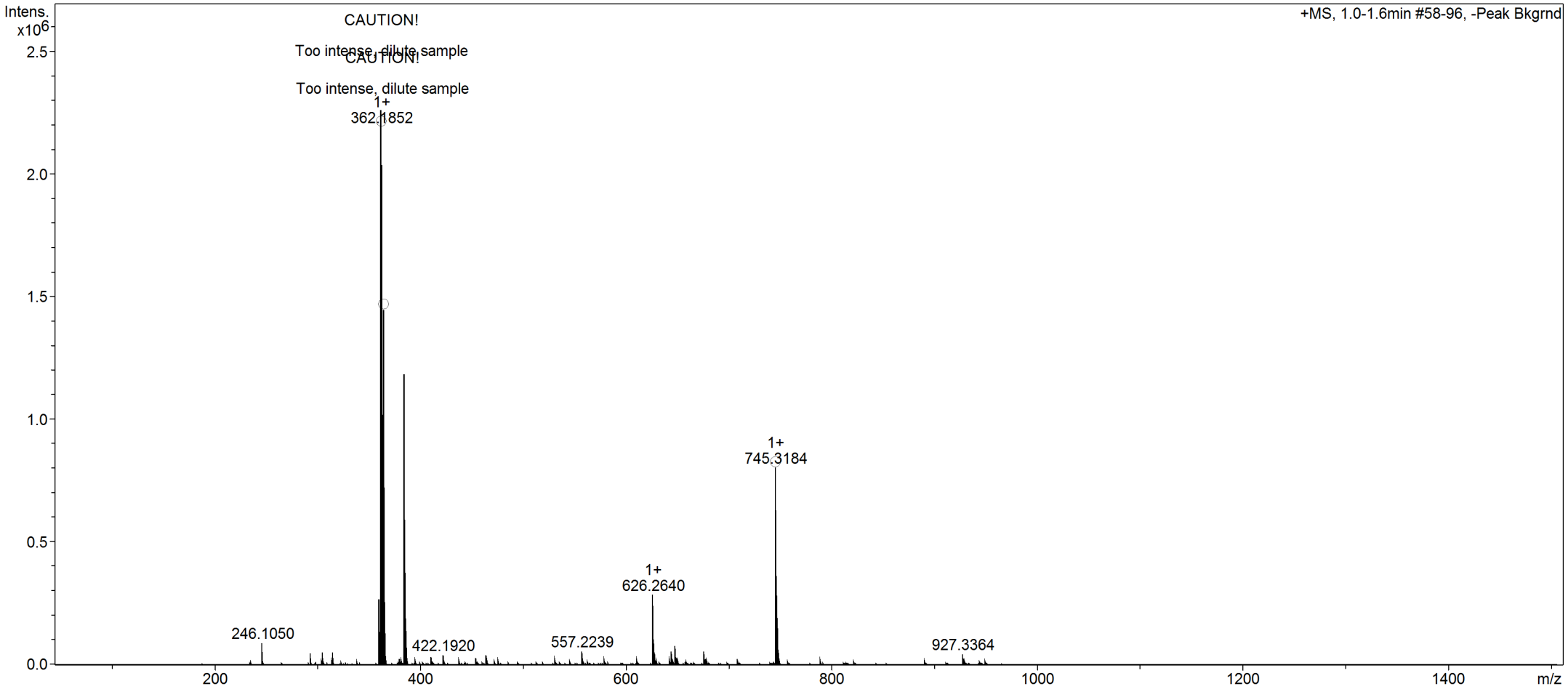
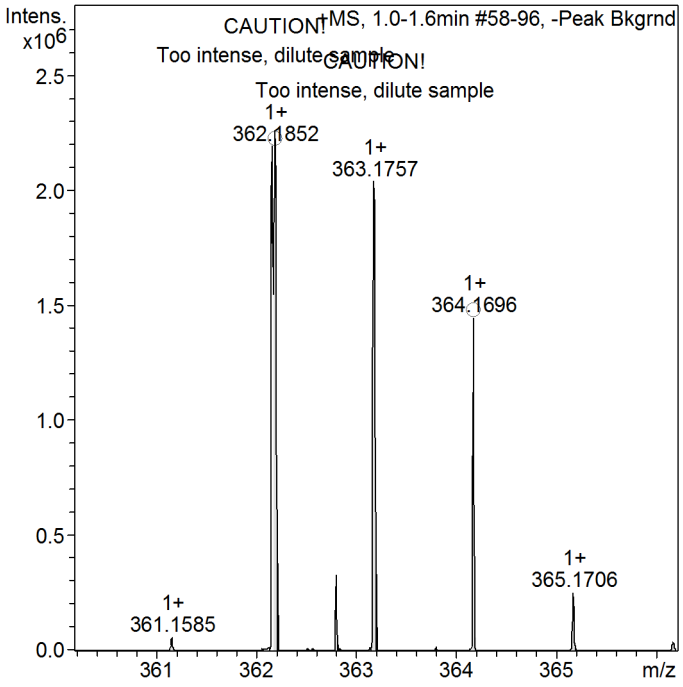
School of Chemistry Mass Spectrometry Service

SampleID	NS180 actual	**Submitter**	Namrah Shahid
Sample Description			
Analysis Name	NS180 actual_271454_RD4_01_57892.d	**Supervisor**	Malcolm Halcrow
Method	3a_AccMass_Loop_Positive.m	**Acquisition Date**	13/05/2019 17:58:20
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
362.185220	C22H24N3O2	1+	362.186303	1.1	3.0	n.a.	100.00	C22H23N3O2	M+H
	C22H24N3O2	1+	362.186303	1.1	3.0	n.a.	100.00	C22H20N2O2	M+NH4
	C20H25N3NaO2	1+	362.183898	-1.3	-3.7	n.a.	100.00	C20H25N3O2	M+Na
	C17H29KN3O3	1+	362.184050	-1.2	-3.2	n.a.	100.00	C17H29N3O3	M+K
	C23H26NNa2	1+	362.185515	0.3	0.8	n.a.	100.00	C23H27N	M+Na2-H
	C8H22N13Na2O	1+	362.186017	0.8	2.2	n.a.	78.18	C8H23N13O	M+Na2-H
364.169597	C11H18N13O2	1+	364.170093	0.5	1.4	5.0	100.00	C11H17N13O2	M+H
	C10H22N9O6	1+	364.168756	-0.8	-2.3	17.1	66.74	C10H21N9O6	M+H
	C11H18N13O2	1+	364.170093	0.5	1.4	5.0	100.00	C11H14N12O2	M+NH4
	C10H22N9O6	1+	364.168756	-0.8	-2.3	17.1	66.74	C10H18N8O6	M+NH4
	C13H23N7NaO4	1+	364.170373	0.8	2.1	3.1	100.00	C13H23N7O4	M+Na
	C12H27N3NaO8	1+	364.169036	-0.6	-1.5	16.5	87.03	C12H27N3O8	M+Na
	C10H27KN7O5	1+	364.170525	0.9	2.5	38.6	100.00	C10H27N7O5	M+K
	C15H28NNa2O6	1+	364.170653	1.1	2.9	2.7	71.49	C15H29NO6	M+Na2-H
	C12H20N11Na2	1+	364.169305	-0.3	-0.8	5.9	100.00	C12H21N11	M+Na2-H
745.318404	C38H50KN4O9	1+	745.320937	2.5	3.4	27.6	27.88	C38H50N4O9	M+K
	C37H54KO13	1+	745.319600	1.2	1.6	32.5	66.31	C37H54O13	M+K
	C35H42KN14O3	1+	745.319589	1.2	1.6	33.2	65.55	C35H42N14O3	M+K
	C34H46KN10O7	1+	745.318252	-0.2	-0.2	37.3	100.00	C34H46N10O7	M+K
	C46H42KN8	1+	745.316401	-2.0	-2.7	39.1	32.16	C46H42N8	M+K