

School of Chemistry Mass Spectrometry Service

SampleID SG076 tbtq dppb
Sample Description
Analysis Name D:\Data\malcolmhalcrow\cmsgr\SG076 tbtq dppb_170867_GD2_01_23916.d
Method 3c_AccMass_Loop_High_Pos.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

Submitter

Sam Greatorex

Supervisor

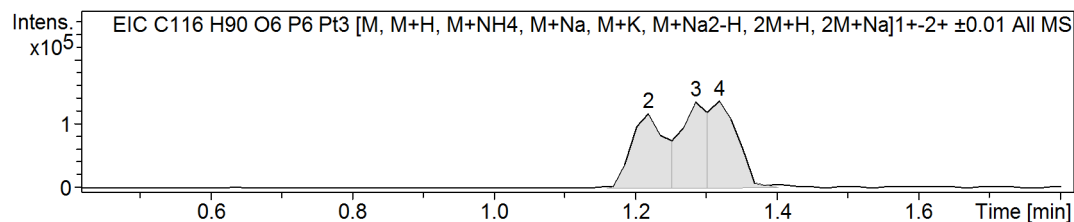
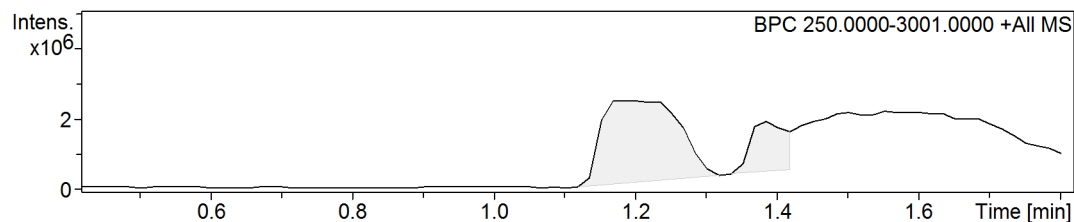
Malcolm Halcrow

Acquisition Date

23/06/2016 13:31:21

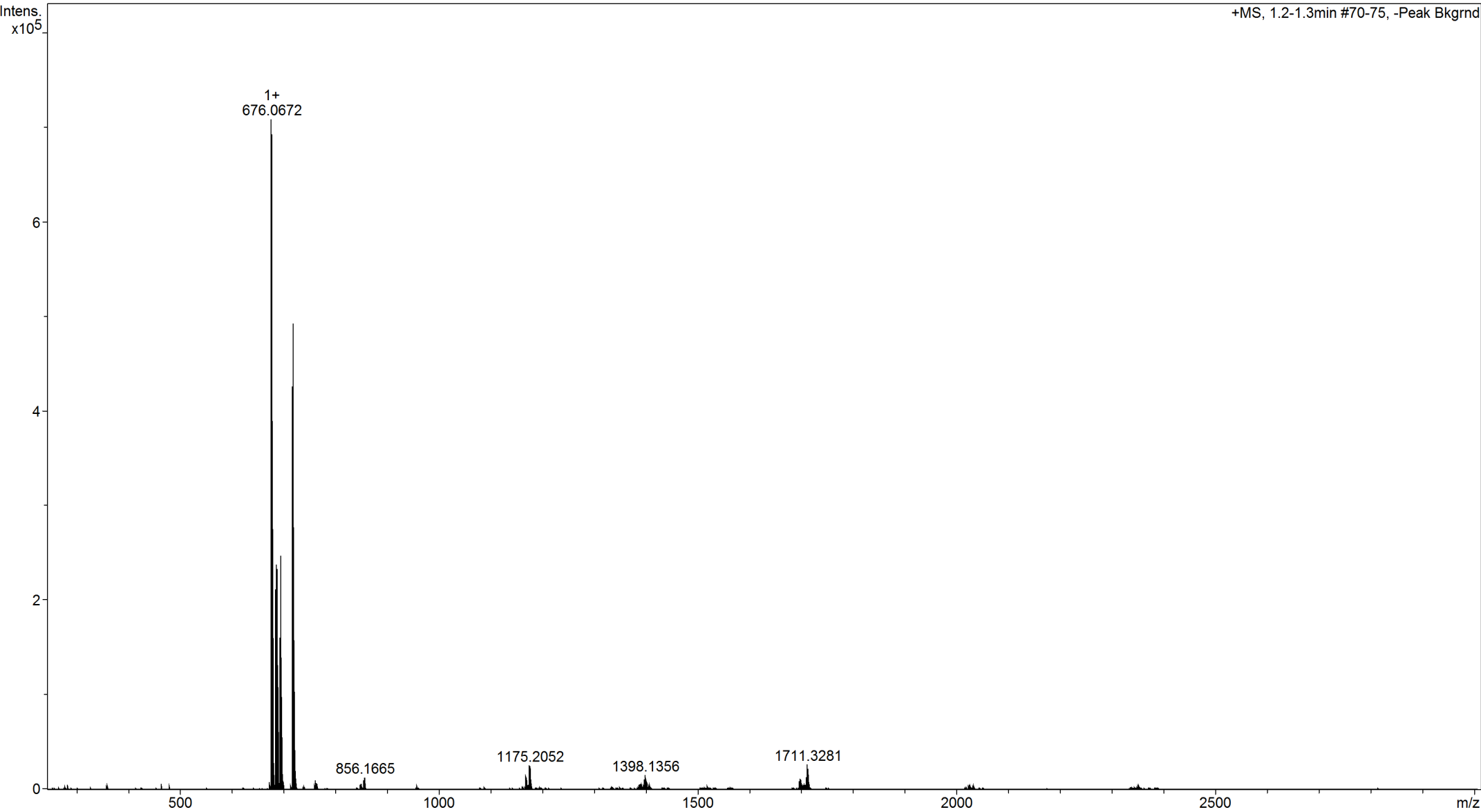
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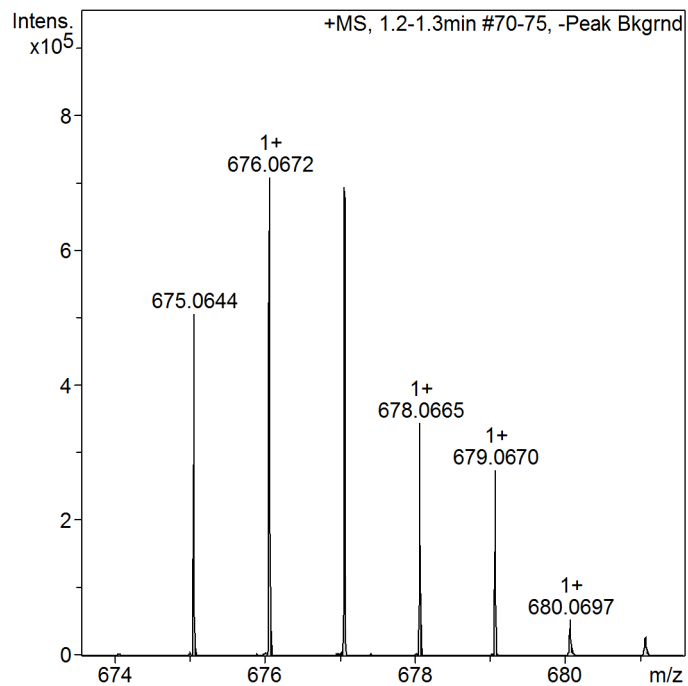
Scan End 3000 m/z



Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 2, 1.2 min	1.22	78.9	no uv	
Cmpd 3, 1.3 min	1.29	no peak	no uv	
Cmpd 4, 1.3 min	1.32	21.1	no uv	





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, 1.2 min

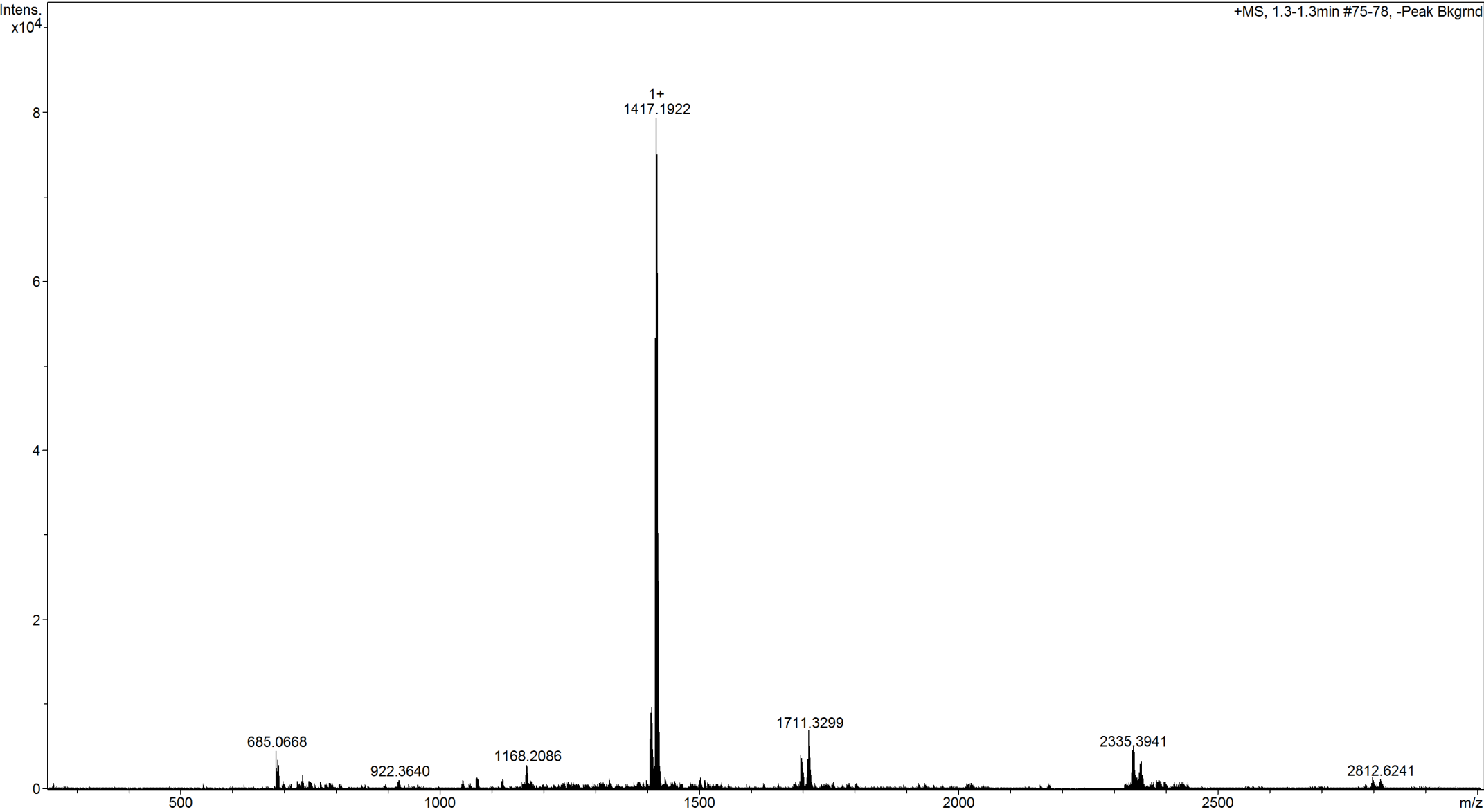
Smart Formula Parameter	Value
Expected Formula	C ₁₁₆ H ₉₀ O ₆ Pt ₃
Adducts Considered	;M;;M+H;;M+NH ₄ ;;M+Na;;M+K;;M+Na ₂ -H;;2M+H;;2M+Na;

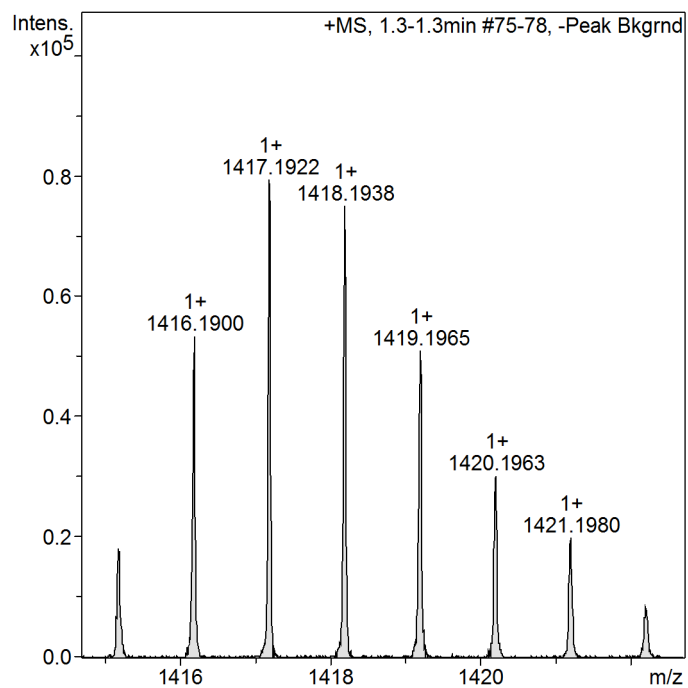
Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	
Formula Search Maximum	P 12 Pt 6

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	both
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80

Cmpd 3, 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 3, 1.3 min

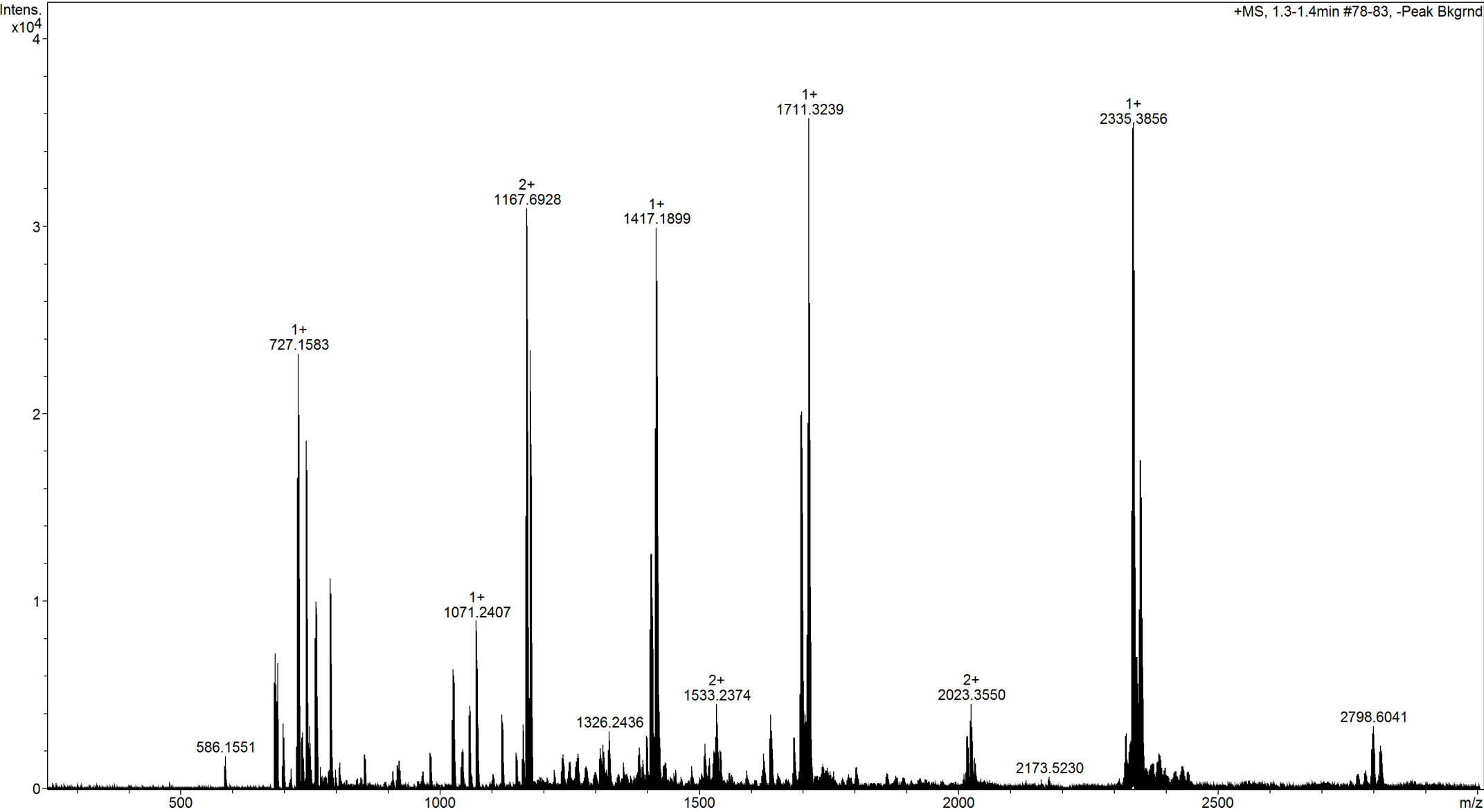
Smart Formula Parameter	Value
Expected Formula	C ₁₁₆ H ₉₀ O ₆ Pt ₃
Adducts Considered	;M;;M+H;;M+NH ₄ ;;M+Na;;M+K;;M+Na ₂ -H;;2M+H;;2M+Na;

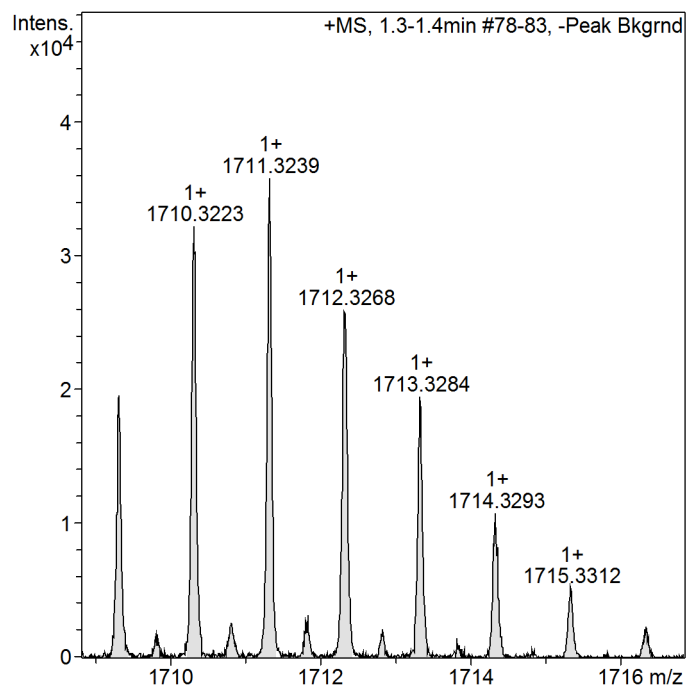
Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	
Formula Search Maximum	P 12 Pt 6

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	both
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80

Cmpd 4, 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 4, 1.3 min

Smart Formula Parameter	Value
Expected Formula	C ₁₁₆ H ₉₀ O ₆ Pt ₃
Adducts Considered	;M;;M+H;;M+NH ₄ ;;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	P 12 Pt 6

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	both
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80