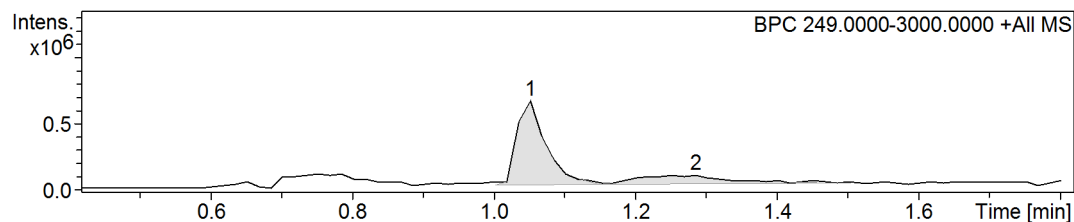


School of Chemistry Mass Spectrometry Service

SampleID S01-180 Ligand
Sample Description
Analysis Name D:\Data\michaelehardie\cmso\S01-180 Ligand_145656_BE8_01_16198.d
Method 3c_AccMass_Loop_High_Pos.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

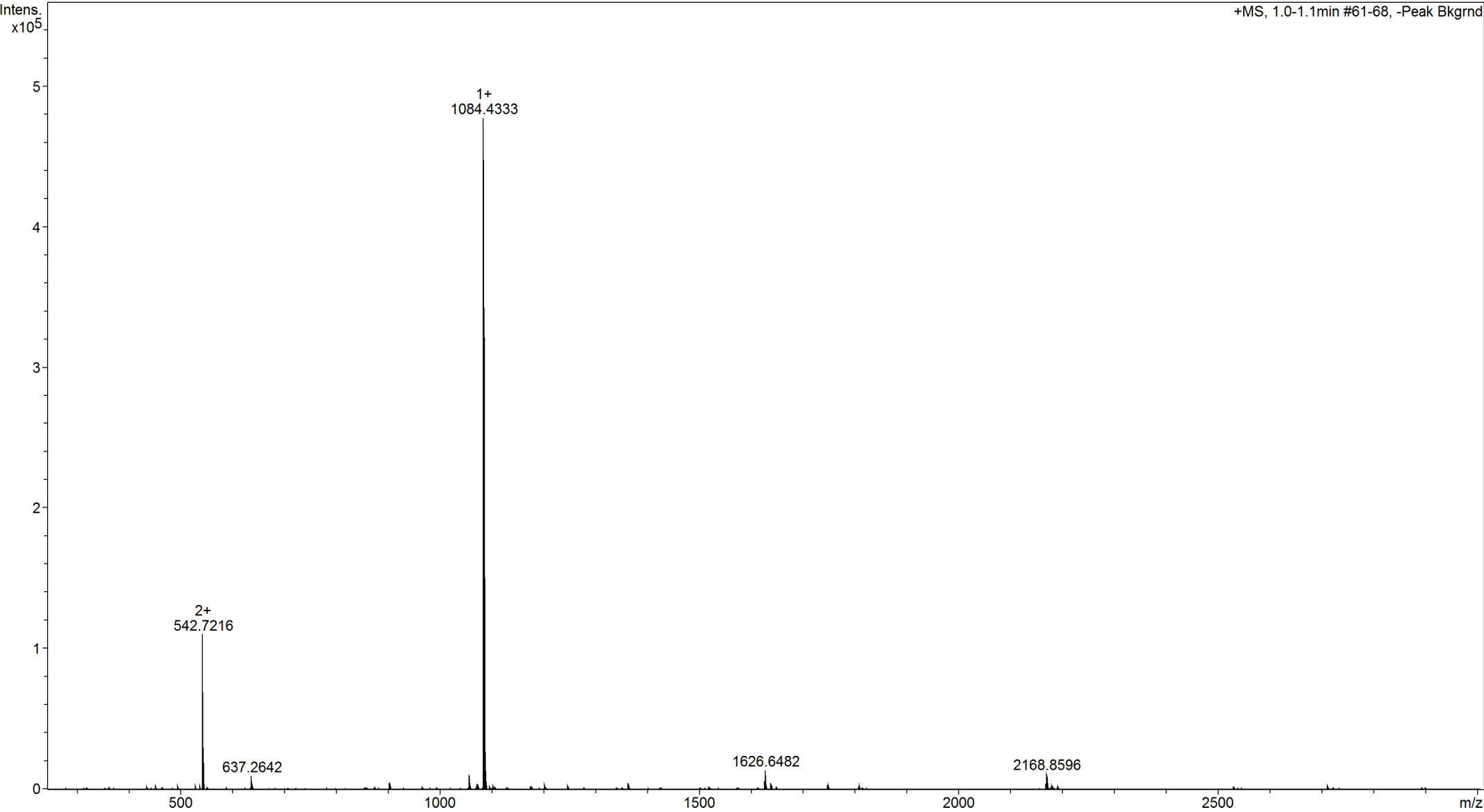
Submitter Sam Oldknow
Supervisor Michael Hardie
Acquisition Date 26/10/2015 12:33:33
Scan Begin 250 m/z **Scan End** 3000 m/z

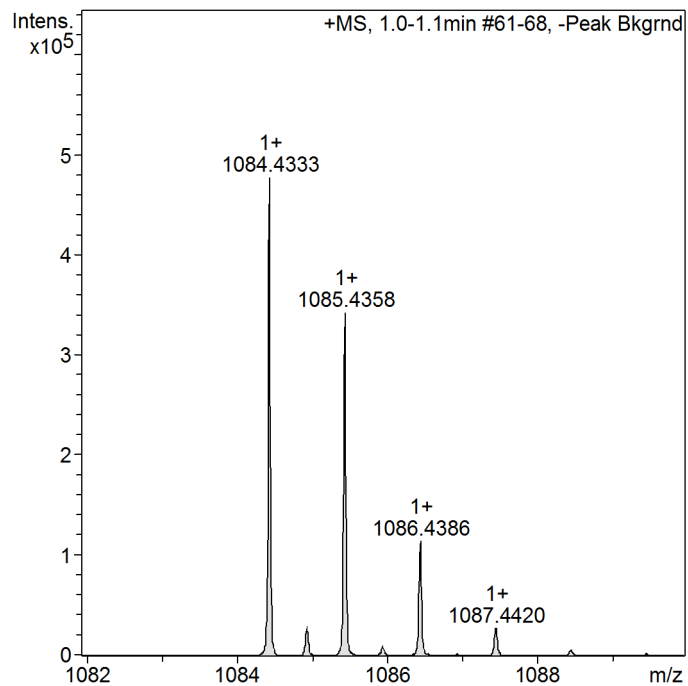


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.1 min	1.05	74.7	no uv	
Cmpd 2, 1.3 min	1.29	25.3	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

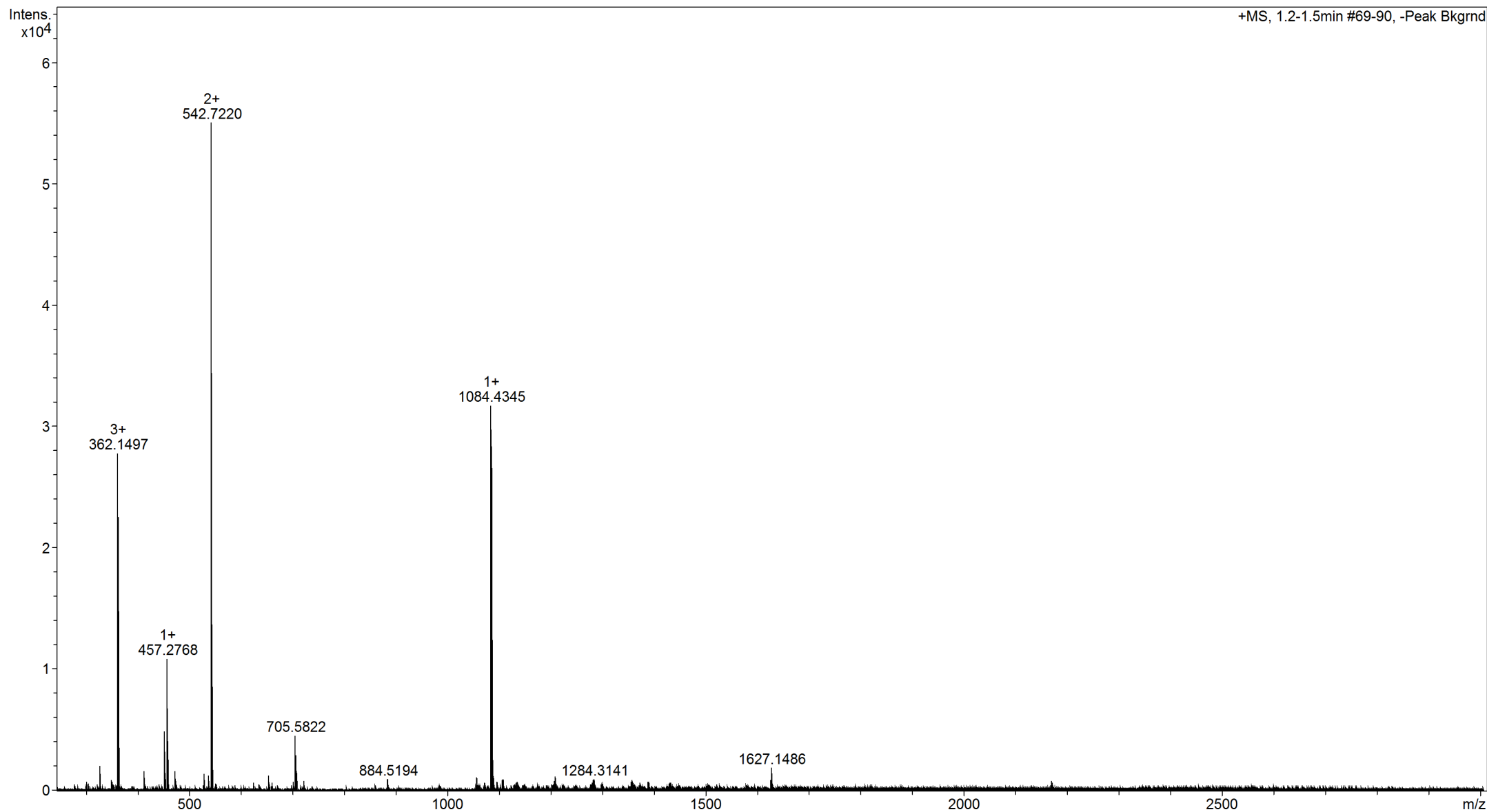
Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M;;M+H;;M+NH4;;M+Na;;M+K;;M+Na2-H;;2M+H;;2M+Na;

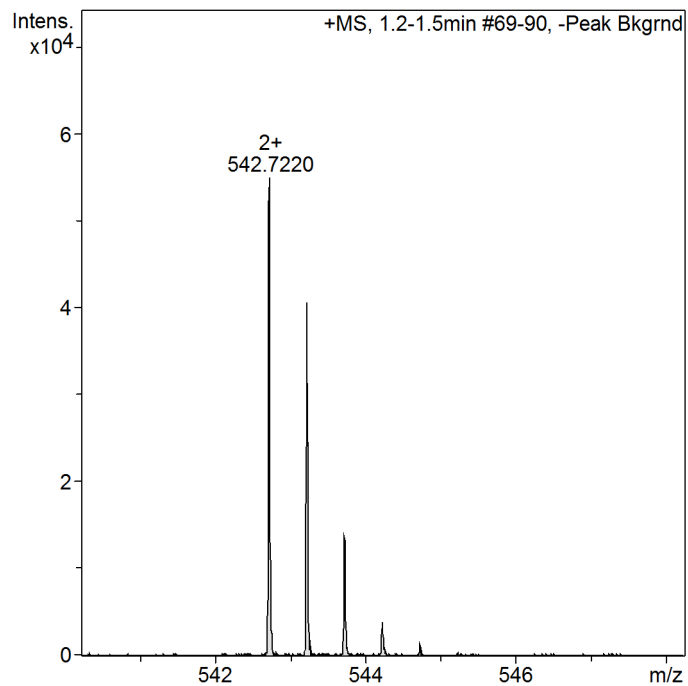
Smart Formula Search Parameters
CHNO and adducts considered implicitly

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, 1.3 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, 1.3 min

Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M;;M+H;;M+NH4;;M+Na;;M+K;;M+Na2-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