

School of Chemistry Mass Spectrometry Service

SampleID FTG BA-hydra cage from NMR

Sample Description

Analysis Name D:\Data\michaelehardie\chmft\FTG BA-hydra cage from NMR_1717_GA8_01_24135.d

Method 3c_AccMass_Loop_High_Pos.m

Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

Submitter

Flora Thorp-Greenwood

Supervisor

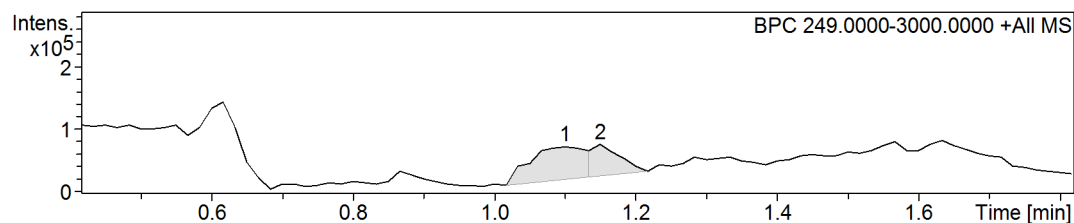
Michaele Hardie

Acquisition Date

01/07/2016 16:15:01

Scan Begin 250 m/z

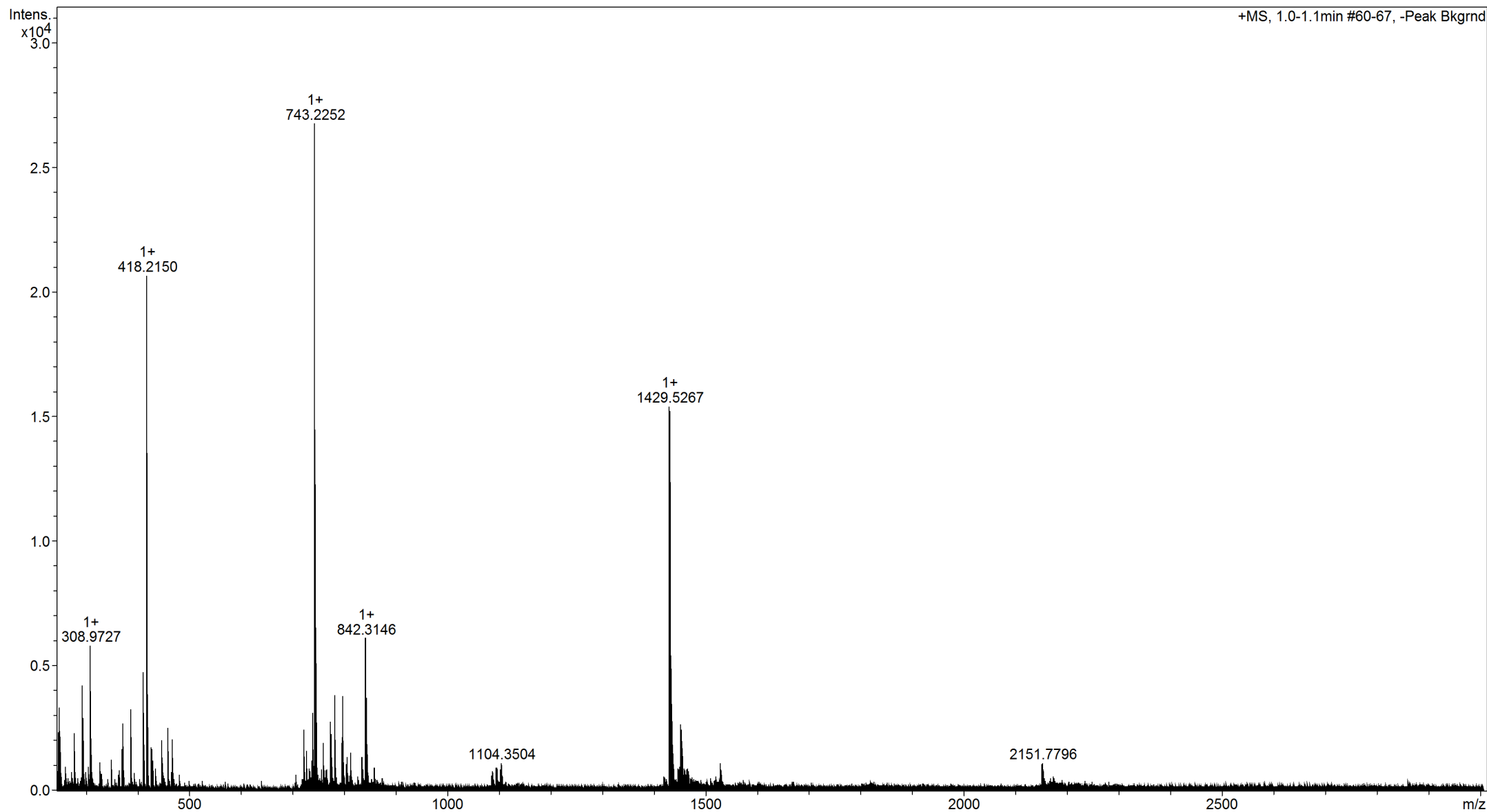
Scan End 3000 m/z

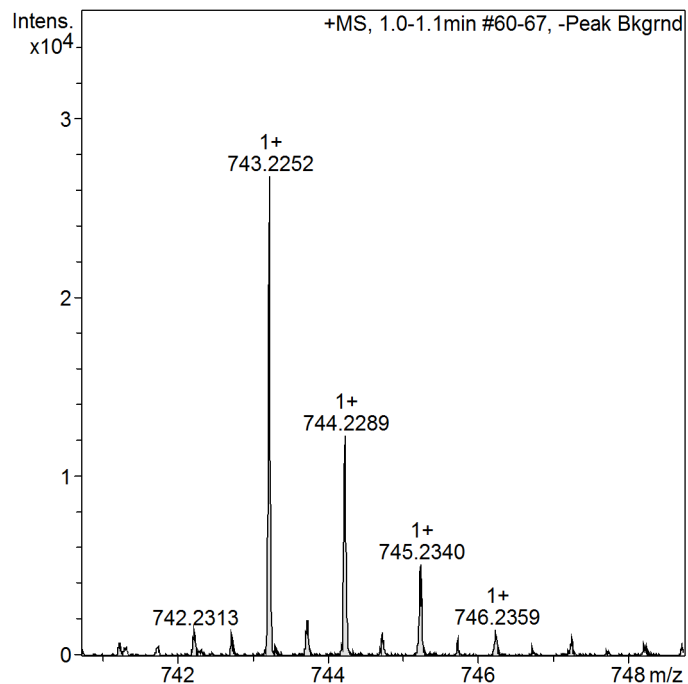


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.1 min	1.10	66.5	no uv	
Cmpd 2, 1.1 min	1.15	33.5	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

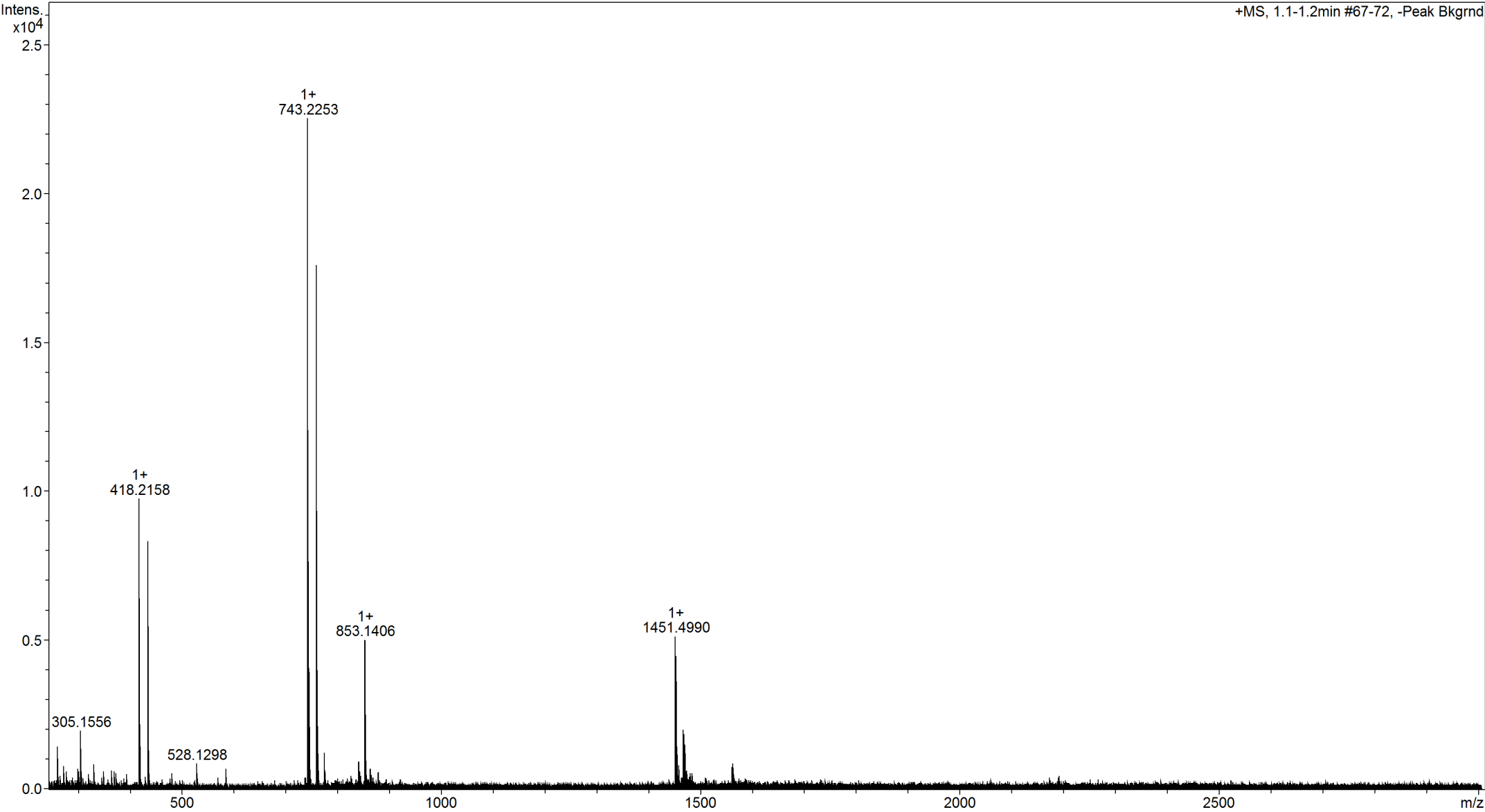
Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M;;M+H;;M+NH4;;M+Na;;M+K;;M+Na2-H;;2M+H;;2M+Na;

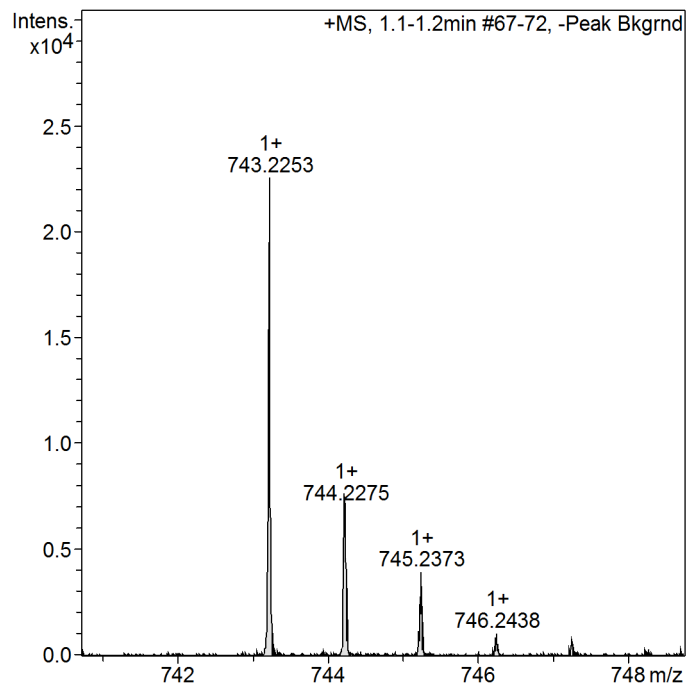
Smart Formula Search Parameters
CHNO and adducts considered implicitly

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, 1.1 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 2, 1.1 min

Smart Formula Parameter	Value
Expected Formula	
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

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