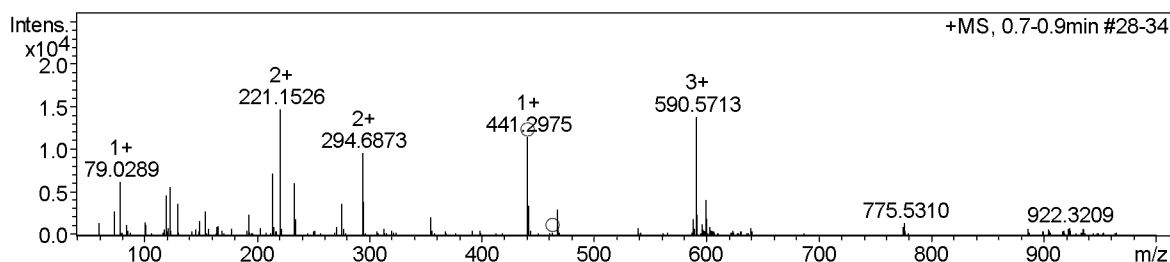




Sample-ID	bralo7_TETA-2Phe	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-2Phe_684257_10_01_15990	Acquisition Date	3/31/2025 1:45:39 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #28-34



#	m/z	I %
1	74.1039	19.1
2	79.0289	42.2
3	120.0834	31.5
4	123.0941	38.8
5	130.1611	24.8
6	214.1801	49.2
7	221.1526	100.0
8	221.6542	29.7
9	234.1609	41.5
10	276.1709	24.9
11	294.6873	65.0
12	295.1911	26.6
13	441.2975	78.3
14	442.2988	23.5
15	467.3119	20.1
16	590.5713	93.6
17	590.9048	91.4
18	591.2375	45.7
19	599.2411	27.9
20	599.5749	27.0

Generate Molecular Formula Parameters

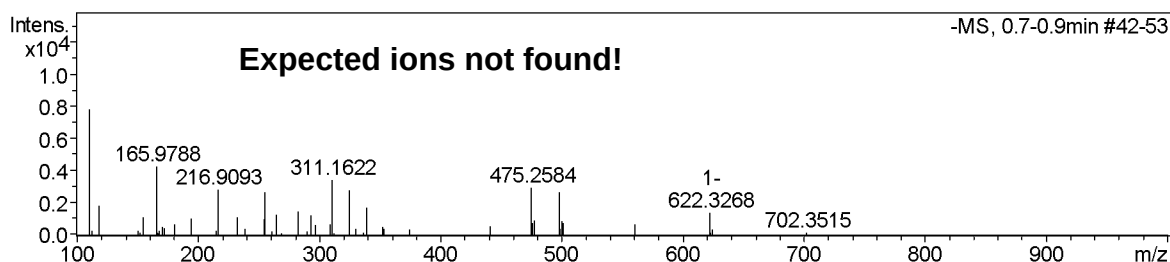
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C24 H36 N6 O2		Adduct(s):		H, Na, NH4, C3H5N2, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	441.2975	441.2973	0.60	0.0081	C24H37N6O2	M+H	1.0078

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



Sample-ID	bralo7_TETA-2Phe	Lab	C13
Submitter	Lewis O'Shaughnessy (bralo7)	Supervisor	Z_NO SUPERVISOR z_NO SUPERVISOR
Analysis Name	bralo7_TETA-2Phe_684257_10_01_15990	Acquisition Date	3/31/2025 2:08:45 PM
Ionisation Mode	8.d ESI Negative	Instrument	Bruker MicroTOF

-MS, 0.7-0.9min #42-53



#	m/z	I %
1	110.9756	100.0
2	118.9419	23.2
3	154.9167	14.2
4	165.9788	54.9
5	194.9277	13.7
6	216.9093	36.6
7	232.8749	14.5
8	254.8559	12.8
9	255.2334	34.0
10	265.1482	16.7
11	283.2639	19.2
12	293.1771	15.7
13	311.1622	43.8
14	325.1840	35.5
15	339.1985	21.7
16	475.2584	38.0
17	477.2577	12.5
18	498.2597	33.8
19	500.2578	11.1
20	622.3268	18.0

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		C24 H36 N6 O2		Adduct(s):		H, radical	

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

