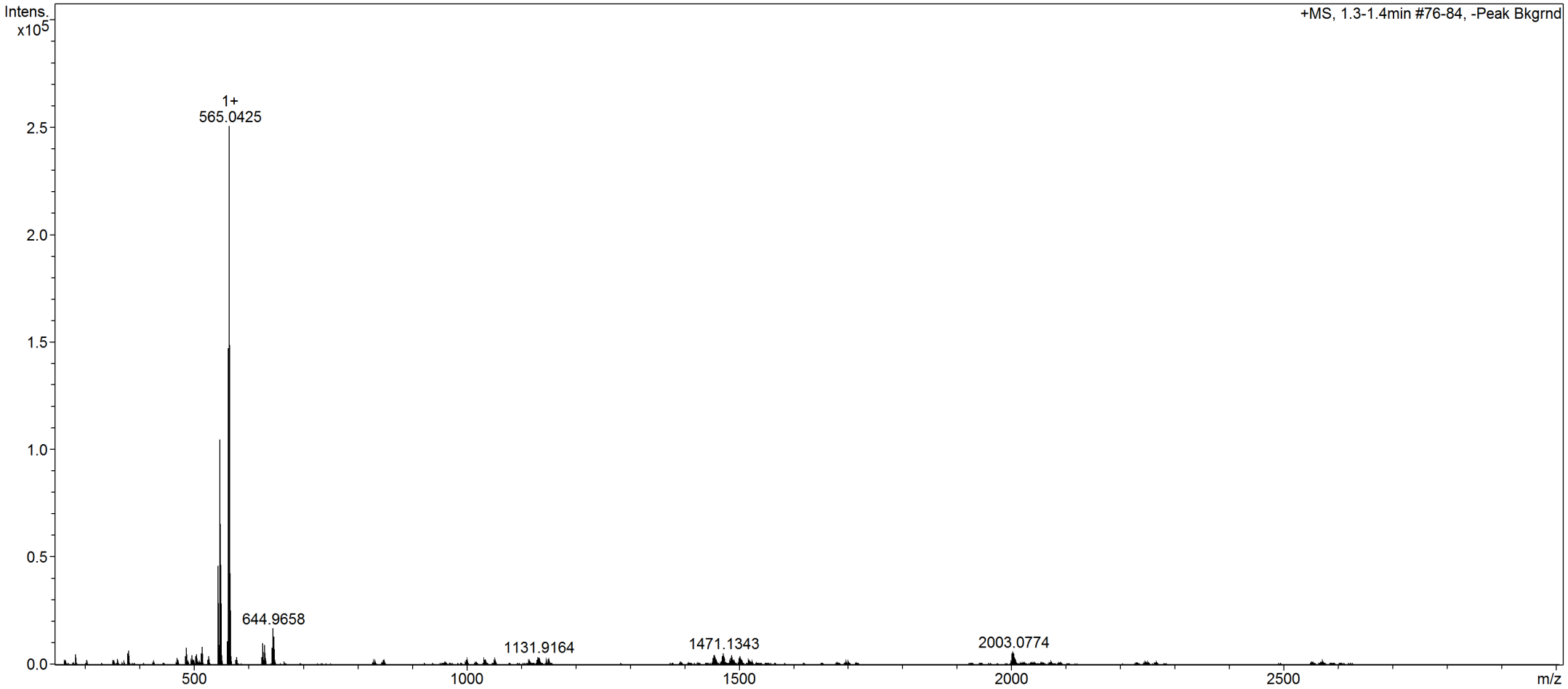
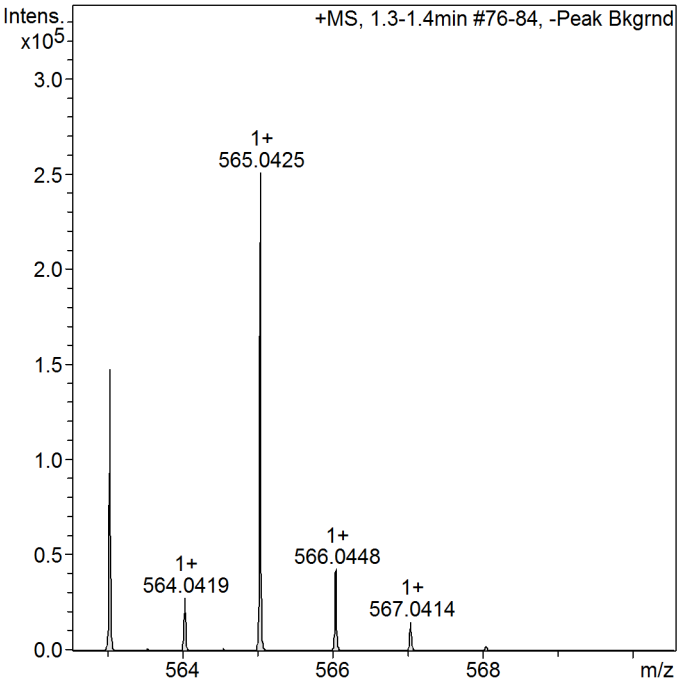
School of Chemistry Mass Spectrometry Service

SampleID	VP58 5microL	**Submitter**	Vikki Pritchard
Sample Description			
Analysis Name	VP58 5microL_78554_GE5_01_797.d	**Supervisor**	Michaele Hardie
Method	3c_AccMass_Loop_High_Pos.m	**Acquisition Date**	03/07/2013 17:49:55
Instrument	maXis impact	**Source Type** ESI	**Ion Polarity** Positive
Scan Begin 250 m/z	**Scan End** 3000 m/z		





Smart Formula Parameter	Value
Expected Formula	C69H54Br3N6O15Re3
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	Br 6 Re 6
Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	both
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