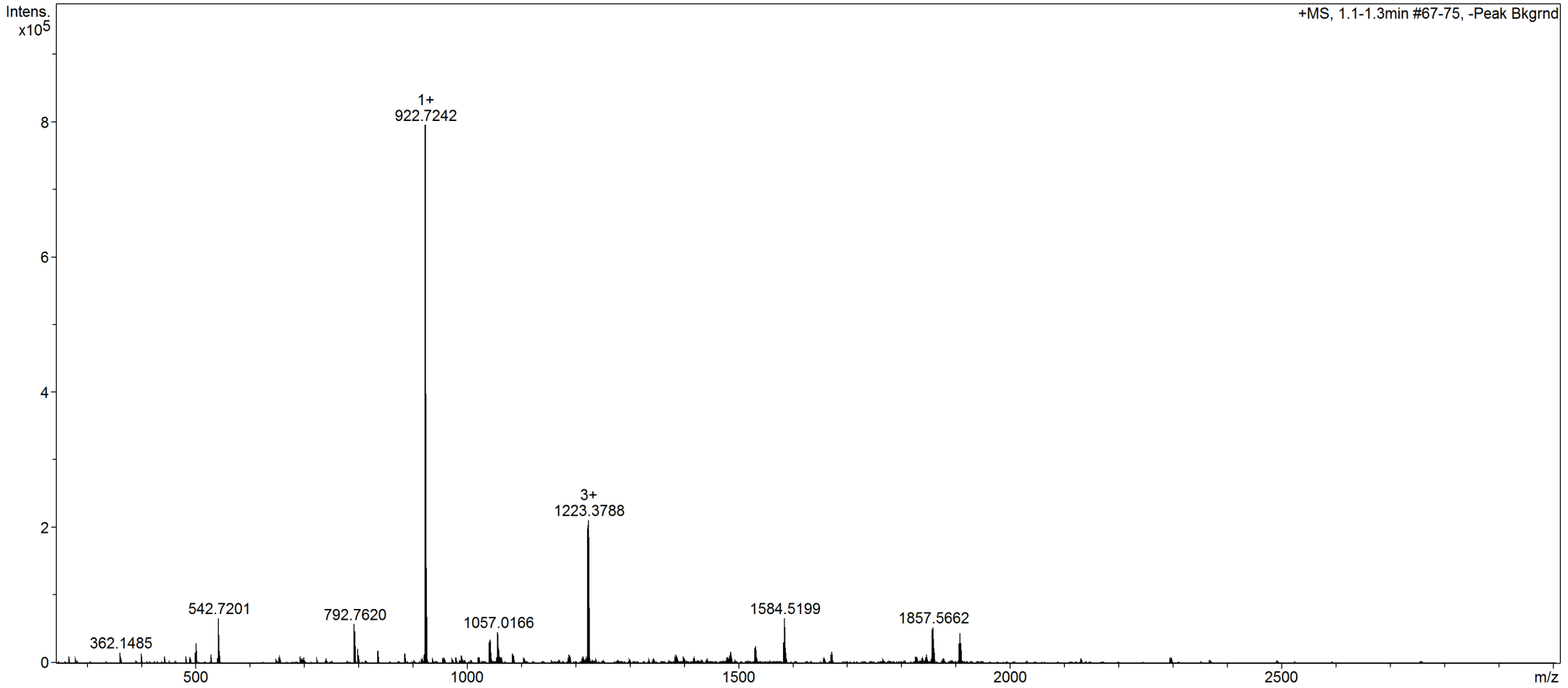
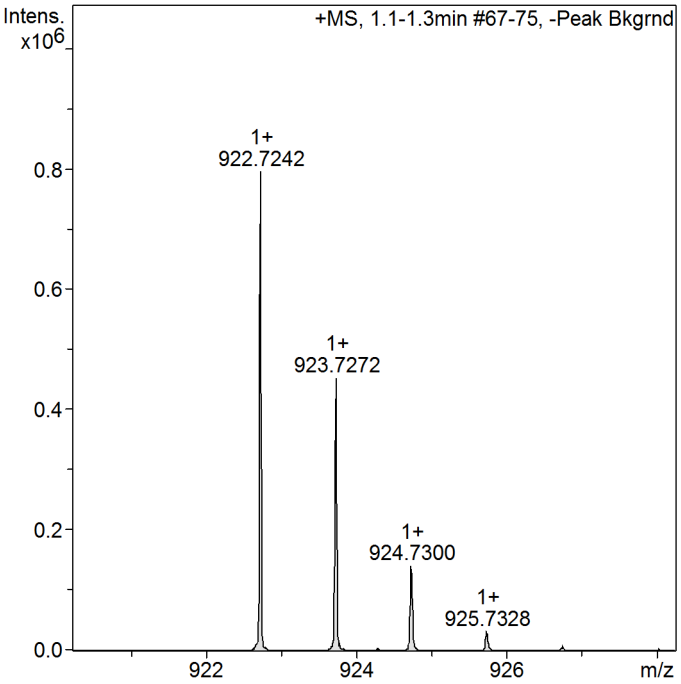
School of Chemistry Mass Spectrometry Service

SampleID	S02-214 DCM				**Submitter**	Sam Oldknow	
Sample Description							
Analysis Name	S02-214 DCM_153621_RE2_01_18576.d				**Supervisor**	Michaele Hardie	
Method	3c_AccMass_Loop_High_Pos.m				**Acquisition Date**	20/01/2016 12:39:40	
Instrument	maXis impact	**Source Type**	ESI	**Ion Polarity**	Positive	**Scan Begin** 250 m/z	**Scan End** 3000 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

Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M;;M+H;;M+NH4;;M+Na;;M+K;;M+Na2-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