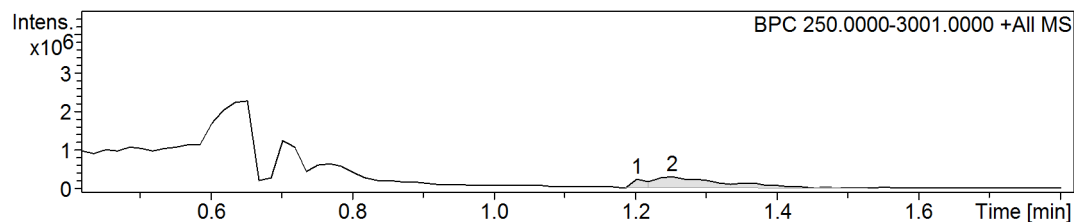


# School of Chemistry Mass Spectrometry Service

**SampleID** S02-226 POWDER  
**Sample Description**  
**Analysis Name** D:\Data\michaelehardie\cmso\S02-226 POWDER\_156629\_GD8\_01\_19245.d  
**Method** 3c\_AccMass\_Loop\_High\_Pos.m  
**Instrument** maXis impact **Source Type** ESI **Ion Polarity** Positive

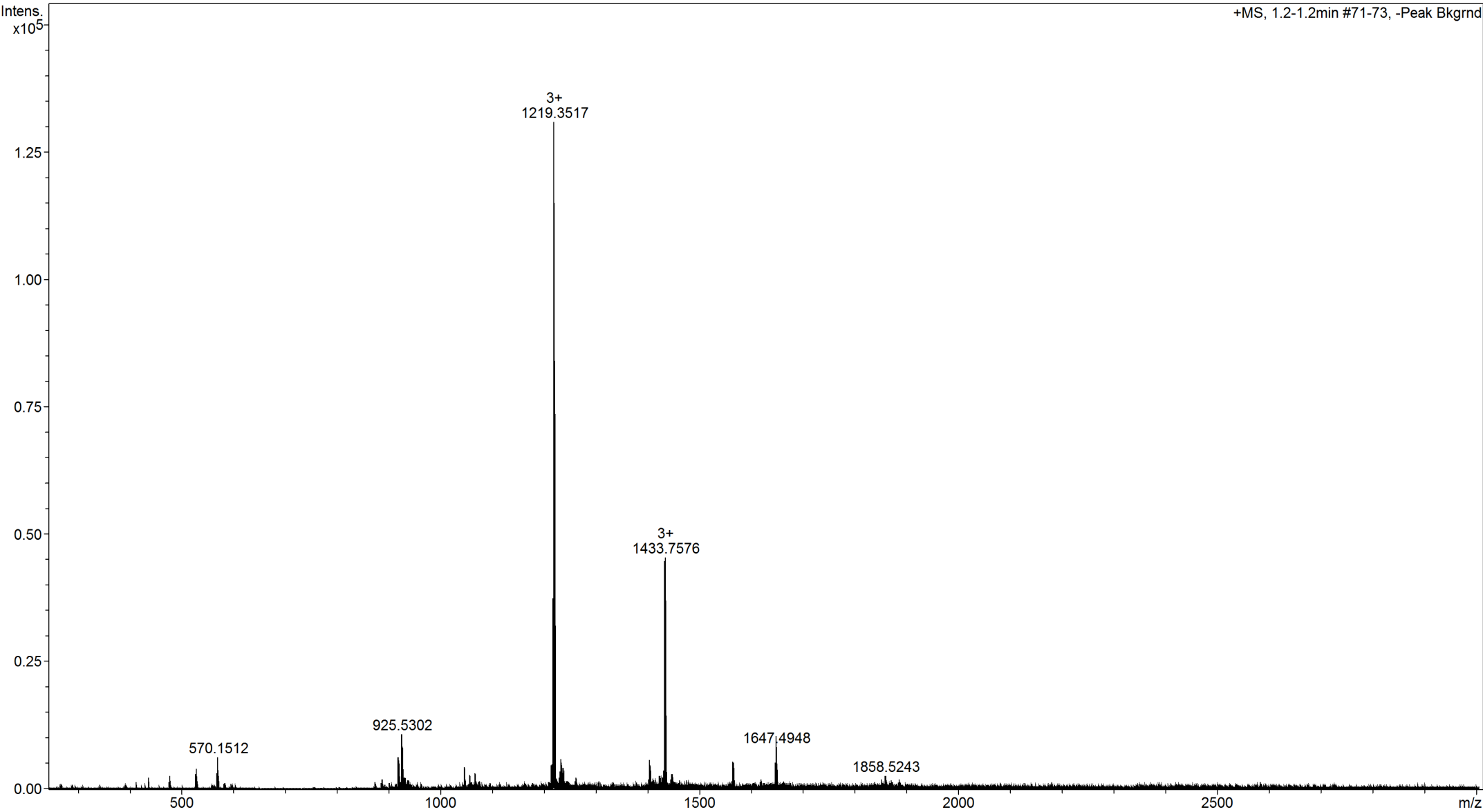
**Submitter** Sam Oldknow  
**Supervisor** Michael Hardie  
**Acquisition Date** 16/02/2016 13:48:24  
**Scan Begin** 250 m/z **Scan End** 3000 m/z

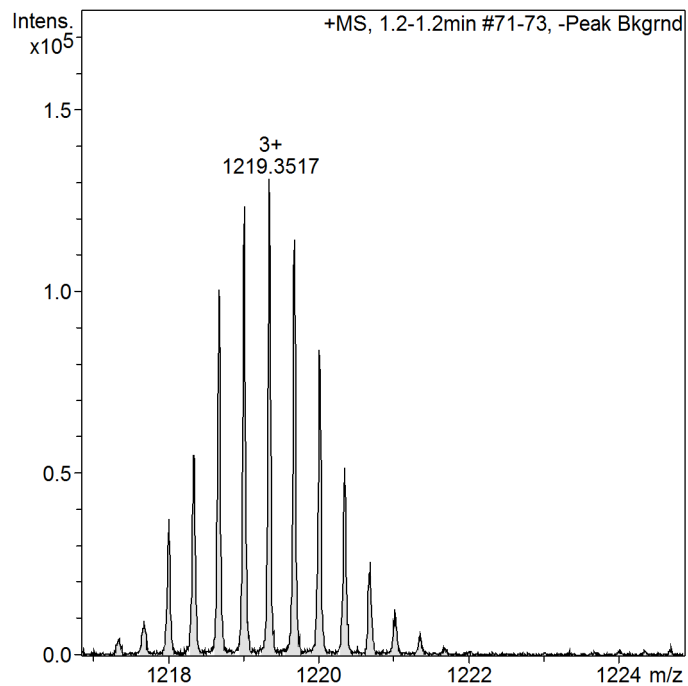


## Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.2 min	1.20	13.4	no uv	
Cmpd 2, 1.3 min	1.25	86.6	no uv	

Cmpd 1, 1.2 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, 1.2 min

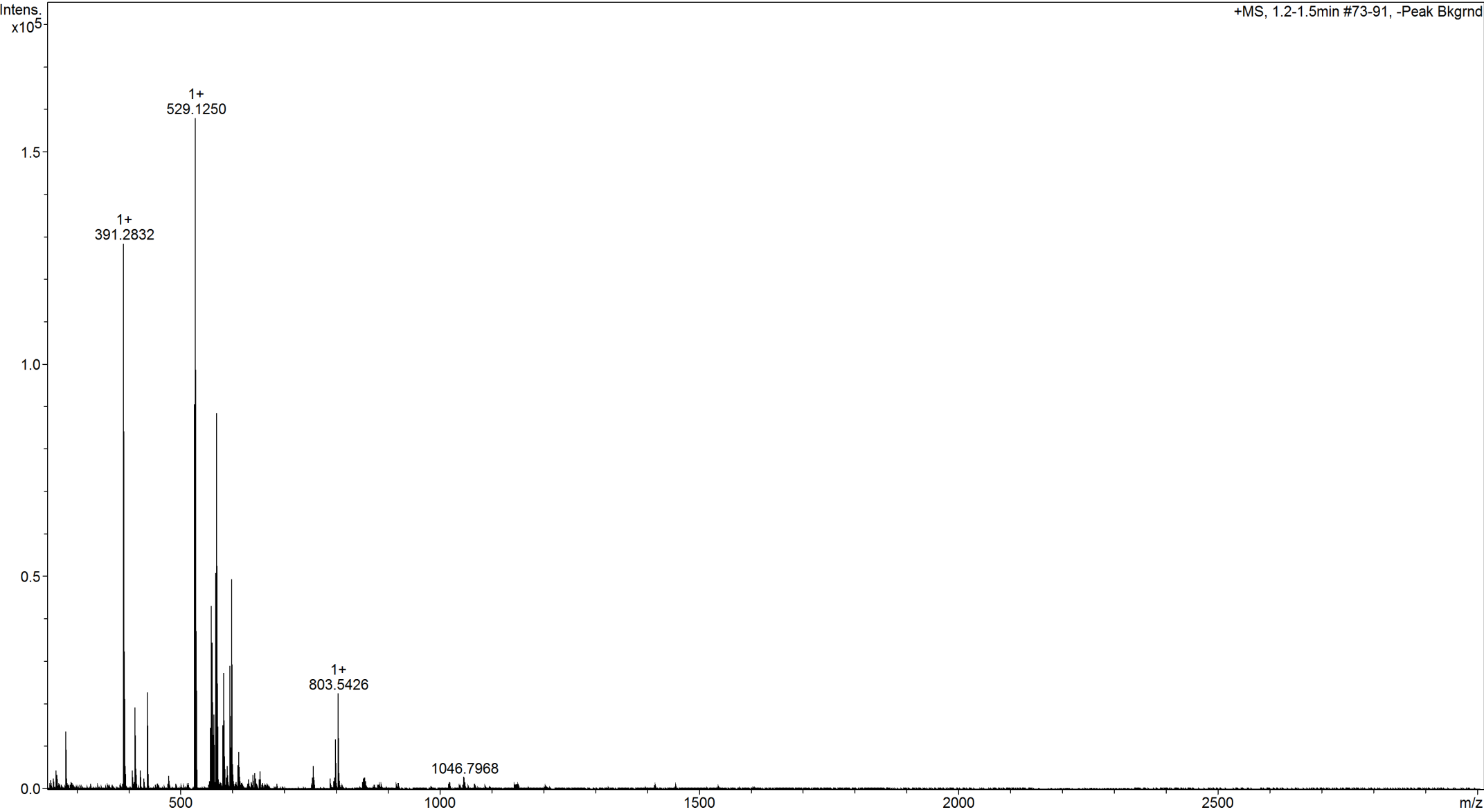
Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M;;M+H;;M+NH4;;M+Na;;M+K;;M+Na2-H;;2M+H;;2M+Na;

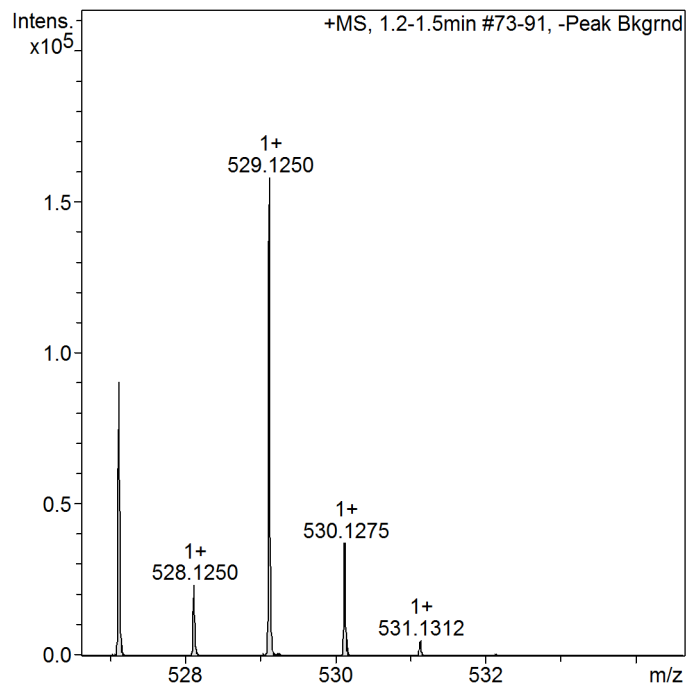
Smart Formula Search Parameters  
CHNO and adducts considered implicitly

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