

School of Chemistry Mass Spectrometry Service

SampleID ER01x4
Sample Description
Analysis Name ER01x4_252163_GD6_01_50922.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Emily Ratcliffe

Supervisor

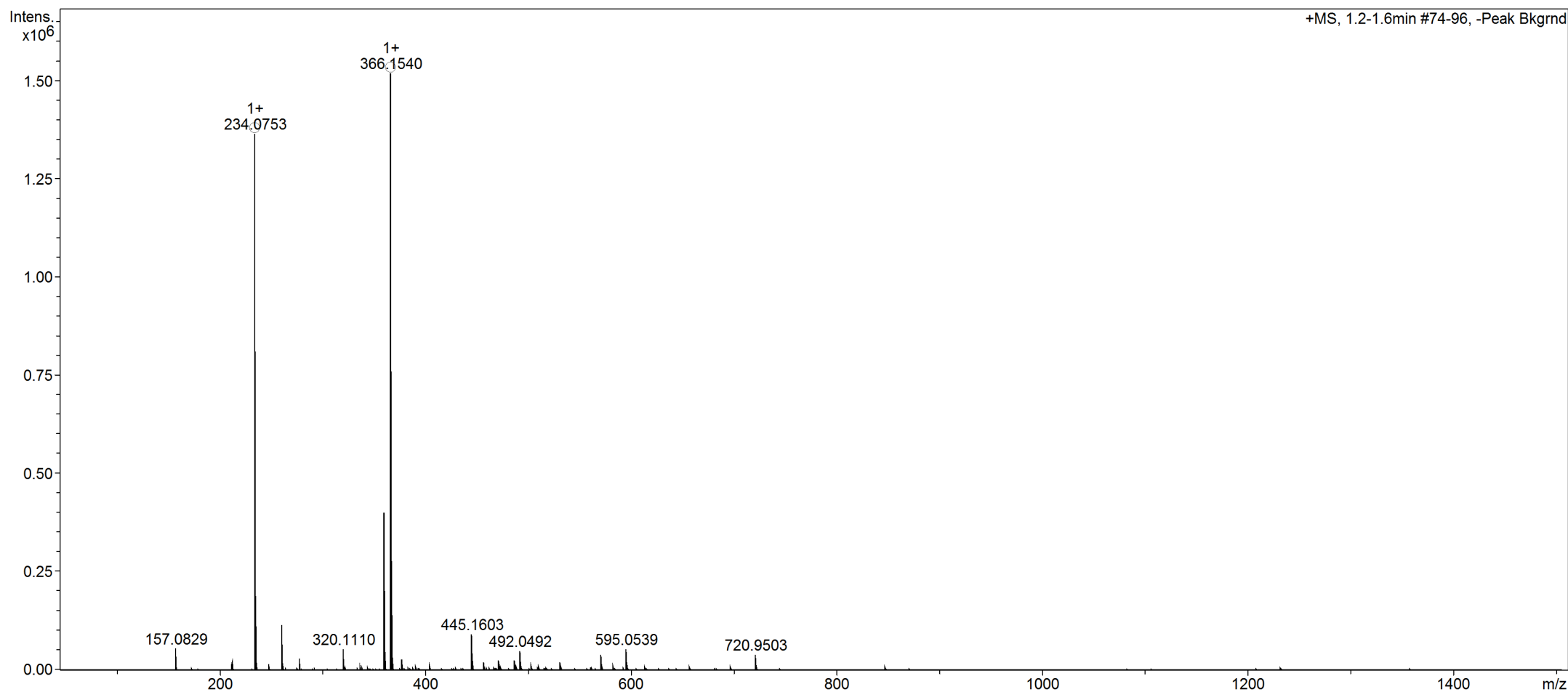
Malcolm Halcrow

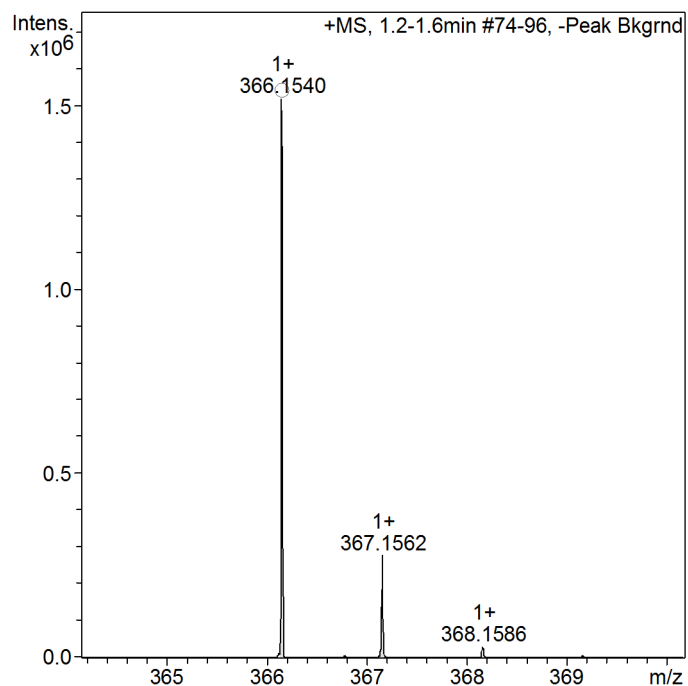
Acquisition Date

15/11/2018 14:59:59

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
234.075307	C12H12NO4	1+	234.076084	0.8	3.3	5.6	100.00	C12H11NO4	M+H
	C12H12NO4	1+	234.076084	0.8	3.3	5.6	100.00	C12H8O4	M+NH4
	C11H9N5Na	1+	234.075016	-0.3	-1.2	0.9	100.00	C11H9N5	M+Na
	C8H13KN5O	1+	234.075168	-0.1	-0.6	39.5	100.00	C8H13N5O	M+K
366.153953	C15H16N11O	1+	366.153381	-0.6	-1.6	12.7	100.00	C15H15N11O	M+H
	C18H24NO7	1+	366.154729	0.8	2.1	14.7	86.82	C18H23NO7	M+H
	C15H16N11O	1+	366.153381	-0.6	-1.6	12.7	100.00	C15H12N10O	M+NH4
	C18H24NO7	1+	366.154729	0.8	2.1	14.7	86.82	C18H20O7	M+NH4
	C17H21N5NaO3	1+	366.153660	-0.3	-0.8	13.8	100.00	C17H21N5O3	M+Na
	C15H21KN9	1+	366.155150	1.2	3.3	36.8	60.36	C15H21N9	M+K
	C14H25KN5O4	1+	366.153812	-0.1	-0.4	38.1	100.00	C14H25N5O4	M+K
	C20H22N3Na2O	1+	366.155277	1.3	3.6	27.8	100.00	C20H23N3O	M+Na2-H

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