

School of Chemistry Mass Spectrometry Service

SampleID ICB-1-65-1
Sample Description
Analysis Name ICB-1-65-1_167404_GE8_01_22611.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Izar Capel

Supervisor

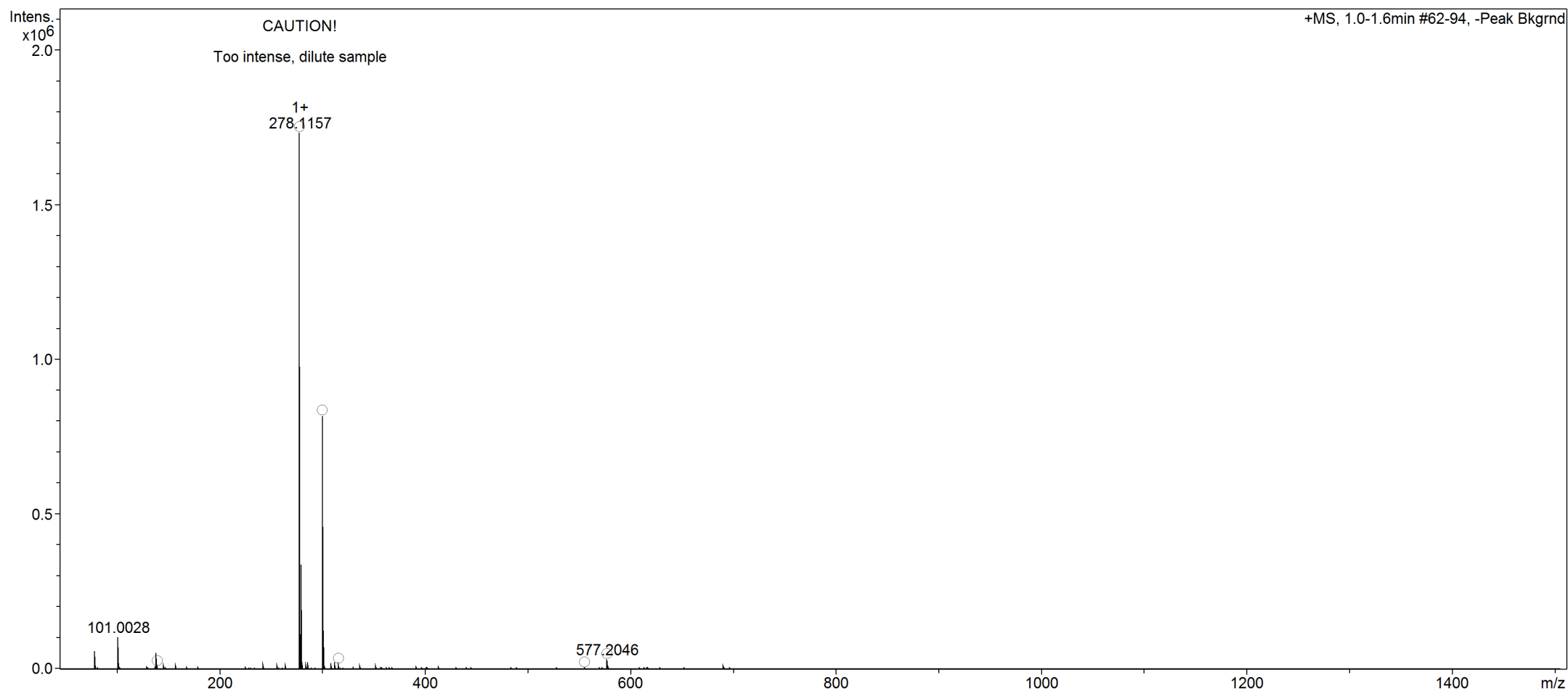
Malcolm Halcrow

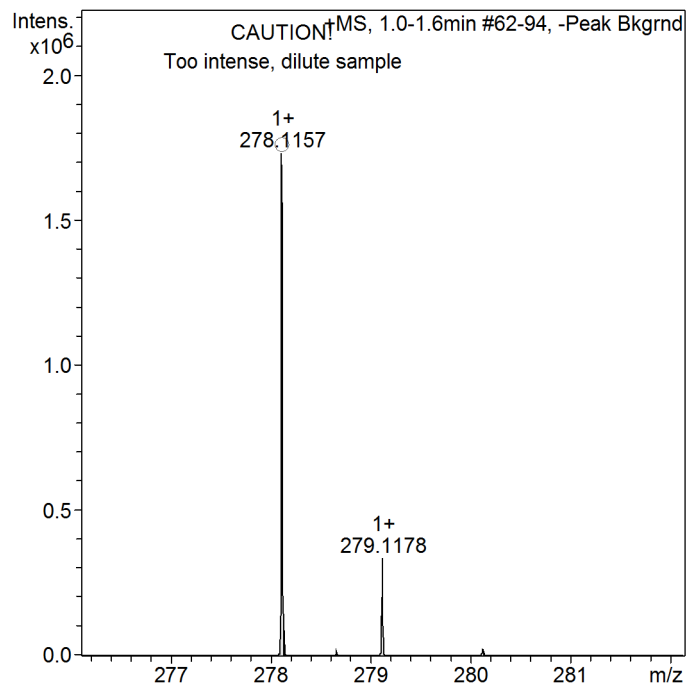
Acquisition Date

24/05/2016 15:51:00

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
139.560877	C14H13N7	2+	139.561073	0.2	1.4	10.8	100.00	C14H11N7	M+H
278.115744	C14H12N7	1+	278.114870	-0.9	-3.1	9.2	100.00		M+H
300.097265	C14H11N7Na	1+	300.096814	-0.5	-1.5	15.7	100.00		M+Na
316.070717	C14H11KN7	1+	316.070751	0.0	0.1	8.5	100.00		M+K
555.222055	C28H23N14	1+	555.222463	0.4	0.7	36.0	100.00		2M+H
577.204643	C28H22N14Na	1+	577.204407	-0.2	-0.4	8.6	100.00		2M+Na

Smart Formula Parameter	Value
Expected Formula	C14H11N7
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

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