

School of Chemistry Mass Spectrometry Service

SampleID CONMA-2
Sample Description
Analysis Name CONMA-2_254269_BD7_01_51482.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Izar Capel

Supervisor

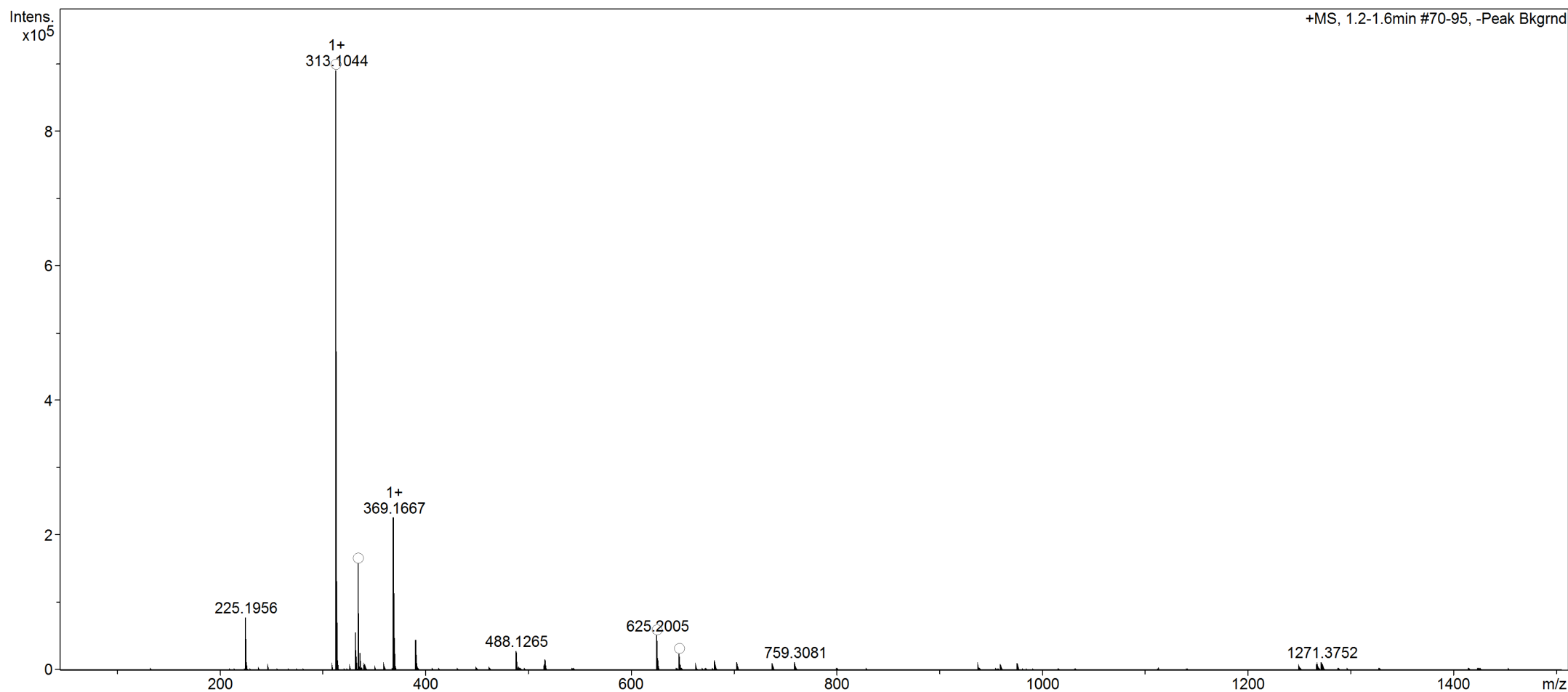
Malcolm Halcrow

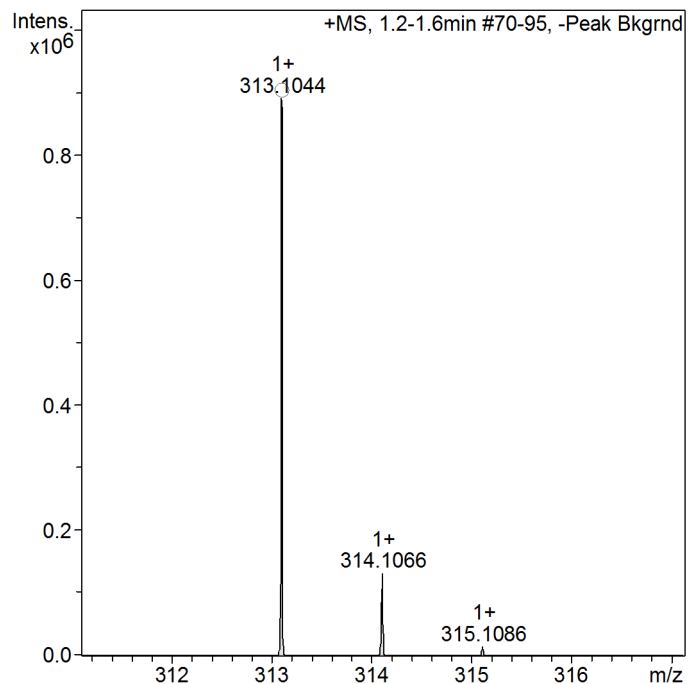
Acquisition Date

30/11/2018 00:11:03

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
313.104401	C ₁₄ H ₁₃ N ₆ O ₃	1+	313.104365	-0.0	-0.1	16.6	100.00	C ₁₄ H ₁₂ N ₆ O ₃	M+H
335.085912	C ₁₄ H ₁₂ N ₆ NaO ₃	1+	335.086309	0.4	1.2	10.9	100.00		M+Na
625.200538	C ₂₈ H ₂₅ N ₁₂ O ₆	1+	625.201453	0.9	1.5	6.2	100.00		2M+H
647.181751	C ₂₈ H ₂₄ N ₁₂ NaO ₆	1+	647.183397	1.6	2.5	13.4	100.00		2M+Na

Smart Formula Parameter	Value
Expected Formula	C ₁₄ H ₁₂ N ₆ O ₃
Adducts Considered	

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