical	

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



Sample-ID	bralo7_Boc-P-OSu	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_Boc-P-OSu_684158_72_01_159832	Acquisition Date	3/28/2025 2:39:55 PM
Ionisation Mode	d ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	302.1365	8.2
2	385.1375	17.1
3	389.2520	8.9
4	417.1642	67.3
5	418.1659	14.8
6	447.2935	21.3
7	454.2547	8.1
8	505.3355	22.7
9	563.3765	13.9
10	617.4595	7.2
11	664.2845	9.1
12	747.2863	30.3
13	748.2900	11.8
14	779.3128	78.9
15	780.3162	32.2
16	781.3179	8.7
17	811.3408	100.0
18	812.3410	42.4
19	813.3421	11.7
20	833.3193	9.3

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		C18 H22 N2 O6		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	385.1375	385.1370	1.20	0.0030	C18H22N2NaO6	M+Na	22.9898
1	380.1801	380.1816	4.10	0.0677	C18H26N3O6	M+H4N	18.0344

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

