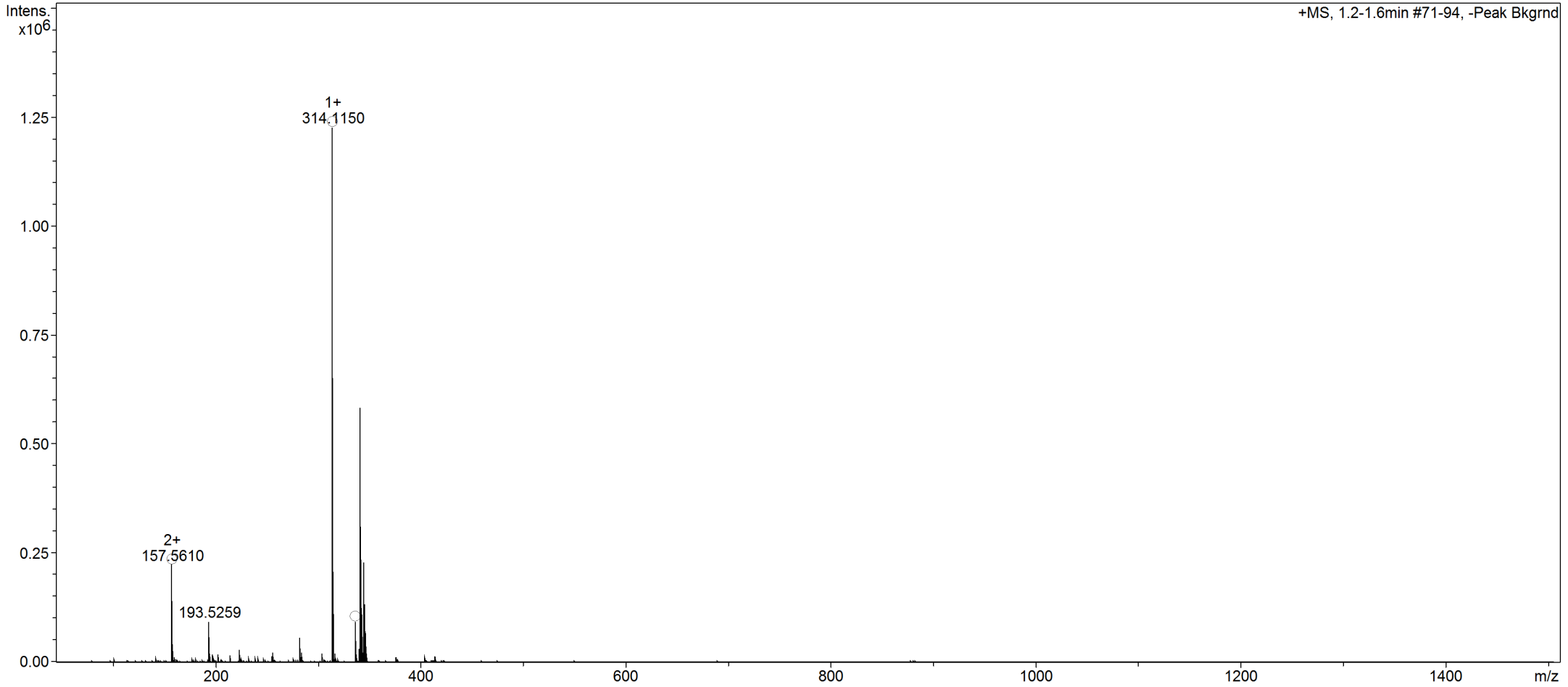
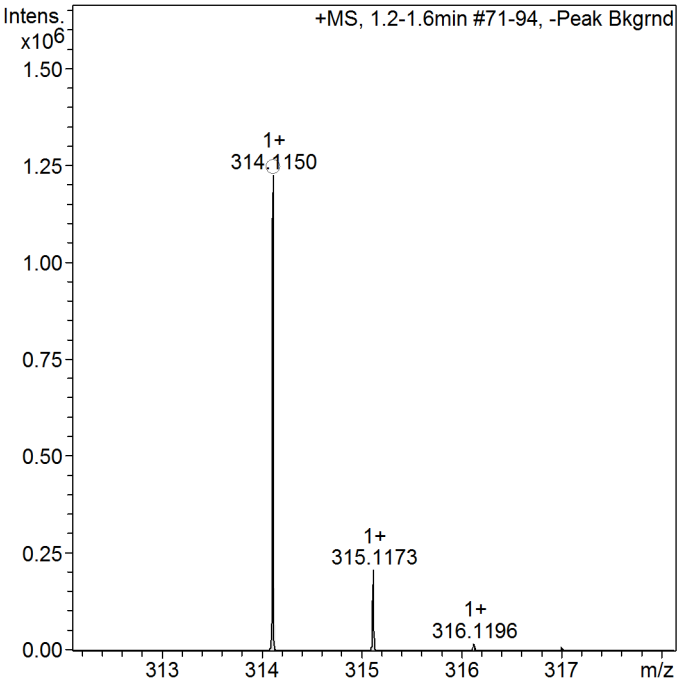
School of Chemistry Mass Spectrometry Service

SampleID	RK171				**Submitter**	Rafal Kulmaczewski	
Sample Description							
Analysis Name	RK171_175258_GB4_01_25434.d				**Supervisor**	Malcolm Halcrow	
Method	3a_AccMass_Loop_Positive.m				**Acquisition Date**	19/08/2016 08:09:06	
Instrument	maXis impact	**Source Type**	ESI	**Ion Polarity**	Positive	**Scan Begin** 50 m/z	**Scan End** 1500 m/z





Smart Formula Parameter	Value
Expected Formula	C17H11N7
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

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

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
157.560989	C17H13N7	2+	157.561073	0.1	0.5	16.8	100.00	C17 H11 N7	M+H
314.114986	C17H12N7	1+	314.114870	0.1	0.4	24.2	100.00		M+H
336.096837	C17H11N7Na	1+	336.096814	-0.0	-0.1	13.4	100.00	C17 H11 N7	M+Na