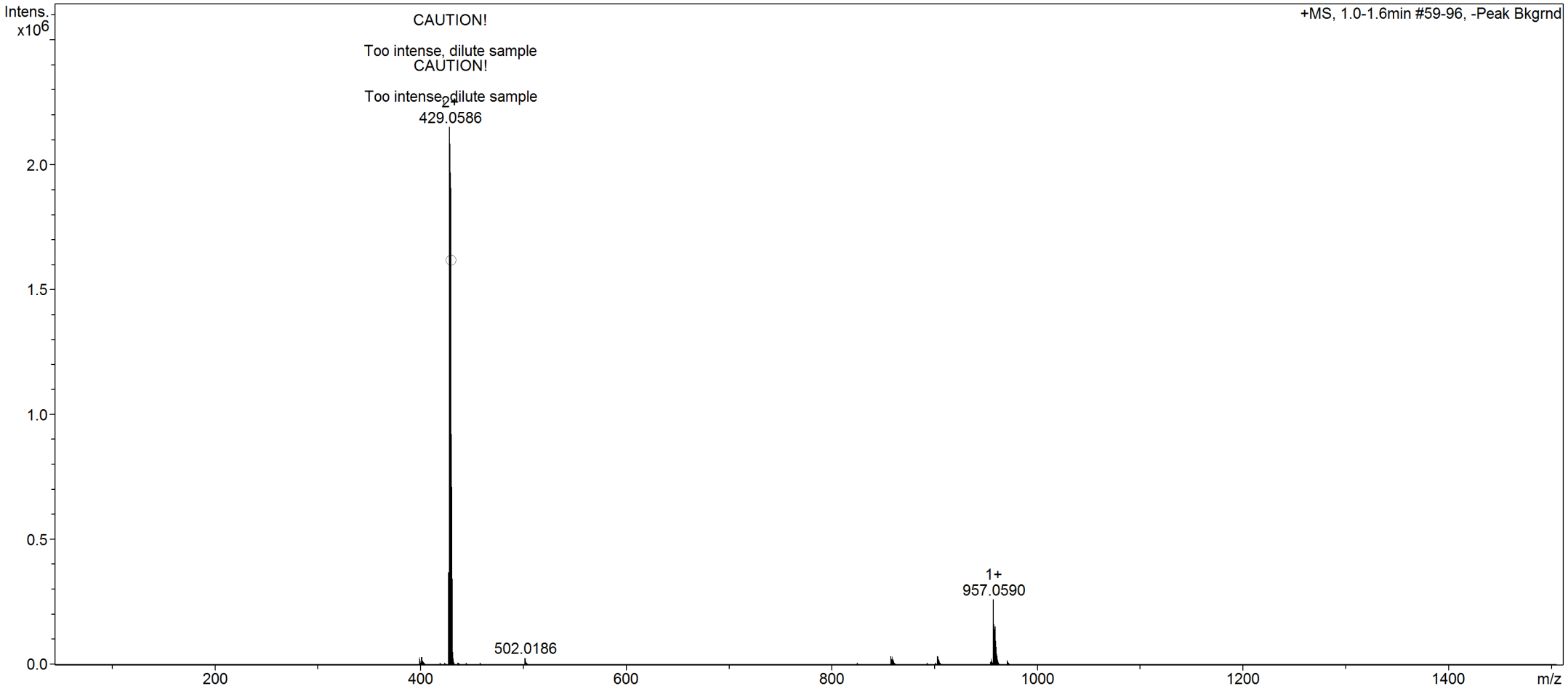
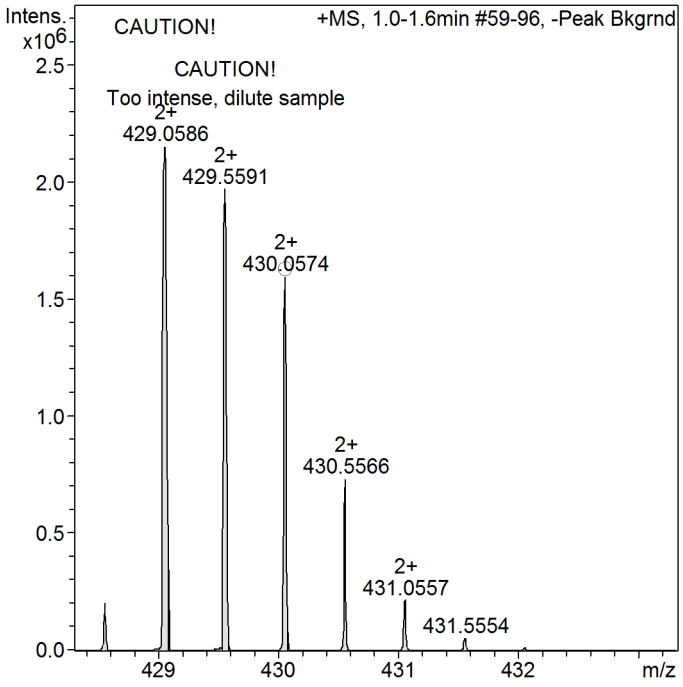
School of Chemistry Mass Spectrometry Service

SampleID	NS236	**Submitter**	Namrah Shahid
Sample Description			
Analysis Name	NS236_289953_BD6_01_65137.d	**Supervisor**	Malcolm Halcrow
Method	3a_AccMass_Loop_Positive.m	**Acquisition Date**	22/11/2019 17:17:21
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

Calibration failed!
Concentration too high. Dilute sample!

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
430.057395	C37H16N16O11	2+	430.058674	1.3	3.0	4.3	64.44	C37H14N16O11	M+H
	C34H8N26O5	2+	430.058000	0.6	1.4	10.4	84.37	C34H6N26O5	M+H
	C39H28N2O21	2+	430.058679	1.3	3.0	10.6	57.43	C39H26N2O21	M+H
	C36H20N12O15	2+	430.058005	0.6	1.4	10.8	83.53	C36H18N12O15	M+H
	C33H12N22O9	2+	430.057331	-0.1	-0.1	14.3	100.00	C33H10N22O9	M+H
	C35H4N30O	2+	430.058669	1.3	3.0	16.9	51.05	C35H2N30O	M+H
	C30H4N32O3	2+	430.056657	-0.7	-1.7	19.4	65.78	C30H2N32O3	M+H
	C35H24N8O19	2+	430.057337	-0.1	-0.1	22.1	85.15	C35H22N8O19	M+H
	C32H16N18O13	2+	430.056663	-0.7	-1.7	24.0	59.73	C32H14N18O13	M+H
	C29H8N28O7	2+	430.055989	-1.4	-3.3	27.3	37.36	C29H6N28O7	M+H
	C37H16N16O11	2+	430.058674	1.3	3.0	4.3	64.44	C37H8N14O11	M+NH4
	C34H8N26O5	2+	430.058000	0.6	1.4	10.4	84.37	C34N24O5	M+NH4
	C39H28N2O21	2+	430.058679	1.3	3.0	10.6	57.43	C39H20O21	M+NH4
	C36H20N12O15	2+	430.058005	0.6	1.4	10.8	83.53	C36H12N10O15	M+NH4
	C33H12N22O9	2+	430.057331	-0.1	-0.1	14.3	100.00	C33H4N20O9	M+NH4
	C35H24N8O19	2+	430.057337	-0.1	-0.1	22.1	85.15	C35H16N6O19	M+NH4
	C32H16N18O13	2+	430.056663	-0.7	-1.7	24.0	59.73	C32H8N16O13	M+NH4
	C29H8N28O7	2+	430.055989	-1.4	-3.3	27.3	37.36	C29N26O7	M+NH4
	C46H24N2O16	2+	430.055743	-1.7	-3.8	30.3	29.44	C46H16O16	M+NH4
	C34H28N4O23	2+	430.056668	-0.7	-1.7	33.7	47.44	C34H20N2O23	M+NH4
	C42H28N2Na4O13	2+	430.058559	1.2	2.7	4.9	66.35	C42H28N2Na2O13	M+Na
	C39H20N12Na4O7	2+	430.057885	0.5	1.1	8.4	89.66	C39H20N12Na2O7	M+Na
	C38H24N8Na4O11	2+	430.057217	-0.2	-0.4	10.2	100.00	C38H24N8Na2O11	M+Na
	C36H12N22Na4O	2+	430.057212	-0.2	-0.4	14.3	92.20	C36H12N22Na2O	M+Na
	C35H16N18Na4O5	2+	430.056543	-0.9	-2.0	15.4	65.22	C35H16N18Na2O5	M+Na
	C40H16N16Na4O3	2+	430.058554	1.2	2.7	17.8	52.15	C40H16N16Na2O3	M+Na
	C37H28N4Na4O15	2+	430.056548	-0.8	-2.0	20.3	59.09	C37H28N4Na2O15	M+Na
	C34H20N14Na4O9	2+	430.055874	-1.5	-3.5	23.3	36.82	C34H20N14Na2O9	M+Na
	C36H32Na4O19	2+	430.055879	-1.5	-3.5	31.5	30.45	C36H32Na2O19	M+Na
	C40H28N4Na8O7	2+	430.056428	-1.0	-2.2	11.4	73.15	C40H30N4Na4O7	M+Na2-H
	C41H24N8Na8O3	2+	430.057097	-0.3	-0.7	12.7	100.00	C41H26N8Na4O3	M+Na2-H
	C37H20N14Na8O	2+	430.055754	-1.6	-3.8	17.5	42.44	C37H22N14Na4O	M+Na2-H
	C39H32Na8O11	2+	430.055759	-1.6	-3.8	19.3	41.06	C39H34Na4O11	M+Na2-H
	C45H28N2Na8O5	2+	430.058440	1.0	2.4	19.5	59.44	C45H30N2Na4O5	M+Na2-H

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
	C46H24N6Na8O	2+	430.059108	1.7	4.0	31.2	29.61	C46H26N6Na4O	M+Na2-H
	C46H24N2O16	2+	430.055743	-1.7	-3.8	30.3	29.44	C23H11NO8	2M+H
	C44H12N16O6	2+	430.055738	-1.7	-3.9	40.1	22.81	C22H5N8O3	2M+H