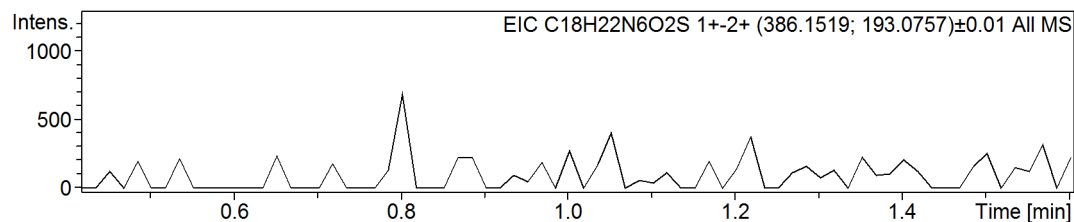
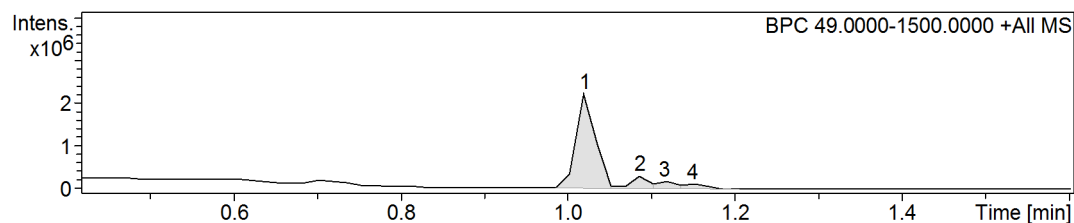


School of Chemistry Mass Spectrometry Service

SampleID SEN-F6
Sample Description
Analysis Name D:\Data\malcolmhalcrow\cmic\SEN-F6_240702_RA2_01_47486.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

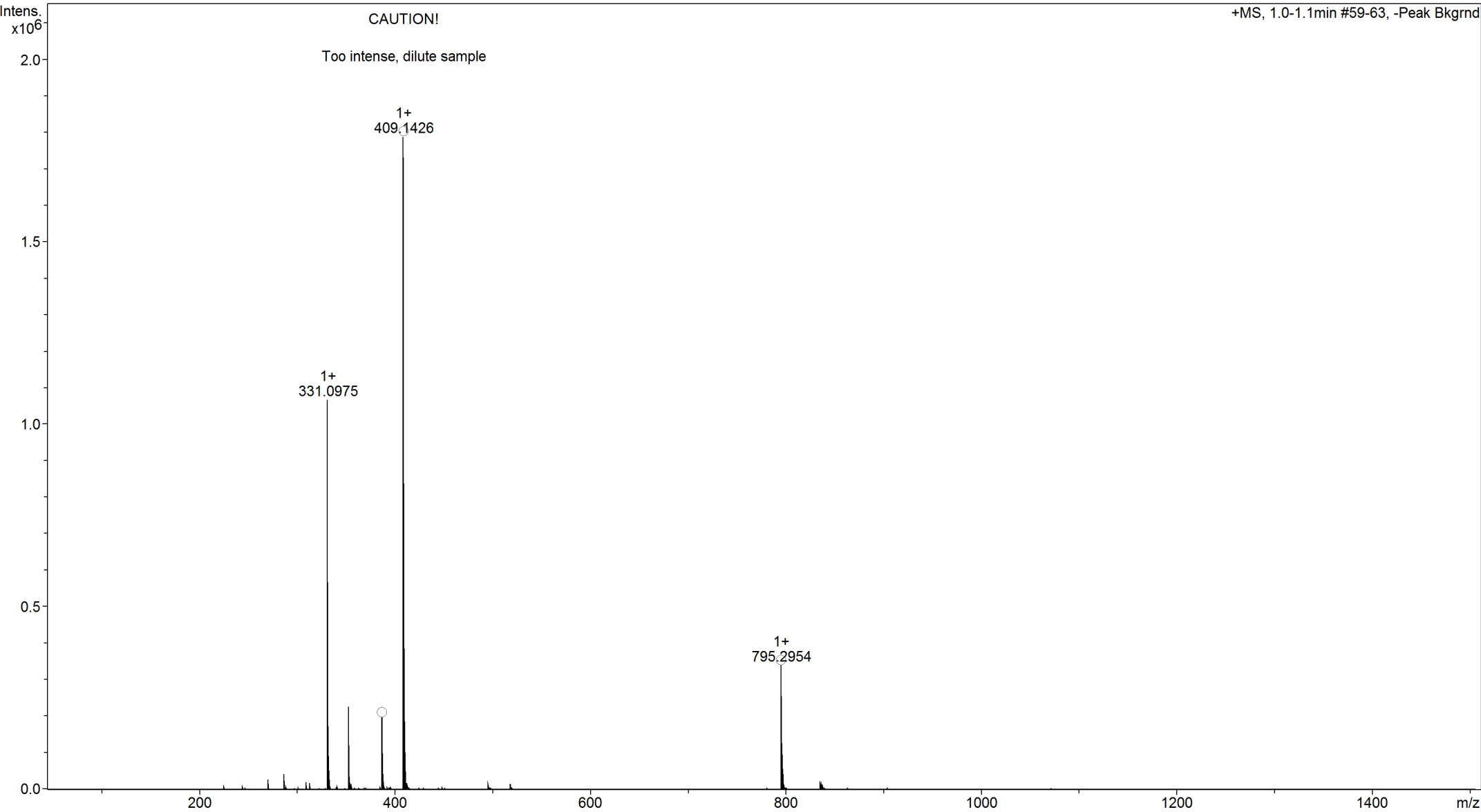
Submitter Izar Capel
Supervisor Malcolm Halcrow
Acquisition Date 20/06/2018 00:56:31
Scan Begin 50 m/z **Scan End** 1500 m/z

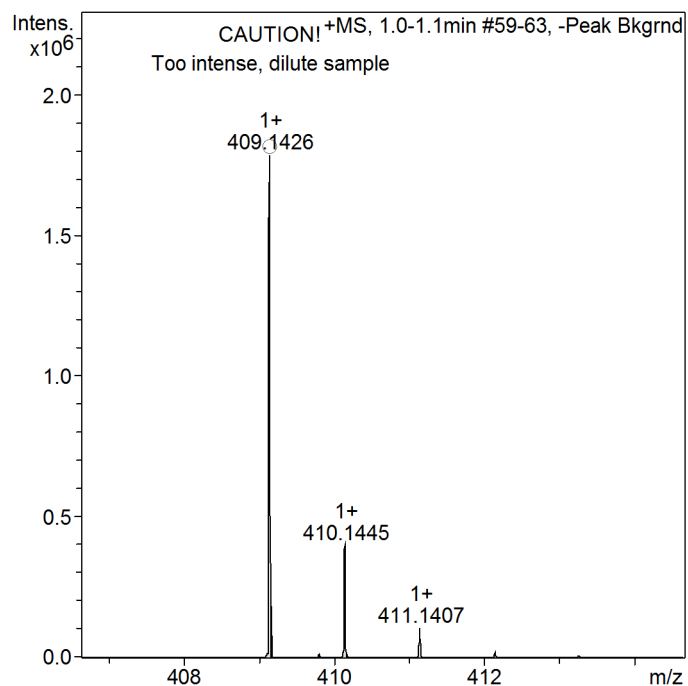


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.0 min	1.02	79.8	no uv	C18H22N6O2S
Cmpd 2, 1.1 min	1.09	9.9	no uv	C18H22N6O2S
Cmpd 3, 1.1 min	1.12	5.8	no uv	C18H22N6O2S
Cmpd 4, 1.1 min	1.15	4.6	no uv	C18H22N6O2S

Cmpd 1, 1.0 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, 1.0 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
387.159783	C18H23N6O2S	1+	387.159771	-0.0	-0.0	9.8	100.00	C18H22N6O2S	M+H
409.142632	C18H22N6NaO2S	1+	409.141716	-0.9	-2.2	8.2	100.00		M+Na
795.295362	C36H44N12NaO4S2	1+	795.294211	-1.2	-1.4	39.7	100.00		2M+Na

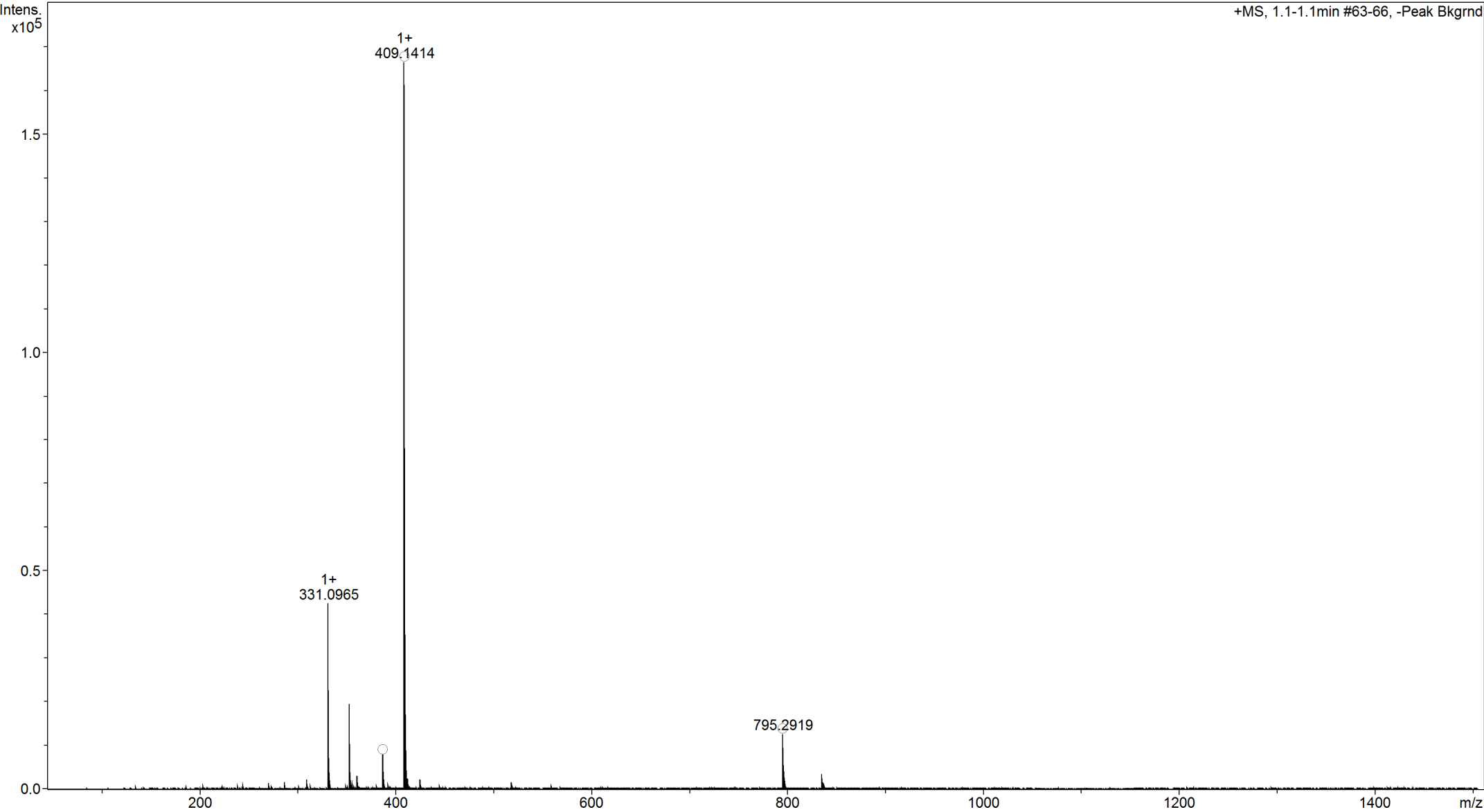
Smart Formula Parameter	Value
Expected Formula	C18H22N6O2S
Adducts Considered	

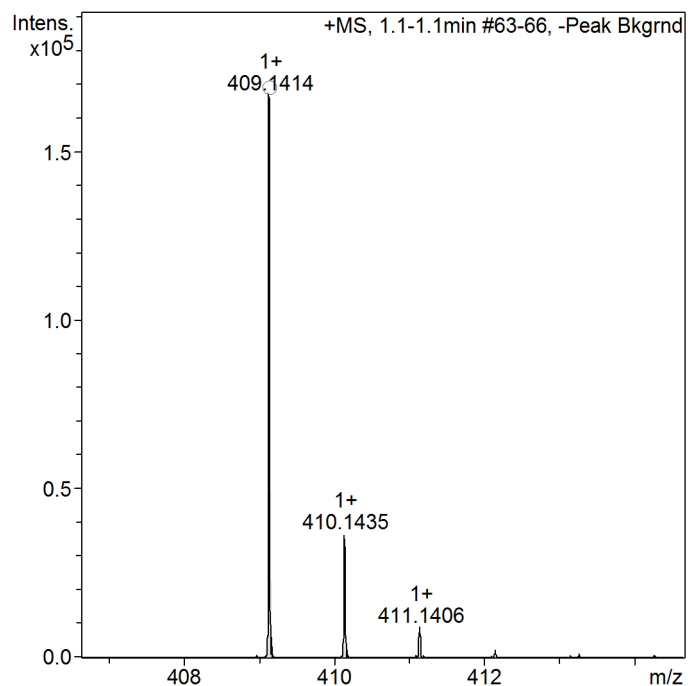
Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	
Formula Search Maximum	S 2

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

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
387.159879	C18H23N6O2S	1+	387.159771	-0.1	-0.3	37.5	100.00	C18H22N6O2S	M+H
409.141361	C18H22N6NaO2S	1+	409.141716	0.4	0.9	11.6	100.00		M+Na
795.291950	C36H44N12NaO4S2	1+	795.294211	2.3	2.8	20.8	100.00		2M+Na

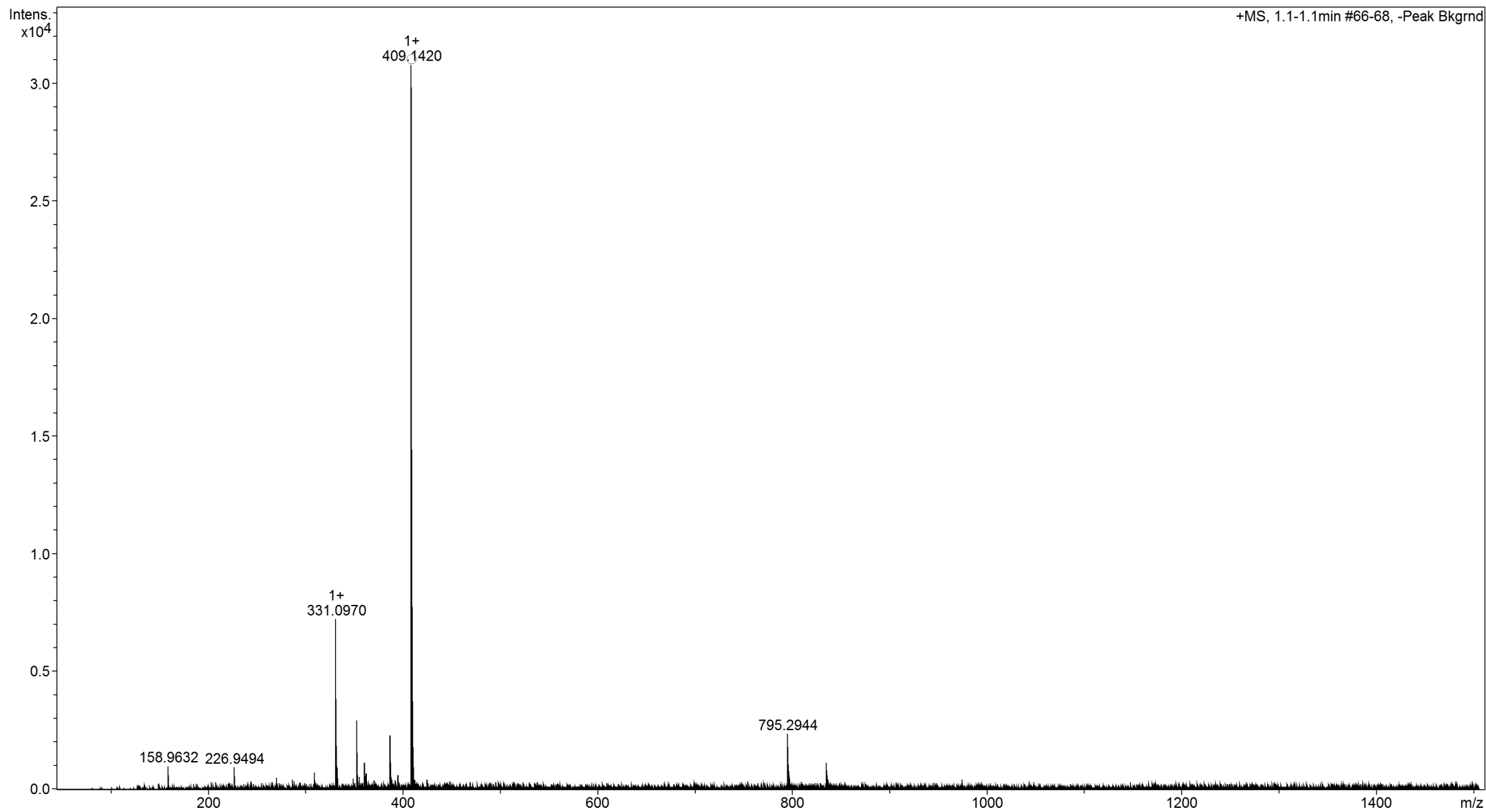
Smart Formula Parameter	Value
Expected Formula	C18H22N6O2S
Adducts Considered	

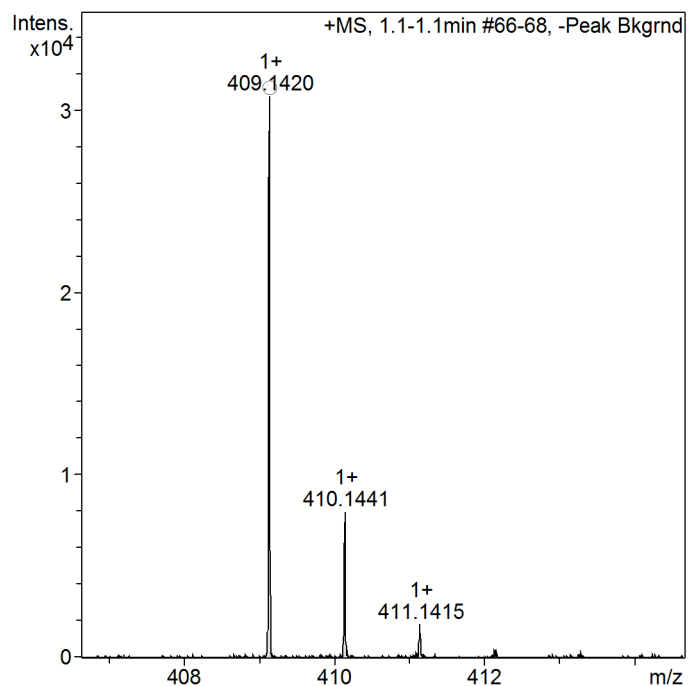
Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	
Formula Search Maximum	S 2

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 3, 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 3, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
409.141956	C ₁₈ H ₂₂ N ₆ NaO ₂ S	1+	409.141716	-0.2	-0.6	19.0	100.00	C ₁₈ H ₂₂ N ₆ O ₂ S	M+Na

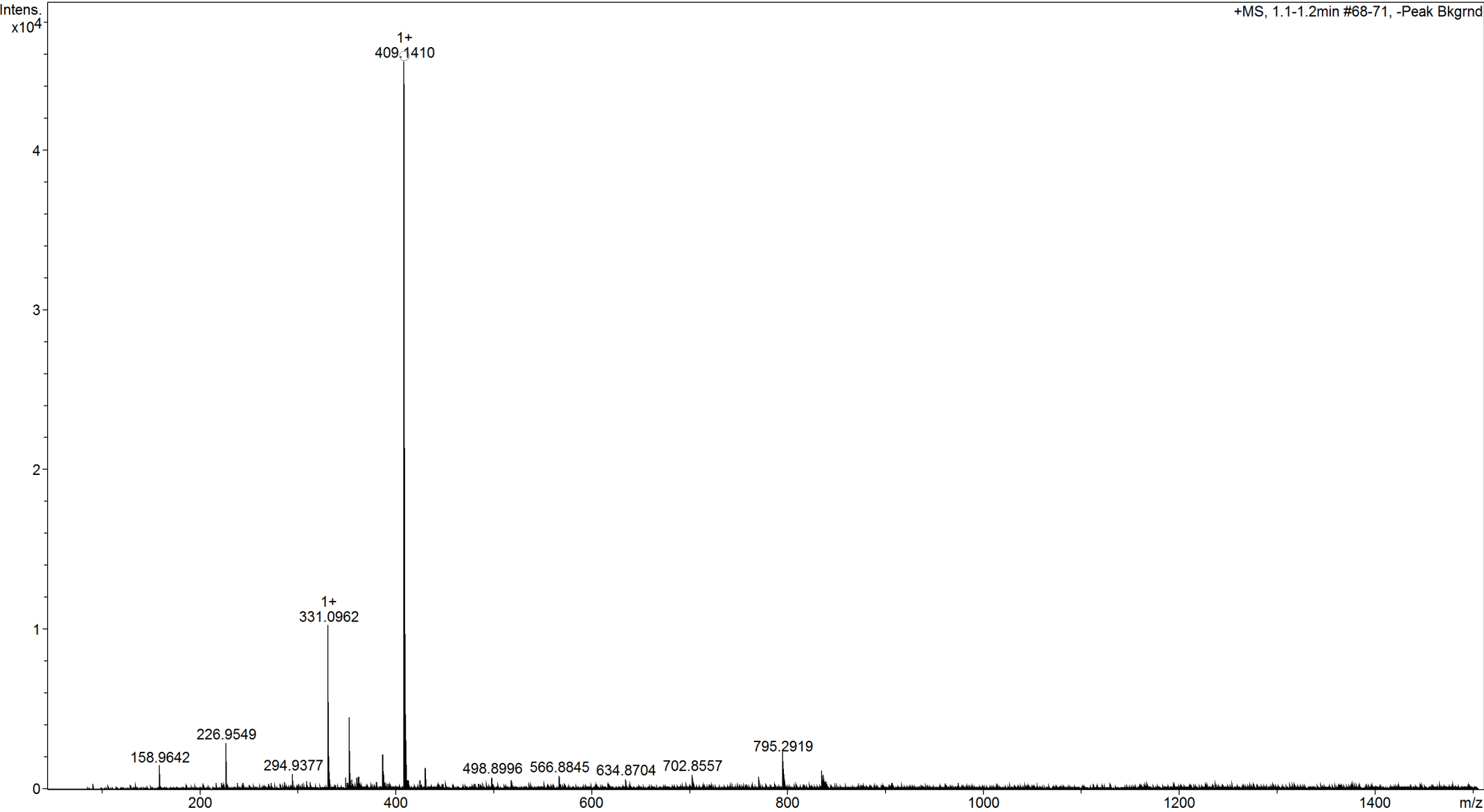
Smart Formula Parameter	Value
Expected Formula	C ₁₈ H ₂₂ N ₆ O ₂ S
Adducts Considered	

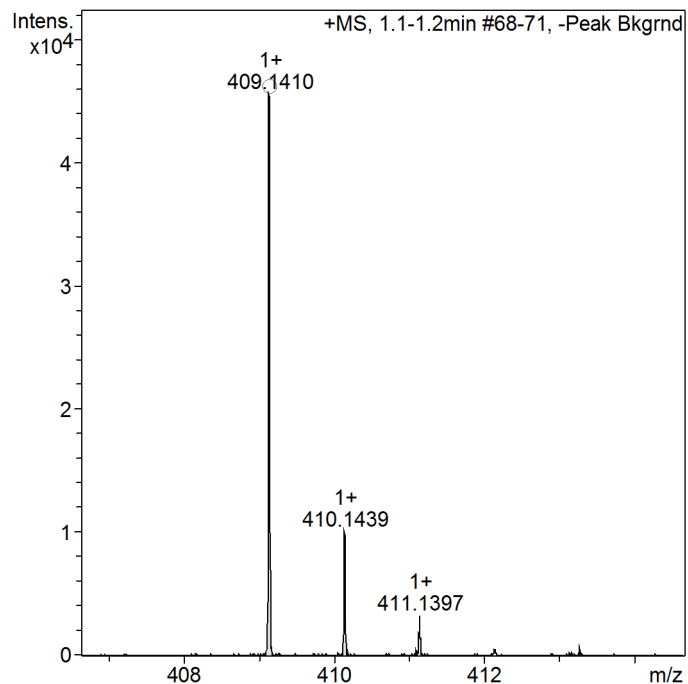
Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	
Formula Search Maximum	S 2

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 4, 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 4, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
409.141028	C ₁₈ H ₂₂ N ₆ NaO ₂ S	1+	409.141716	0.7	1.7	7.4	100.00	C ₁₈ H ₂₂ N ₆ O ₂ S	M+Na

Smart Formula Parameter	Value
Expected Formula	C ₁₈ H ₂₂ N ₆ O ₂ S
Adducts Considered	

Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	
Formula Search Maximum	S 2

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