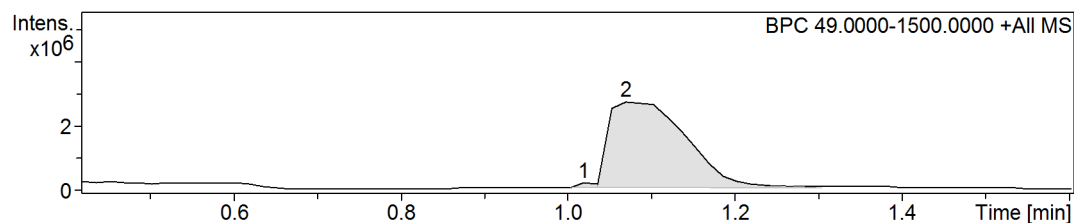


School of Chemistry Mass Spectrometry Service

SampleID 4-318
Sample Description
Analysis Name D:\Data\michaelehardie\cmhdj\4-318_187944_BA2_01_29099.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

Submitter HAYDER ARKAWAZI

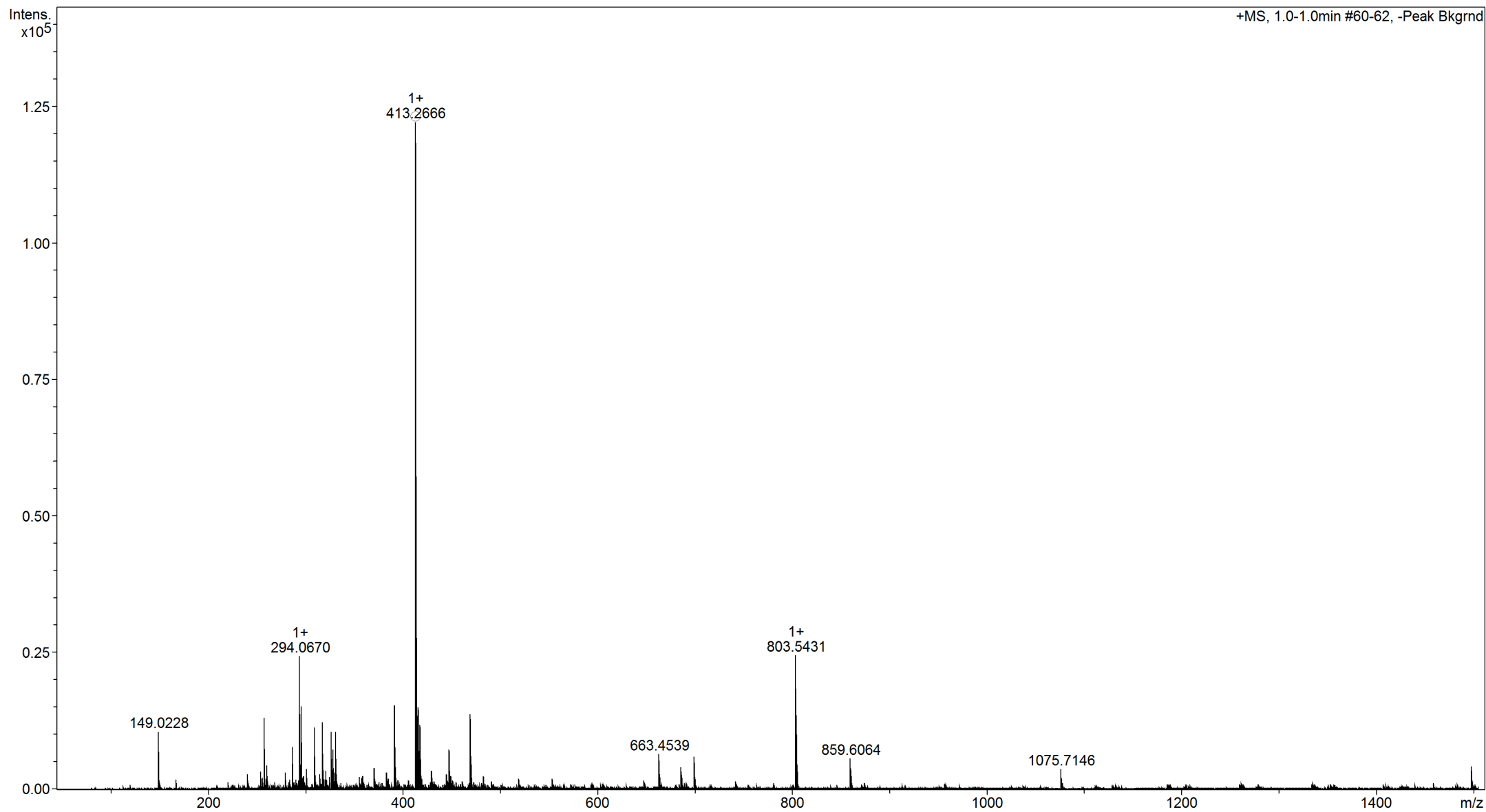
Supervisor Michael Hardie
Acquisition Date 16/12/2016 15:00:42
Scan Begin 50 m/z **Scan End** 1500 m/z

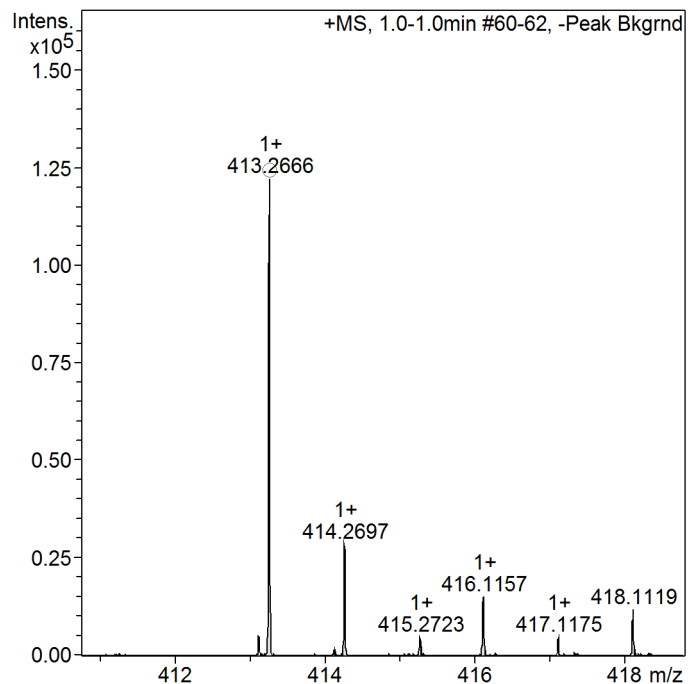


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.0 min	1.02	1.2	no uv	
Cmpd 2, 1.1 min	1.07	98.8	no uv	

Cmpd 1, 1.0 min





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

Cmpd 1, 1.0 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
413.266612	C22H33N6O2	1+	413.265951	-0.7	-1.6	15.3	100.00	C22 H32 N6 O2	M+H
	C22H33N6O2	1+	413.265951	-0.7	-1.6	15.3	100.00	C22 H29 N5 O2	M+NH4
	C24H38NaO4	1+	413.266230	0.4	0.9	15.9	100.00	C24 H38 O4	M+Na
	C25H34N4Na	1+	413.267568	-1.0	-2.3	27.5	57.78	C25 H34 N4	M+Na
	C10H30N16NaO	1+	413.268070	1.5	3.5	39.0	23.90	C10 H30 N16 O	M+Na
	C21H42KO5	1+	413.266383	-0.2	-0.6	36.5	100.00	C21 H42 O5	M+K
	C22H38KN4O	1+	413.267720	1.1	2.7	37.3	62.54	C22 H38 N4 O	M+K
	C23H35N4Na2	1+	413.265162	-1.5	-3.5	19.5	100.00	C23 H36 N4	M+Na2-H
	C24H38NaO4	1+	413.266230	0.4	0.9	15.9	100.00	C12 H19 O2	2M+Na

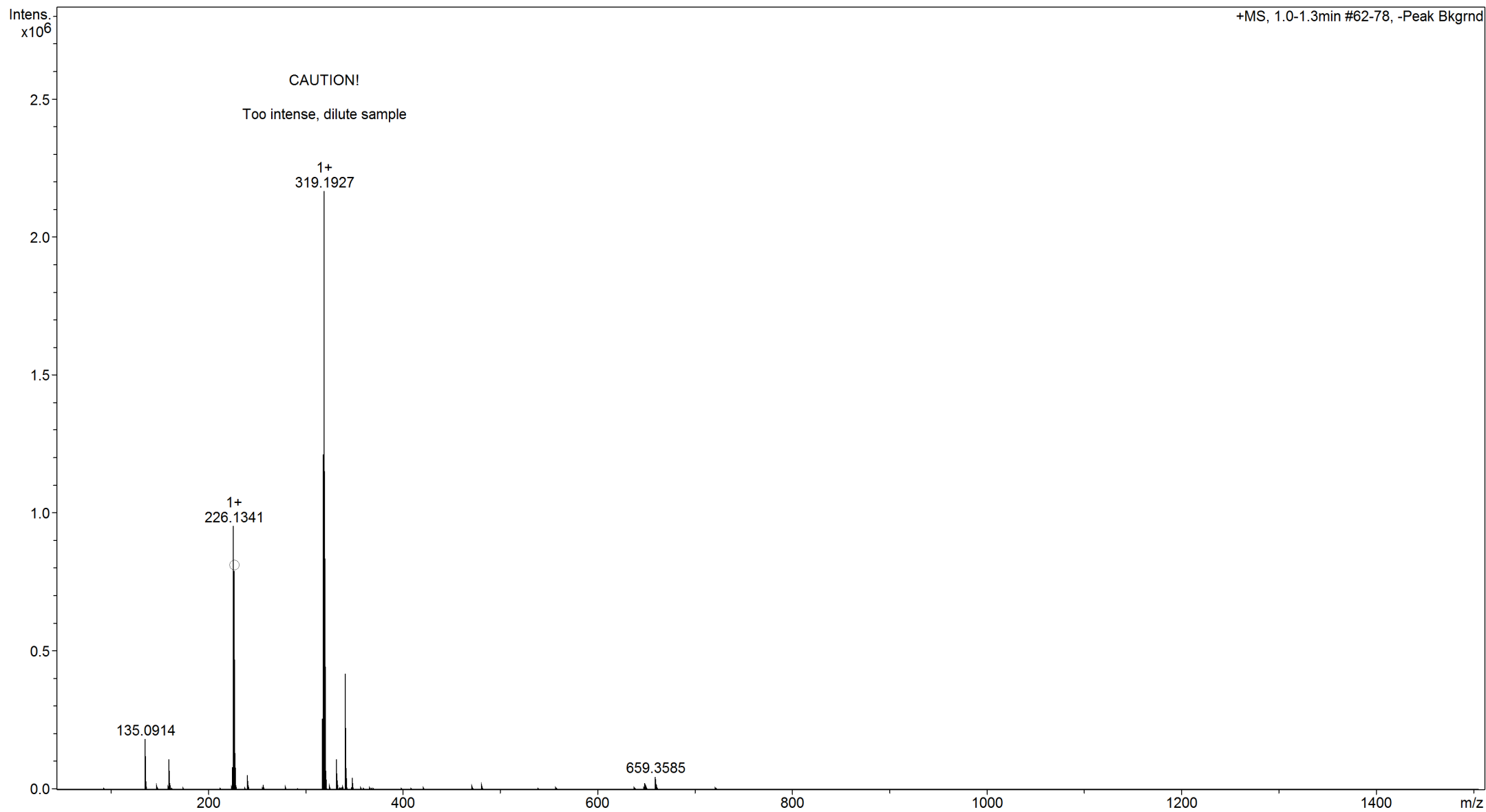
Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;

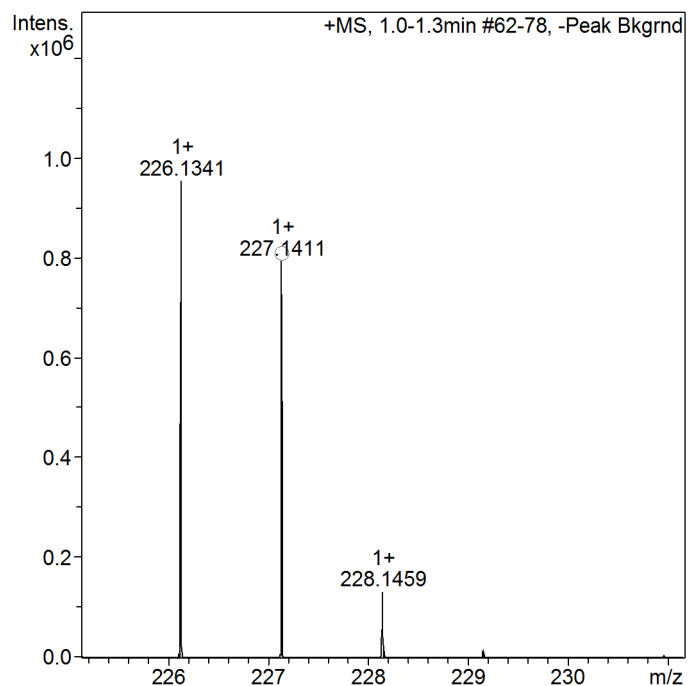
Smart Formula Search Parameters
CHNO and adducts considered
implicitly

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

Cmpd 2, 1.1 min





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

Cmpd 2, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
227.141054	C14H20NaO	1+	227.140636	0.4	1.8	6.7	100.00	C14 H19 Na O	M+H
	C14H20NaO	1+	227.140636	0.4	1.8	6.7	100.00	C14 H20 Na O	M+NH4
	C14H20NaO	1+	227.140636	0.4	1.8	6.7	100.00	C14 H20 O	M+Na

Smart Formula Parameter	Value
Expected Formula	
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