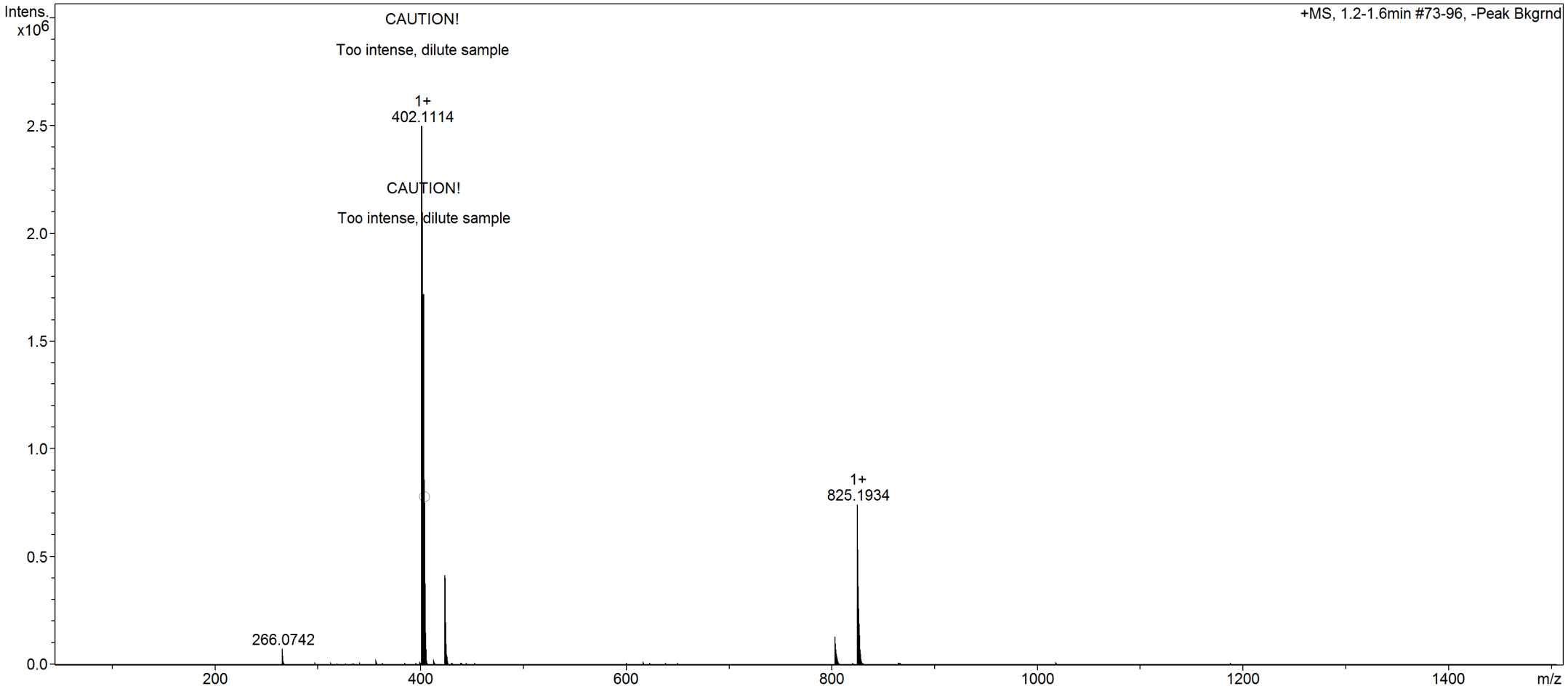
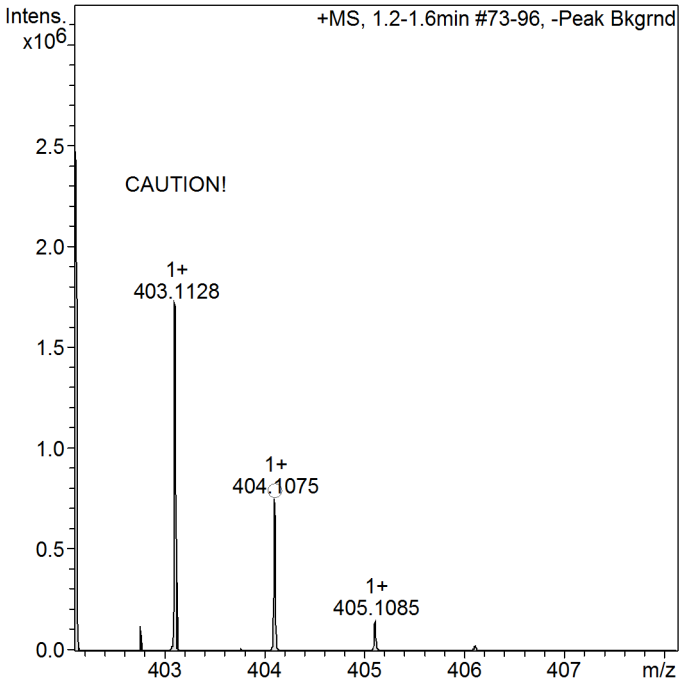
School of Chemistry Mass Spectrometry Service

SampleID	NS140 ppt	**Submitter**	Namrah Shahid
Sample Description			
Analysis Name	NS140 ppt_261279_GE4_01_54061.d	**Supervisor**	Malcolm Halcrow
Method	3a_AccMass_Loop_Positive.m	**Acquisition Date**	14/02/2019 16:18:11
Instrument	maXis impact	**Source Type** ESI	**Ion Polarity** Positive
Scan Begin	50 m/z	**Scan End**	1500 m/z





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

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
404.107485	C14H14N9O6	1+	404.106156	-1.3	-3.3	4.8	55.44	C14H13N9O6	M+H
	C18H18N3O8	1+	404.108841	1.4	3.4	9.1	50.48	C18H17N3O8	M+H
	C15H10N13O2	1+	404.107493	0.0	0.0	9.7	100.00	C15H9N13O2	M+H
	C14H14N9O6	1+	404.106156	-1.3	-3.3	4.8	55.44	C14H10N8O6	M+NH4
	C18H18N3O8	1+	404.108841	1.4	3.4	9.1	50.48	C18H14N2O8	M+NH4
	C15H10N13O2	1+	404.107493	0.0	0.0	9.7	100.00	C15H6N12O2	M+NH4
	C16H19N3NaO8	1+	404.106435	-1.0	-2.6	4.0	74.84	C16H19N3O8	M+Na
	C17H15N7NaO4	1+	404.107773	0.3	0.7	9.7	100.00	C17H15N7O4	M+Na
	C18H11N11Na	1+	404.109110	1.6	4.0	23.3	35.60	C18H11N11	M+Na
	C14H19KN7O5	1+	404.107925	0.4	1.1	34.3	100.00	C14H19N7O5	M+K
	C19H20NNa2O6	1+	404.108052	0.6	1.4	10.3	100.00	C19H21NO6	M+Na2-H
	C16H12N11Na2	1+	404.106704	-0.8	-1.9	12.1	86.61	C16H13N11	M+Na2-H