School of Chemistry Mass Spectrometry Service

SampleID 130-MeOH

Sample Description

Analysis Name 130-MeOH_234599_RB8_01_45362.d

Method 3a_AccMass_Loop_Positive.m

Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

Submitter Izar Capel

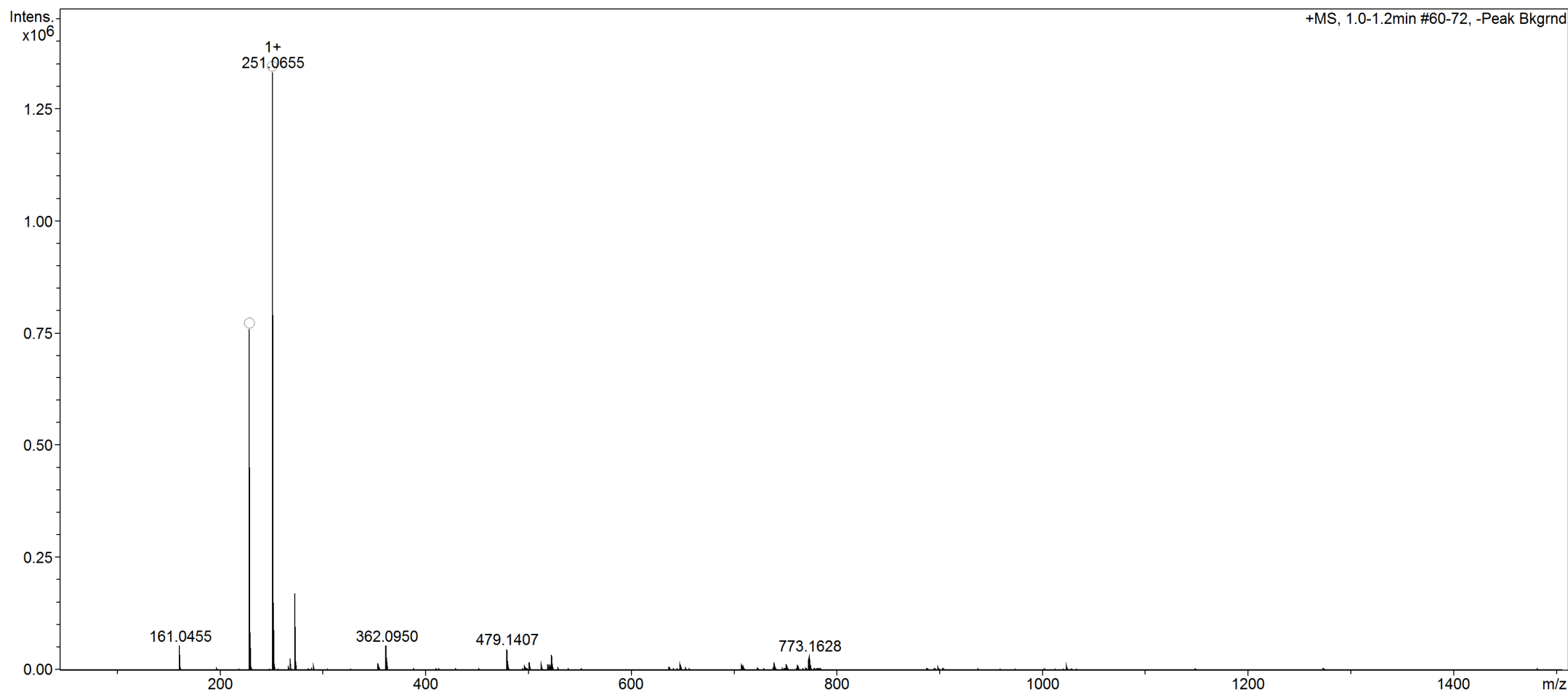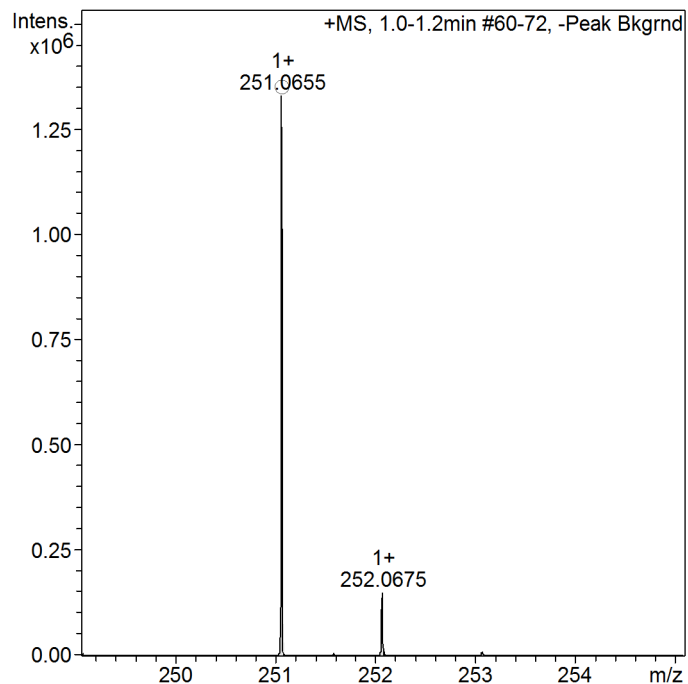**Supervisor** Malcolm Halcrow

Acquisition Date 14/04/2018 19:16:25

Scan Begin 50 m/z **Scan End** 1500 m/z

+MS, 1.0-1.2min #60-72, -Peak Bkgrnd

Intens. x10^6

1+
251.0655

161.0455
362.0950
479.1407
773.1628

Intens.
x10⁶

1+
251.0655

1+
252.0675

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
229.083346	C10H9N6O	1+	229.083235	-0.1	-0.5	13.5	100.00	C10H8N6O	M+H
	C10H9N6O	1+	229.083235	-0.1	-0.5	13.5	100.00	C10H5N5O	M+NH4
	C12H14NaO3	1+	229.083515	0.2	0.7	14.6	100.00	C12H14O3	M+Na
	C9H18KO4	1+	229.083667	0.3	1.4	39.8	100.00	C9H18O4	M+K
251.065543	C11H11N2O5	1+	251.066248	0.7	2.8	11.2	100.00	C11H10N2O5	M+H
	C11H11N2O5	1+	251.066248	0.7	2.8	11.2	100.00	C11H7NO5	M+NH4
	C10H8N6NaO	1+	251.065180	-0.4	-1.4	10.8	100.00	C10H8N6O	M+Na
	C7H12KN6O2	1+	251.065332	-0.2	-0.8	37.1	100.00	C7H12N6O2	M+K
	C12H13Na2O3	1+	251.065459	-0.1	-0.3	11.9	100.00	C12H14O3	M+Na2-H

Smart Formula Parameter	Value
Expected Formula	C11N6H7O
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