

School of Chemistry Mass Spectrometry Service

SampleID TB-004
Sample Description
Analysis Name TB-004 _148772_GD6_01_17074.d
Method 3c_AccMass_Loop_High_Pos.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Therese Berry

Supervisor

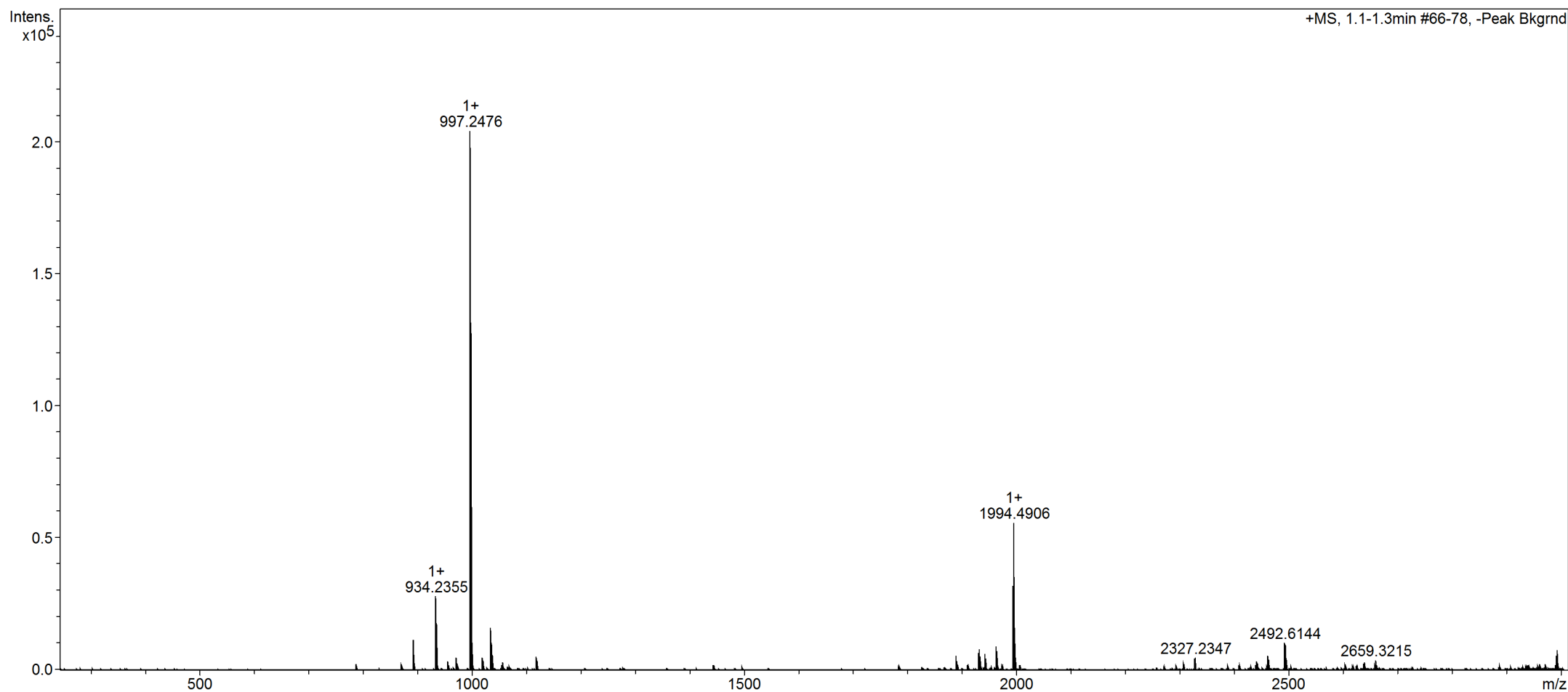
Michael Hardie

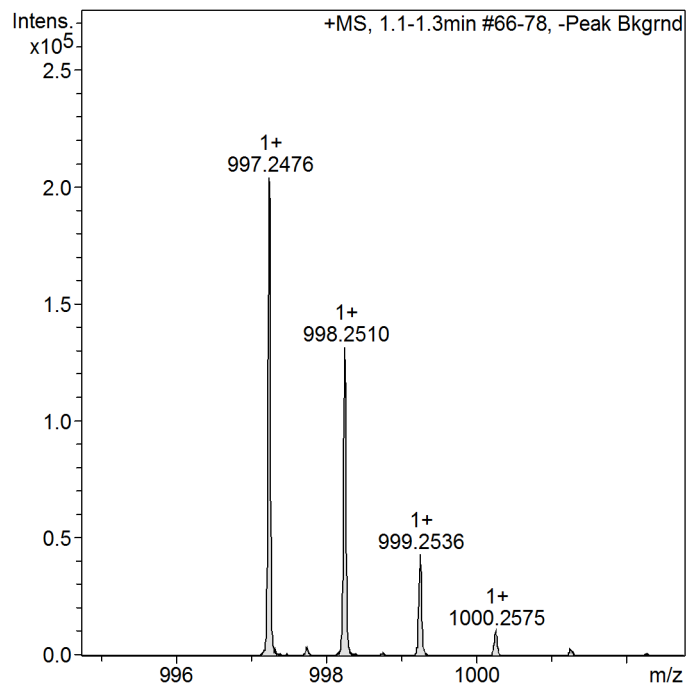
Acquisition Date

18/11/2015 16:26:51

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