

# School of Chemistry Mass Spectrometry Service

**SampleID** 4.314  
**Sample Description**  
**Analysis Name** 4.314\_187956\_BA8\_01\_29105.d  
**Method** 3a\_AccMass\_Loop\_Positive.m  
**Instrument** maXis impact

**Source Type** ESI **Ion Polarity** Positive

**Submitter**

HAYDER ARKAWAZI

**Supervisor**

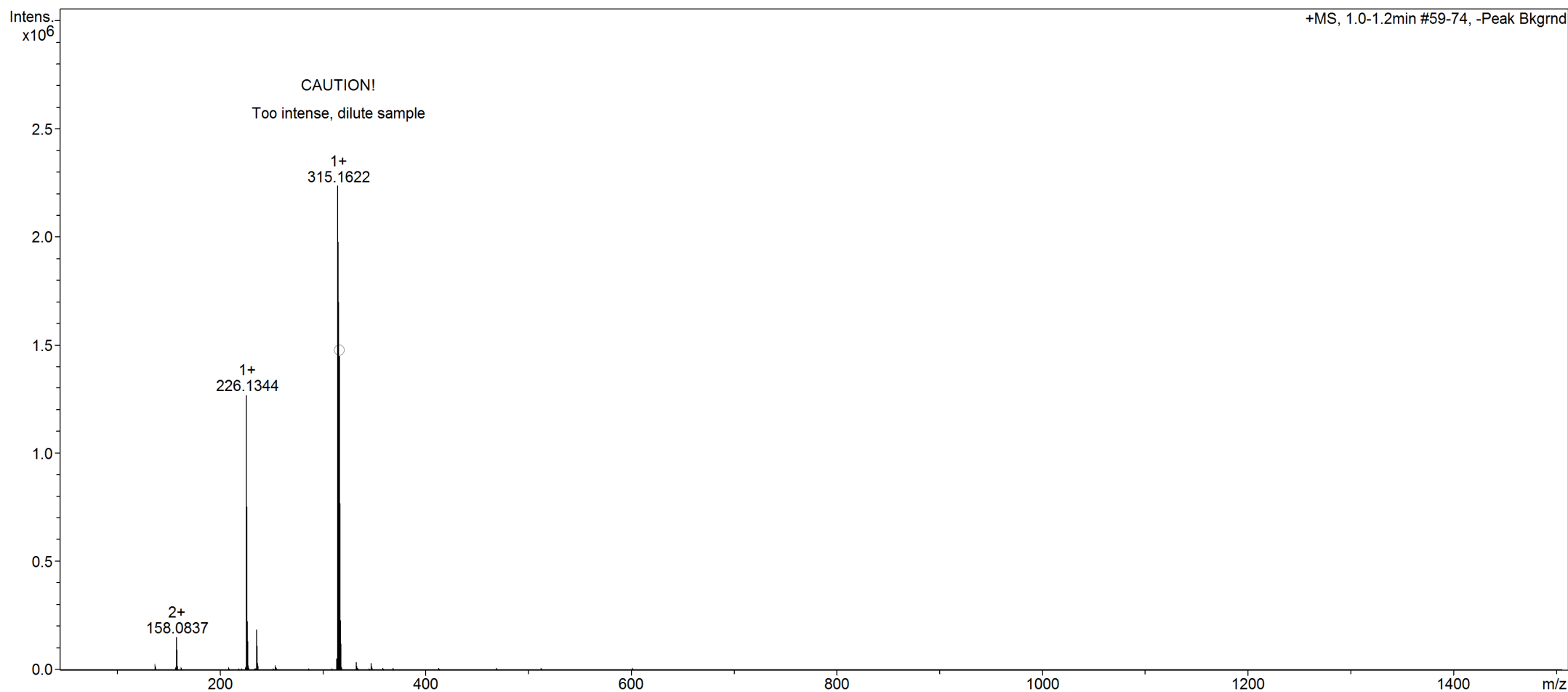
Michaele Hardie

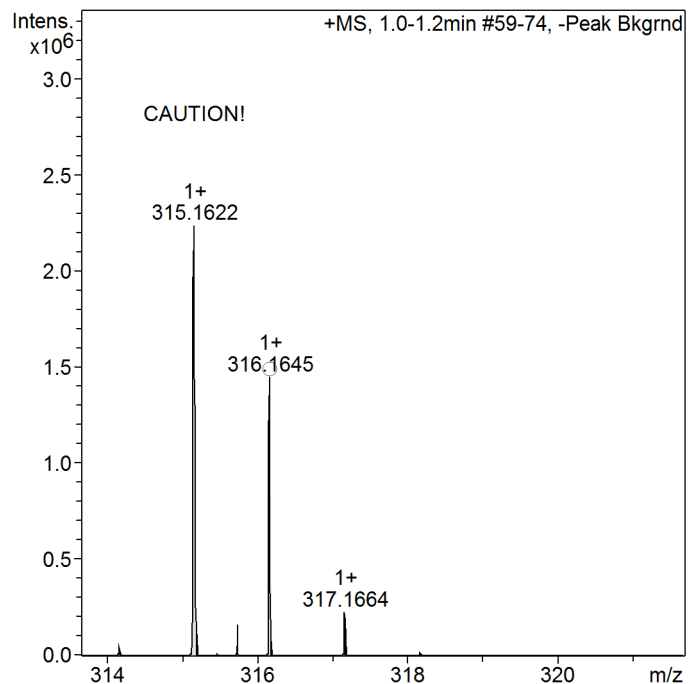
**Acquisition Date**

16/12/2016 16:45:46

**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
316.164501	C13H23KN7	1+	316.164652	0.2	0.5	39.6	100.00	C13 H23 N7	M+K
	C18H24NNa2O	1+	316.164779	0.3	0.9	26.8	100.00	C18 H25 N O	M+Na2-H

Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;

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