

School of Chemistry Mass Spectrometry Service

SampleID S04PY SALT

Sample Description

Analysis Name S04PY SALT_214644_GB8_01_36576.d

Method 3a_AccMass_Loop_Positive.m

Instrument maXis impact

Source Type

ESI

Ion Polarity

Positive

Submitter

Sam Oldknow

Supervisor

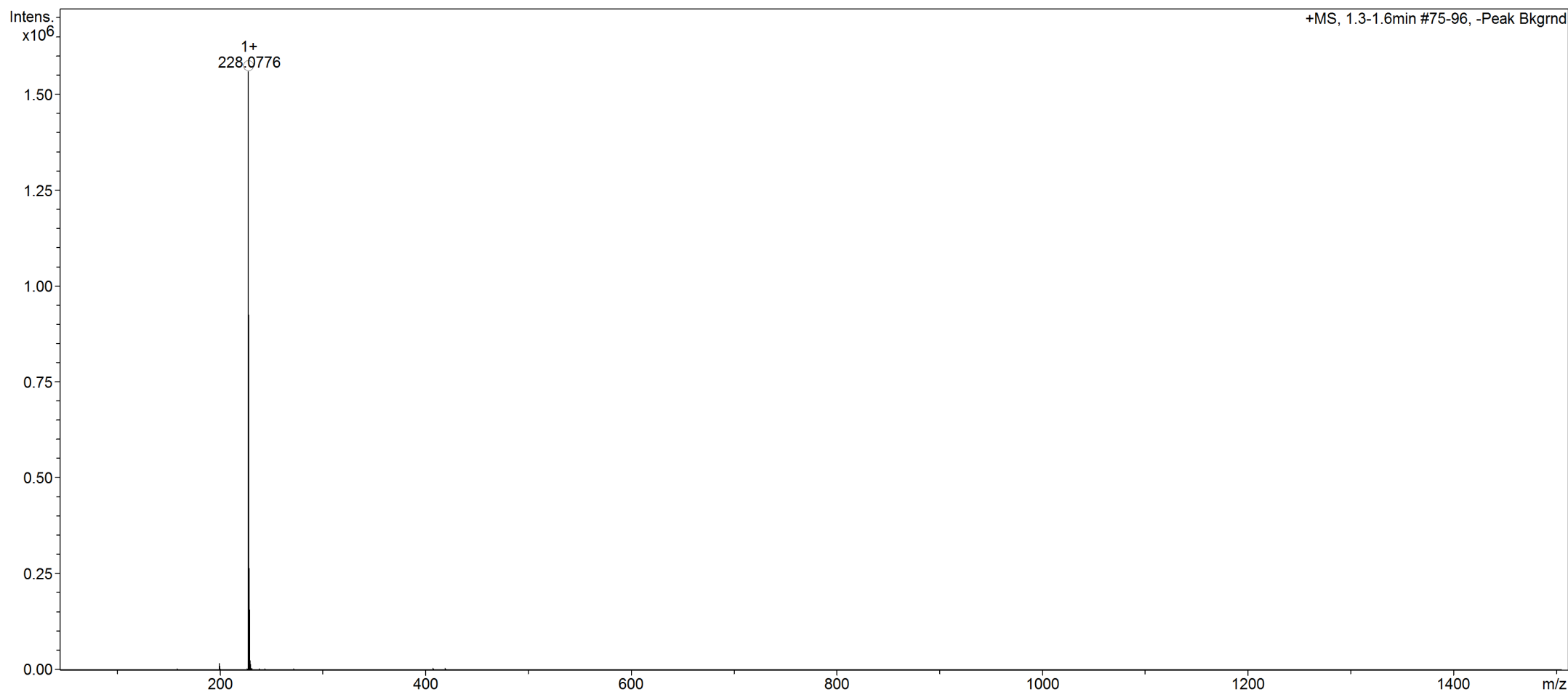
Michael Hardie

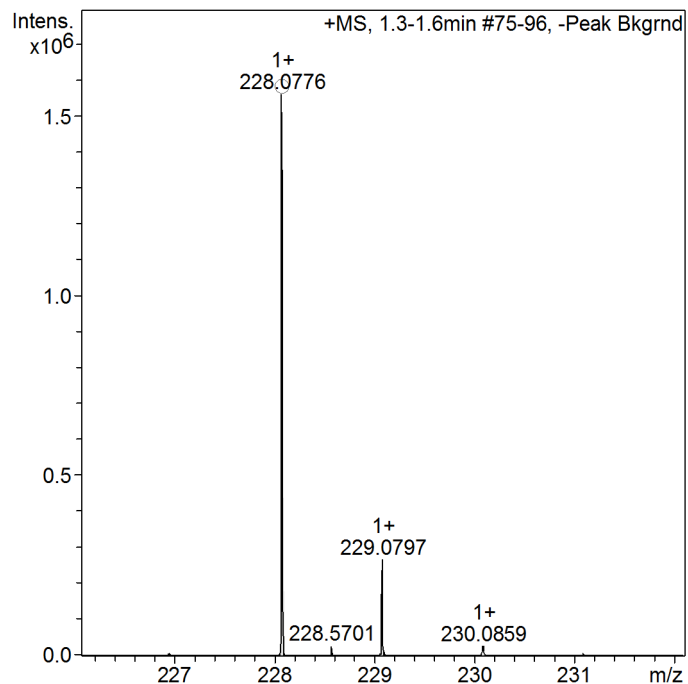
Acquisition Date

20/09/2017 15:12:39

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
228.077605	C12H10N3O2	1+	228.076753	-0.9	-3.7	16.1	100.00	C12H9N3O2	M+H
	C12H10N3O2	1+	228.076753	-0.9	-3.7	16.1	100.00	C12H6N2O2	M+NH4
	C15H11NNa	1+	228.078370	0.8	3.4	2.6	100.00	C15H11N	M+Na
	C12H15KNO	1+	228.078522	0.9	4.0	38.0	100.00	C12H15NO	M+K

Smart Formula Parameter	Value
Expected Formula	
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