

School of Chemistry Mass Spectrometry Service

SampleID 115-good
Sample Description
Analysis Name 115-good_210819_BA4_01_35326.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Izar Capel

Supervisor

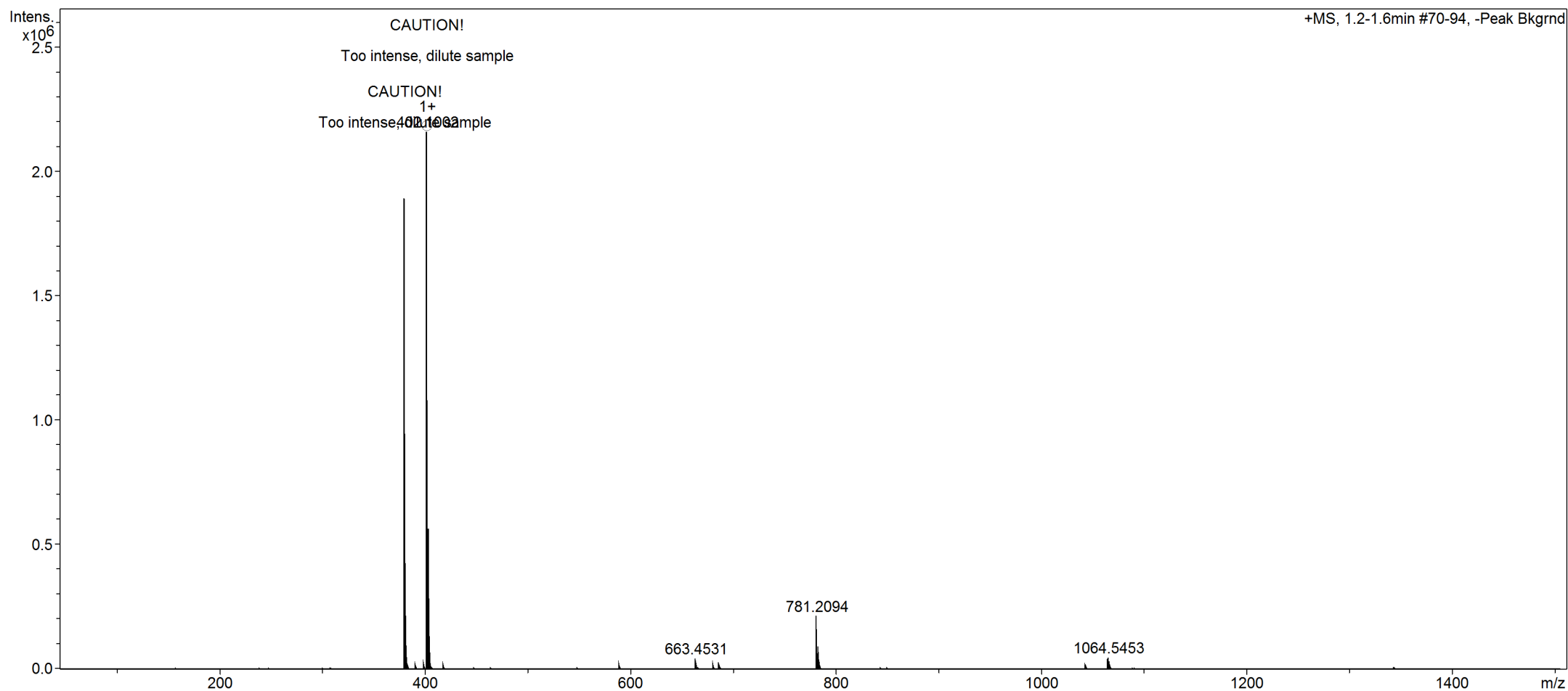
Malcolm Halcrow

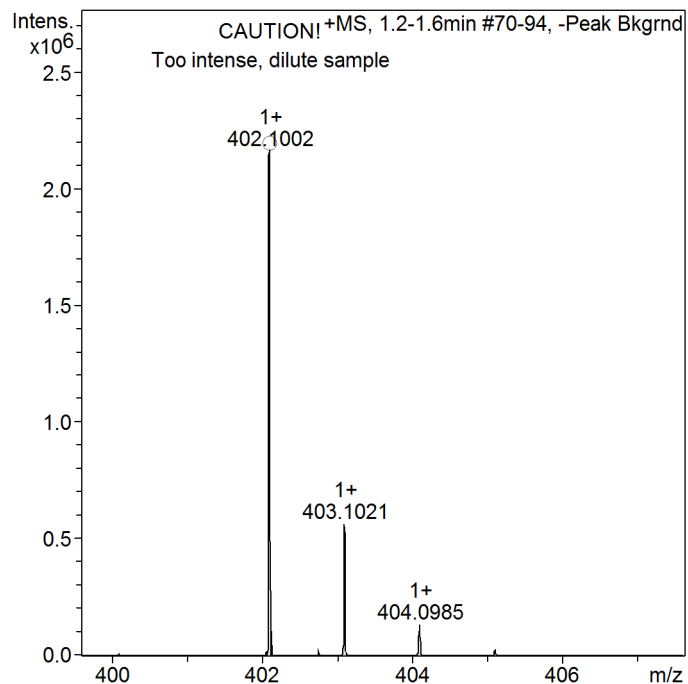
Acquisition Date

27/07/2017 00:06:18

Scan Begin 50 m/z

Scan End 1500 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

Concentration too high. Dilute sample!

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
402.100202	C17H12N11S	1+	402.099237	-1.0	-2.4	14.7	79.71	C17H11N11S	M+H
	C20H20NO6S	1+	402.100585	0.4	1.0	18.3	100.00	C20H19NO6S	M+H
	C17H12N11S	1+	402.099237	-1.0	-2.4	14.7	79.71	C17H8N10S	M+NH4
	C20H20NO6S	1+	402.100585	0.4	1.0	18.3	100.00	C20H16O6S	M+NH4
	C19H17N5NaO2S	1+	402.099517	-0.7	-1.7	15.2	100.00	C19H17N5O2S	M+Na
	C27H13N3Na	1+	402.100168	-0.0	-0.1	26.8	78.74	C27H13N3	M+Na
	C24H17KN3O	1+	402.100320	0.1	0.3	26.4	100.00	C24H17N3O	M+K
	C22H18N3Na2S	1+	402.101134	0.9	2.3	8.5	100.00	C22H19N3S	M+Na2-H

Smart Formula Parameter	Value
Expected Formula	C18H17N5O2S
Adducts Considered	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 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