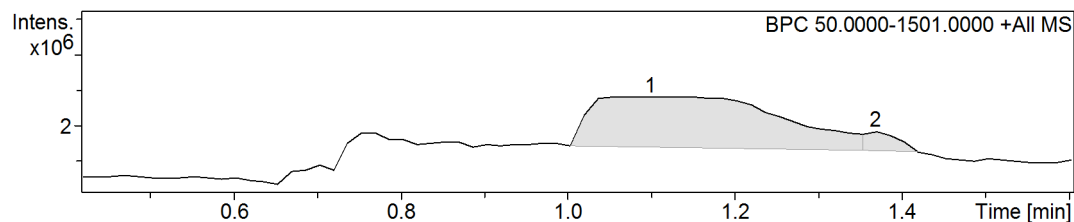


School of Chemistry Mass Spectrometry Service

SampleID RW3B(4)
Sample Description
Analysis Name D:\Data\malcolmhalcrow\cm18rw\RW3B(4)_347289_GC5_01_84570.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

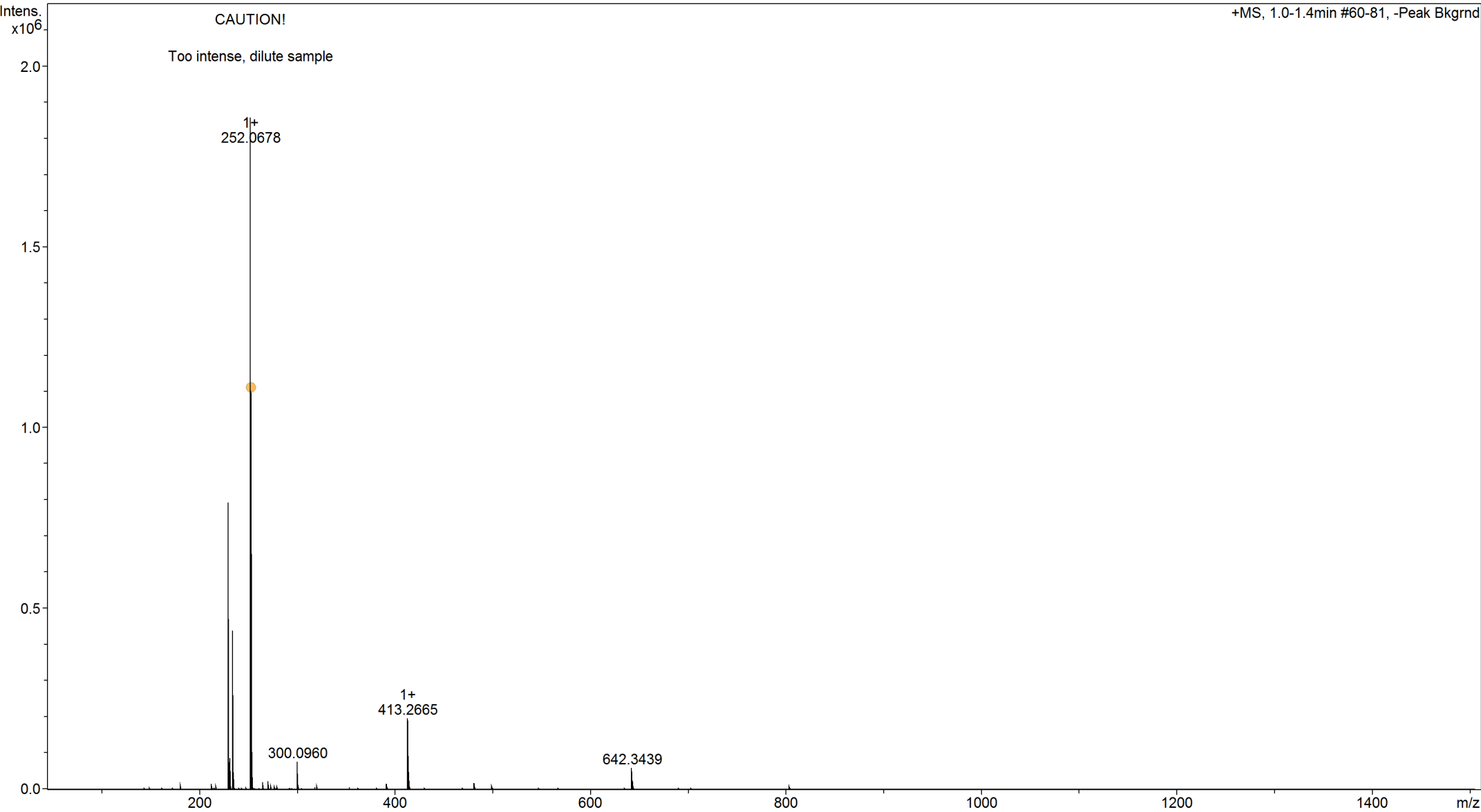
Submitter Rhiannon Watson
Supervisor Malcolm Halcrow
Acquisition Date 16/03/2022 11:22:15
Scan Begin 50 m/z **Scan End** 1500 m/z

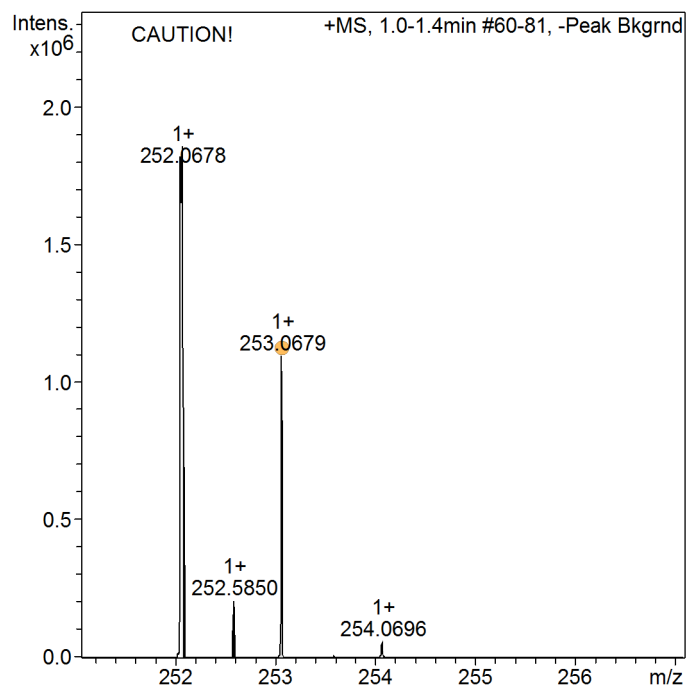


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.1 min	1.10	94.1	no uv	
Cmpd 2, 1.4 min	1.37	5.9	no uv	

Cmpd 1, 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 1, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
253.067908	C8H9N6O4	1+	253.067979	0.1	0.3	34.3	100.00	C8H8N6O4	M+H
	C8H9N6O4	1+	253.067979	0.1	0.3	34.3	100.00	C8H5N5O4	M+NH4
	C7H6N10Na	1+	253.066911	-1.0	-3.9	34.7	73.10	C7H6N10	M+Na
	C10H14NaO6	1+	253.068259	0.4	1.4	35.4	100.00	C10H14O6	M+Na
	C9H11N4Na2O2	1+	253.067191	-0.7	-2.8	35.6	100.00	C9H12N4O2	M+Na2-H
	C10H14NaO6	1+	253.068259	0.4	1.4	35.4	100.00	C5H7O3	2M+Na

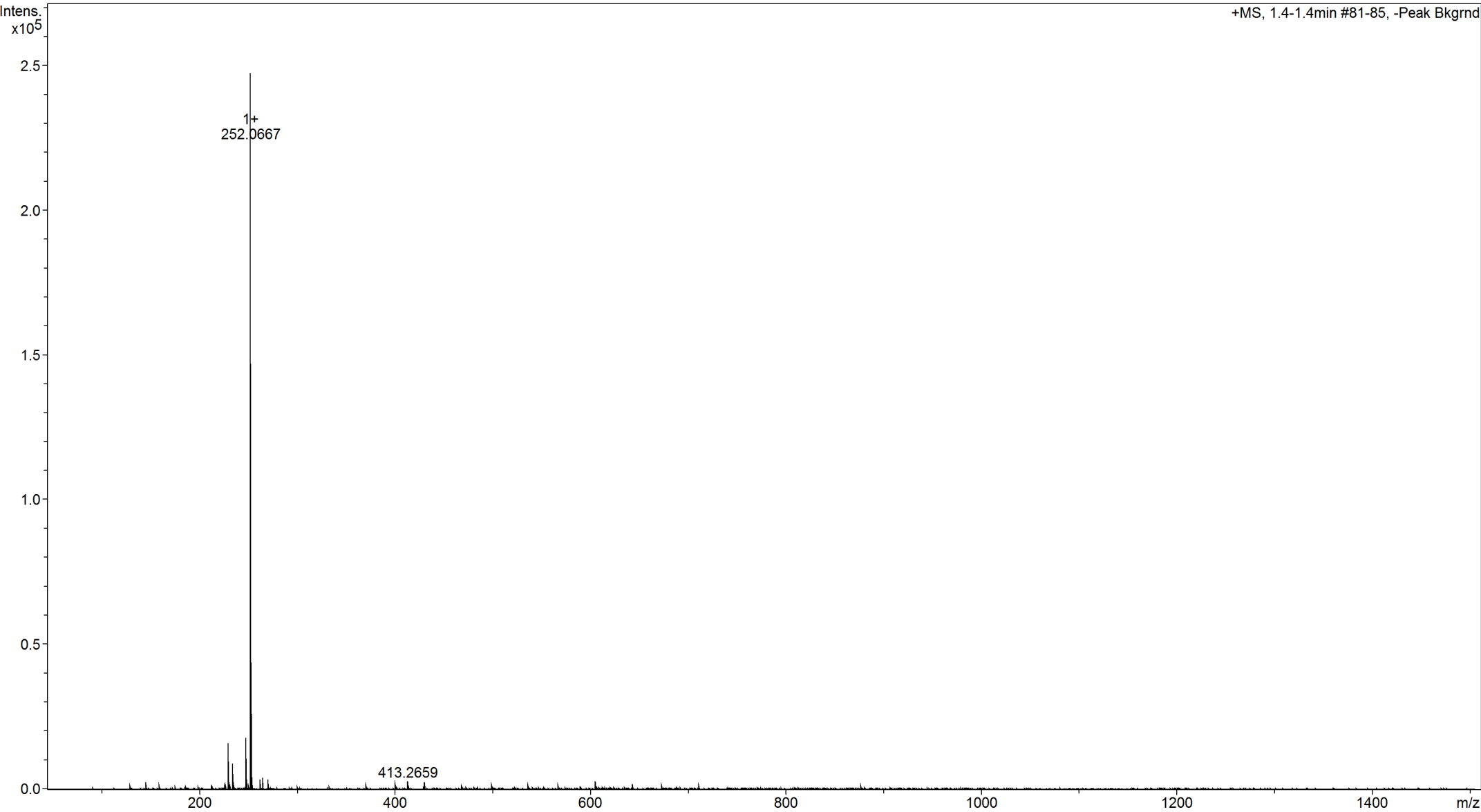
Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	

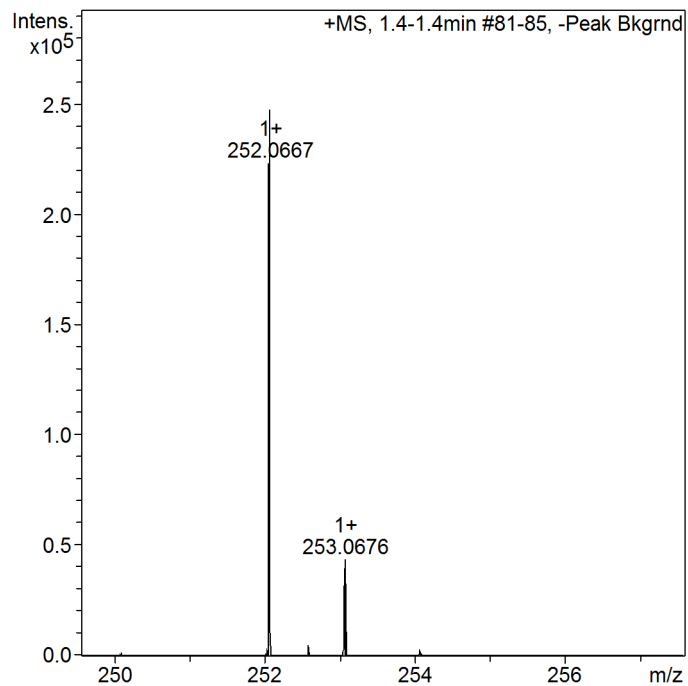
Smart Formula Search Parameters
CHNO and adducts considered implicitly

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

Cmpd 2, 1.4 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, 1.4 min

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