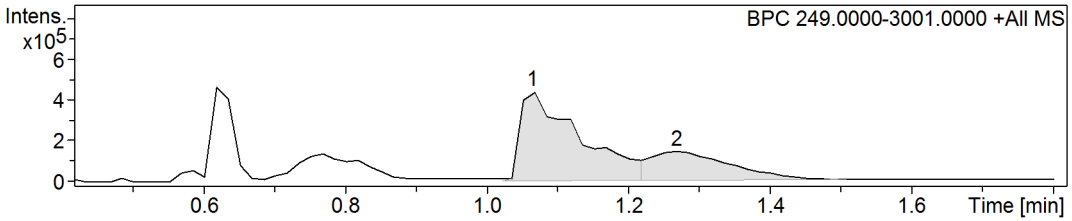
School of Chemistry Mass Spectrometry Service

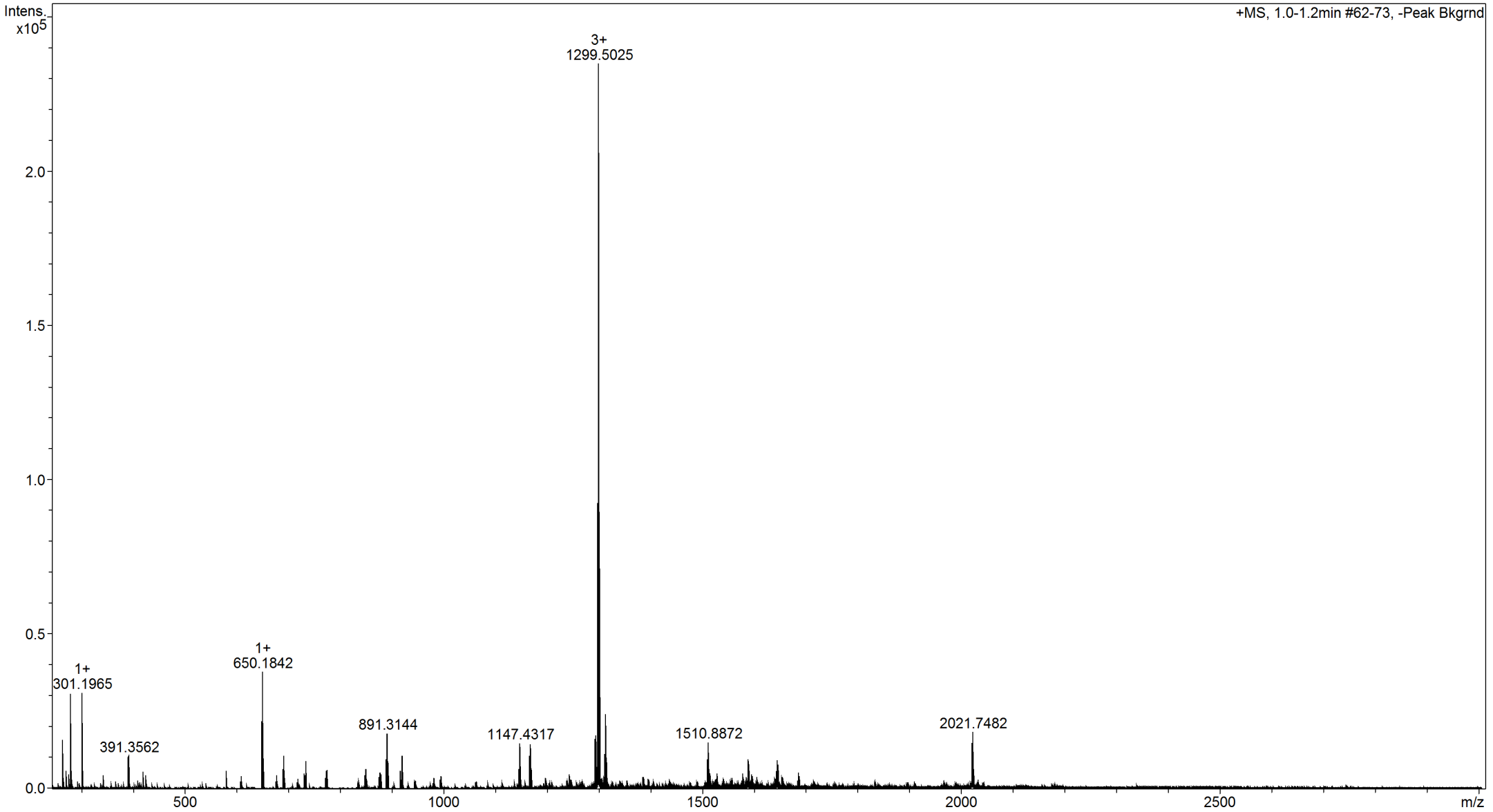
SampleID	S03-369			**Submitter**	Sam Oldknow
Sample Description					
Analysis Name	D:\Data\michaelehardie\cmso\S03-369_201747_BE4_01_32675.d			**Supervisor**	Michaele Hardie
Method	3c_AccMass_Loop_High_Pos.m			**Acquisition Date**	20/04/2017 11:10:54
Instrument	maXis impact	**Source Type**	ESI	**Ion Polarity**	Positive
Scan Begin	250 m/z	**Scan End**	3000 m/z		

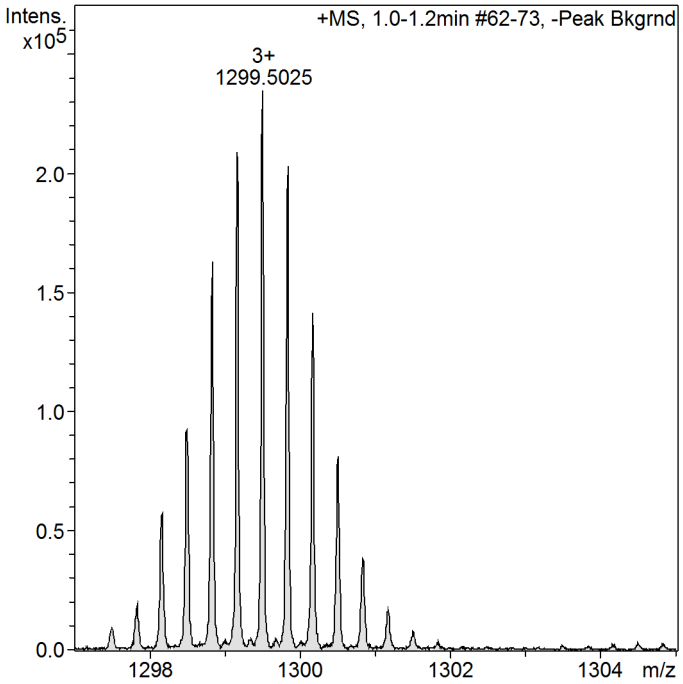


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.1 min	1.06	69.2	no uv	
Cmpd 2, 1.3 min	1.27	30.8	no uv	

Cmpd 1, 1.1 min


Intens.
x10^5
+MS, 1.0-1.2min #62-73, -Peak Bkgrnd
3+
1299.5025
2.0
1.5
1.0
0.5
0.0
1+
301.1965
391.3562
1+
650.1842
891.3144
1147.4317
1510.8872
2021.7482
500
1000
1500
2000
2500
m/z



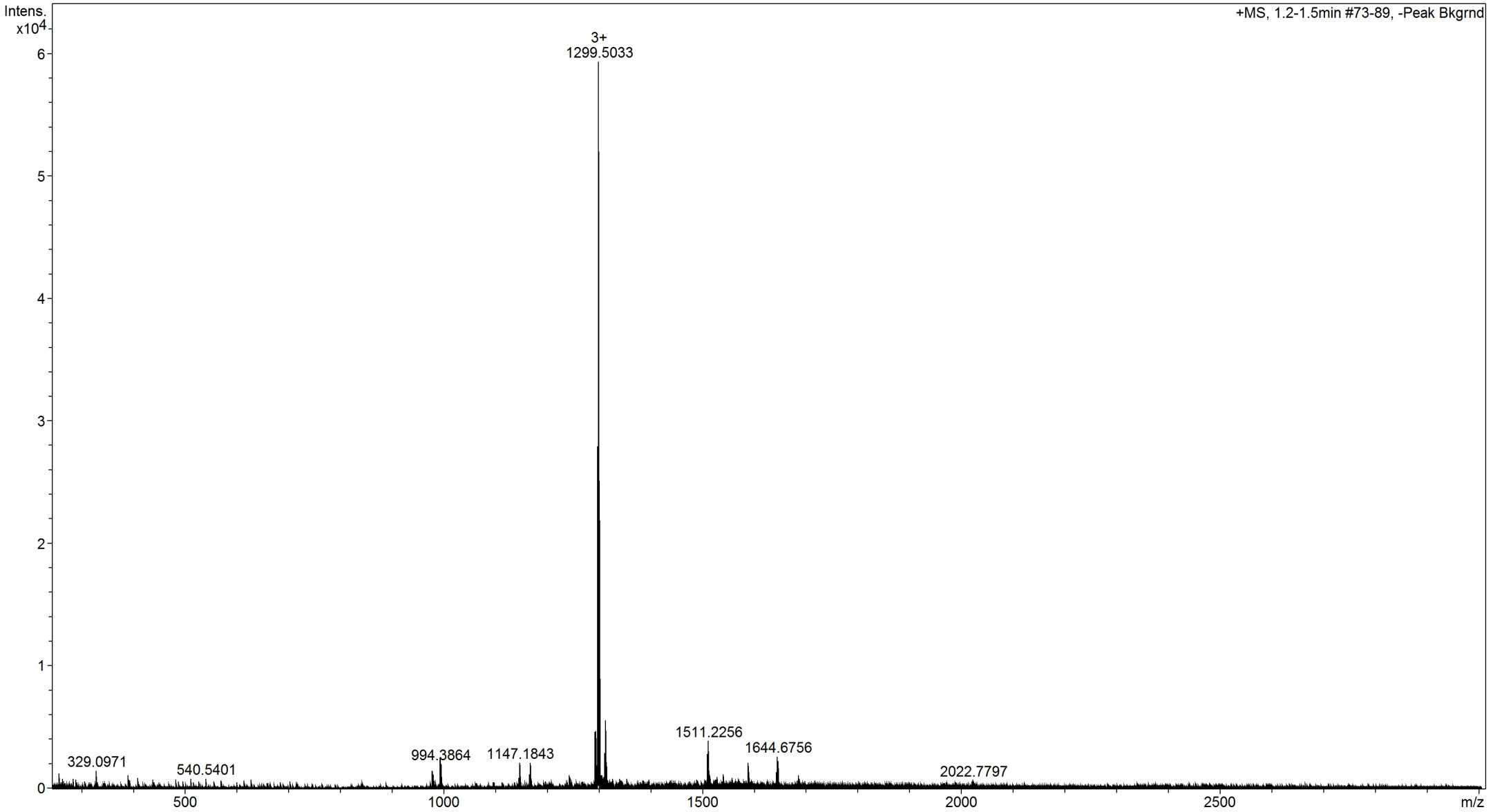
Confirm/Find Formula Results

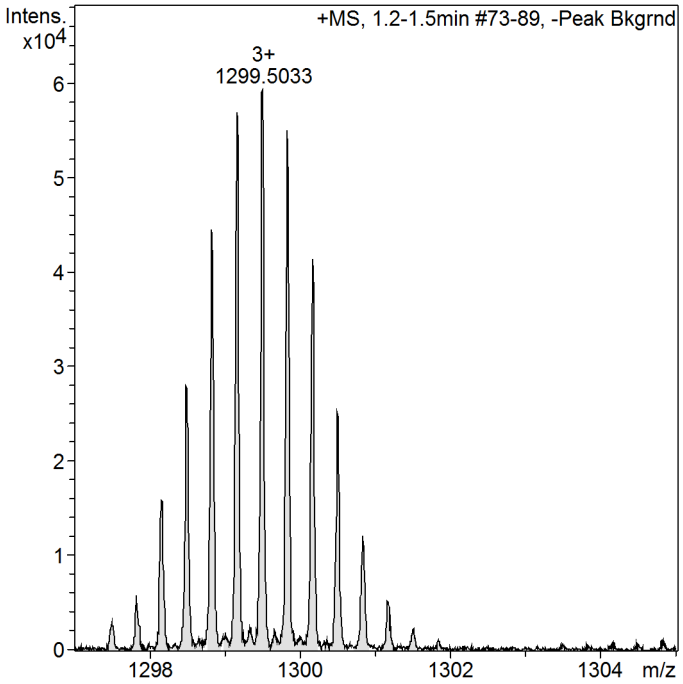
The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Cmpd 1, 1.1 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

Cmpd 2, 1.3 min


Intens.
x10^4
+MS, 1.2-1.5min #73-89, -Peak Bkgrnd
3+
1299.5033
329.0971
540.5401
994.3864
1147.1843
1511.2256
1644.6756
2022.7797
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

Cmpd 2, 1.3 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