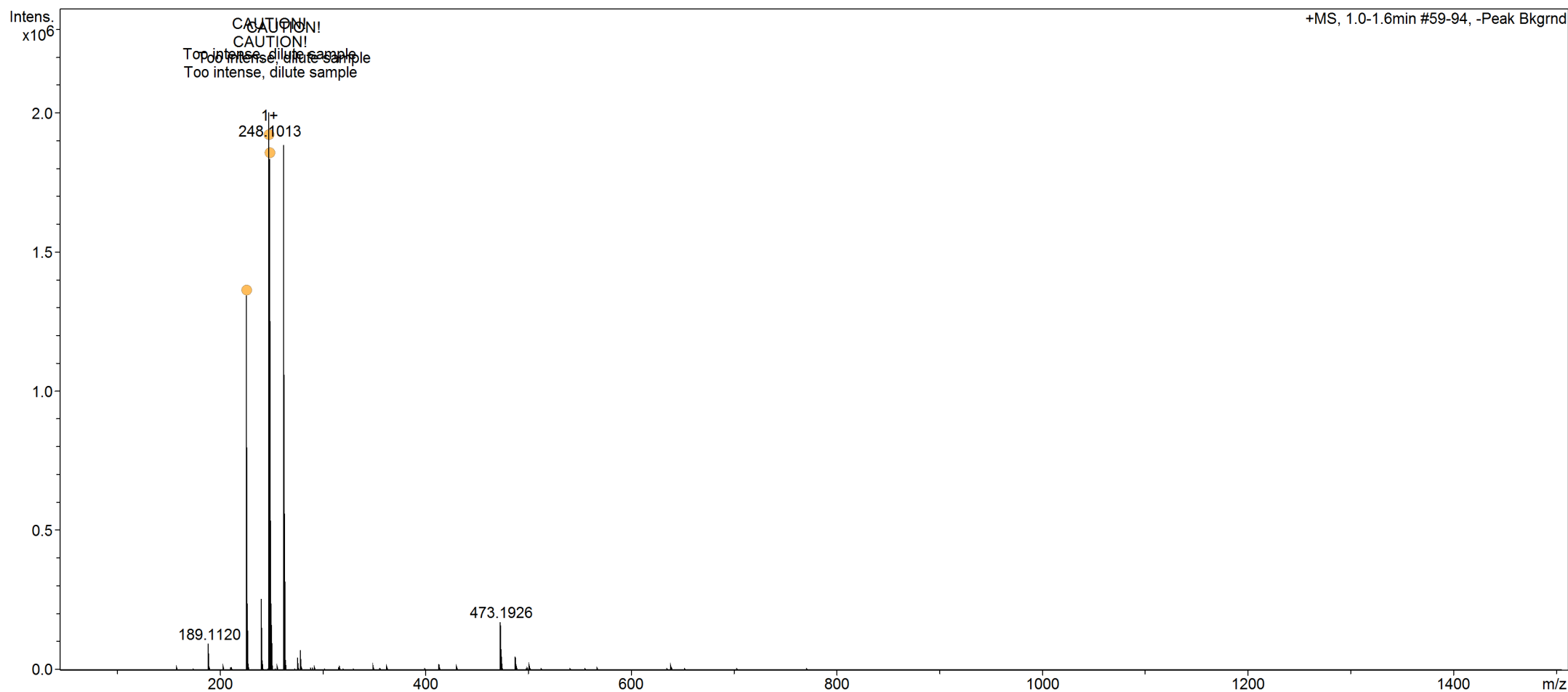
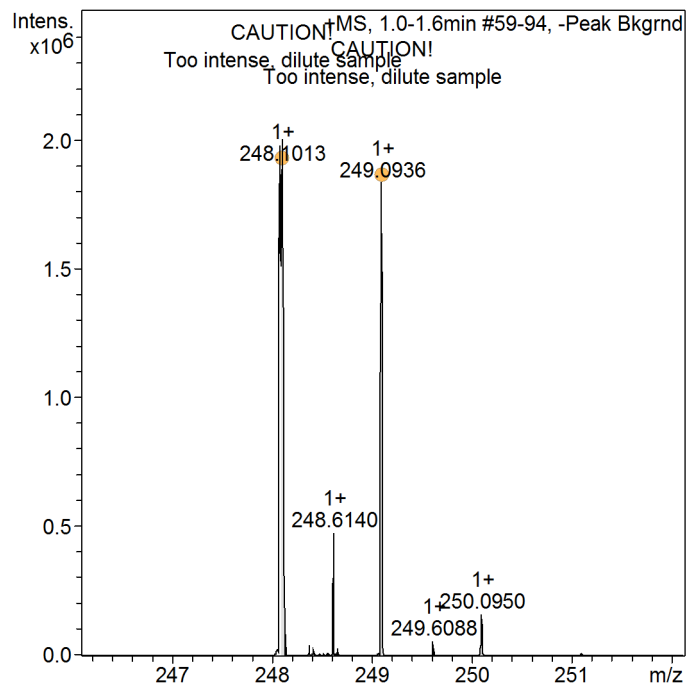


# School of Chemistry Mass Spectrometry Service

**SampleID** RW2A  
**Sample Description**  
**Analysis Name** D:\Data\malcolmhalcrow\cm18rw\RW2A\_347288\_GC4\_01\_84569.d  
**Method** 3a\_AccMass\_Loop\_Positive.m  
**Instrument** maXis impact **Source Type** ESI **Ion Polarity** Positive

**Submitter** Rhiannon Watson  
**Supervisor** Malcolm Halcrow  
**Acquisition Date** 16/03/2022 11:18:10  
**Scan Begin** 50 m/z **Scan End** 1500 m/z





## Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Concentration too high. Dilute sample!

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
226.108493	C12H12N5	1+	226.108722	0.2	1.0	16.0	100.00	C12H11N5	M+H
	C12H12N5	1+	226.108722	0.2	1.0	16.0	100.00	C12H8N4	M+NH4
248.101268	C10H15N3NaO3	1+	248.100562	-0.7	-2.8	n.a.	100.00	C10H15N3O3	M+Na
	C13H16NNa2O	1+	248.102179	0.9	3.7	n.a.	100.00	C13H17NO	M+Na2-H
249.093616	C6H13N6O5	1+	249.094194	0.6	2.3	6.6	100.00	C6H12N6O5	M+H
	C6H13N6O5	1+	249.094194	0.6	2.3	6.6	100.00	C6H9N5O5	M+NH4
	C5H10N10NaO	1+	249.093126	-0.5	-2.0	3.0	100.00	C5H10N10O	M+Na
	C7H15N4Na2O3	1+	249.093405	-0.2	-0.8	5.2	100.00	C7H16N4O3	M+Na2-H

Smart Formula Parameter      Value

Expected Formula

Adducts Considered

Smart Formula Search Parameters

CHNO and adducts considered implicitly

Formula Search Minimum

Formula Search Maximum

Algorithm Parameters

Tolerance      4 ppm

Match to Isotope Pattern(mSigma)      40

Electron Configuration      even

Estimate No of Carbons      yes

Filter by H/C Ratio      0 < H/C < 3

Number of Double Bonds & Rings      0 < rings&DB < 80