

School of Chemistry Mass Spectrometry Service

SampleID ICB-1-16-1
Sample Description solido mojado
Analysis Name ICB-1-16-1_156531_GA5_01_19218.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Izar Capel

Supervisor

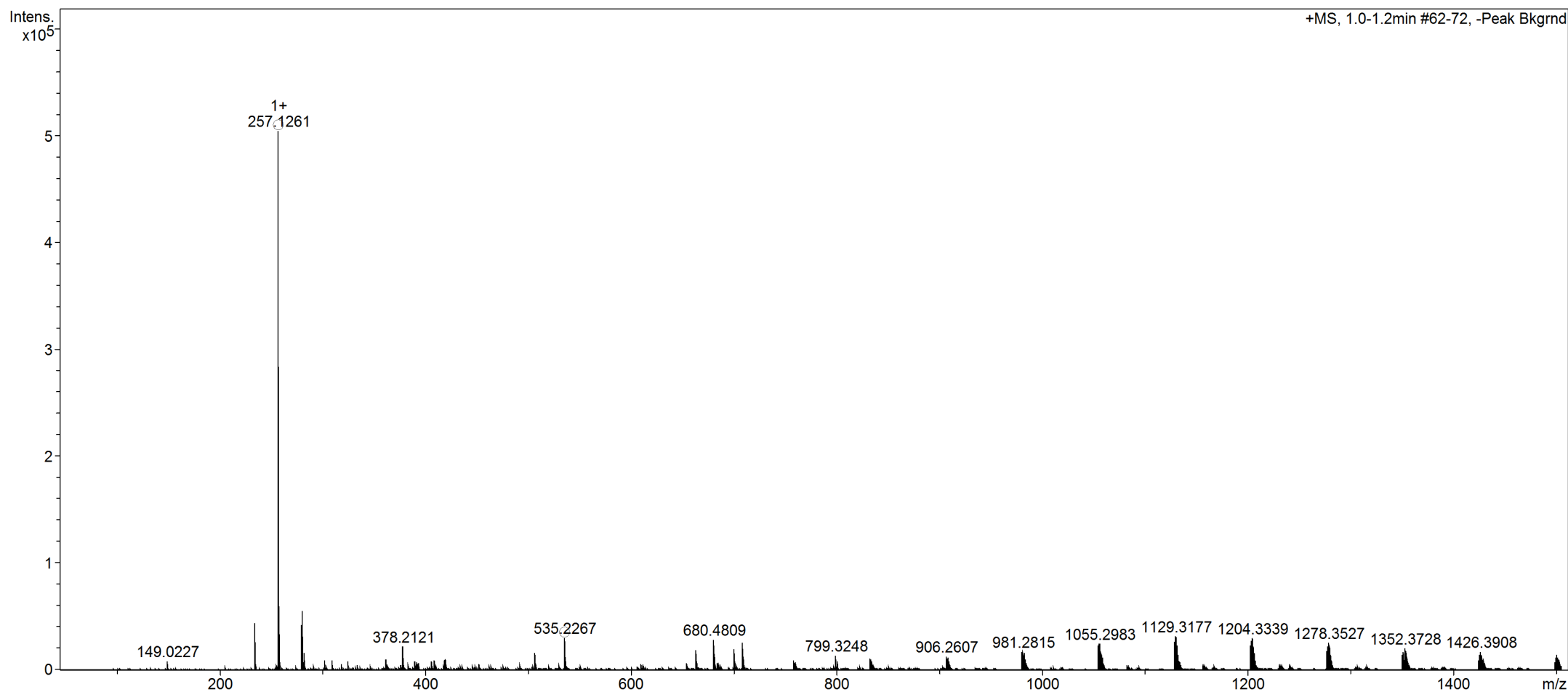
Malcolm Halcrow

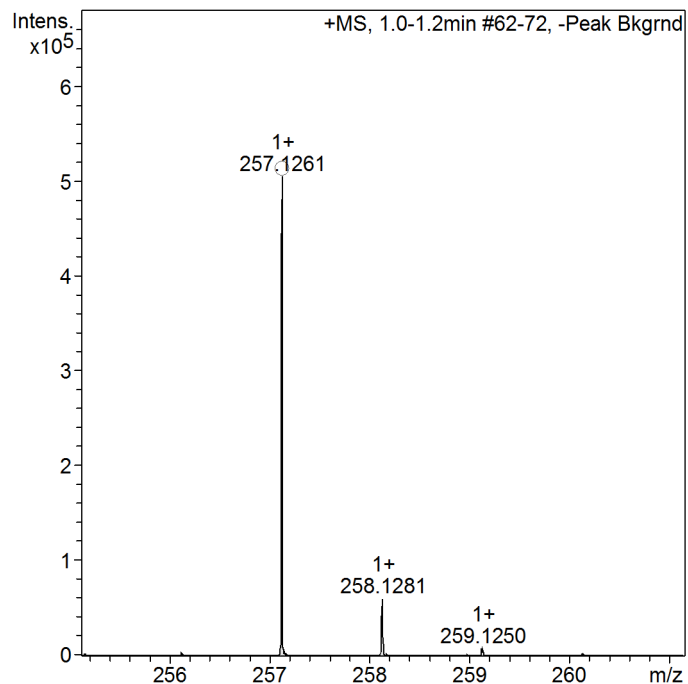
Acquisition Date

15/02/2016 19:53:57

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

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
257.126078	C11H13N8	1+	257.125769	-0.3	-1.2	18.4	100.00	C11 H12 N8	M+H
535.226699	C22H24N16Na	1+	535.226206	0.5	0.9	4.4	100.00	C11 H12 N8	2M+Na

Smart Formula Parameter	Value
Expected Formula	C11N8H12
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