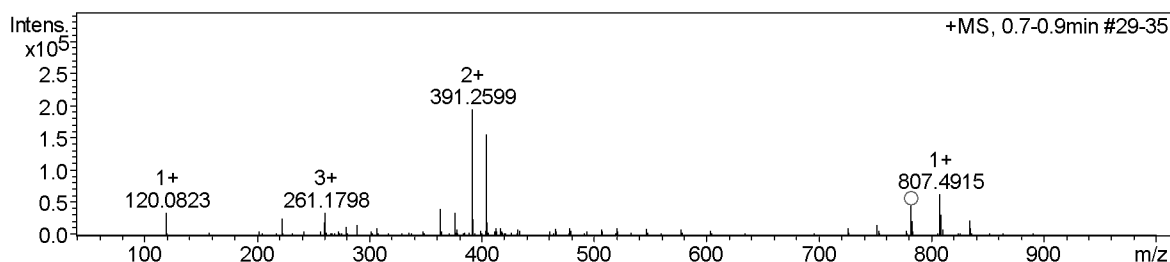




Sample-ID	bralo7_TETA-2C4-2L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-2C4-2L2_684262_16_01_159	Acquisition Date	3/31/2025 2:00:32 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #29-35



#	m/z	I %
1	120.0823	18.0
2	223.1079	13.4
3	260.7026	10.3
4	261.1798	18.2
5	363.2283	21.1
6	363.7280	9.8
7	376.2192	18.3
8	376.7188	8.7
9	391.2599	100.0
10	391.7606	48.6
11	392.2607	13.1
12	404.2493	80.1
13	404.7508	37.2
14	405.2510	10.8
15	751.4261	8.7
16	781.5120	23.8
17	782.5102	11.4
18	807.4915	32.3
19	808.4913	16.3
20	833.4730	12.0

Generate Molecular Formula Parameters

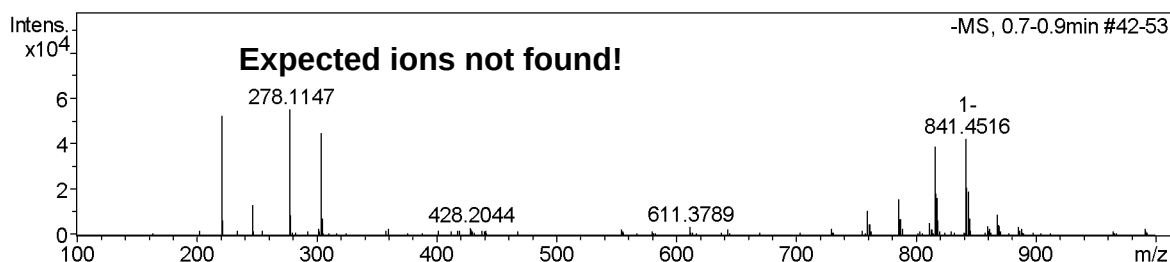
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C40 H64 N10 O6		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	781.5120	781.5083	4.70	0.0015	C40H65N10O6	M+H	1.0078

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



Sample-ID	bralo7_TETA-2C4-2L2	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-2C4-2L2_684262_16_01_159	Acquisition Date	3/31/2025 2:23:42 PM
Ionisation Mode	ESI ⁻ Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	221.0931	94.5
2	222.0962	12.4
3	247.0727	24.2
4	278.1147	100.0
5	279.1164	15.7
6	304.0939	81.0
7	305.0969	13.2
8	759.4084	20.0
9	785.3883	29.0
10	786.3900	12.8
11	787.3880	12.9
12	815.4717	70.5
13	816.4731	33.4
14	817.4708	29.6
15	818.4740	12.2
16	841.4516	76.3
17	842.4544	37.7
18	843.4515	34.5
19	844.4530	13.9
20	867.4303	16.5

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		C40 H64 N10 O6		Adduct(s):		H, radical	

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

