

School of Chemistry Mass Spectrometry Service

SampleID 161

Sample Description

Analysis Name 161_260784_GB1_01_53913.d

Method 3a_AccMass_Loop_Positive.m

Instrument maXis impact

Source Type

ESI

Ion Polarity

Positive

Submitter

Izar Capel

Supervisor

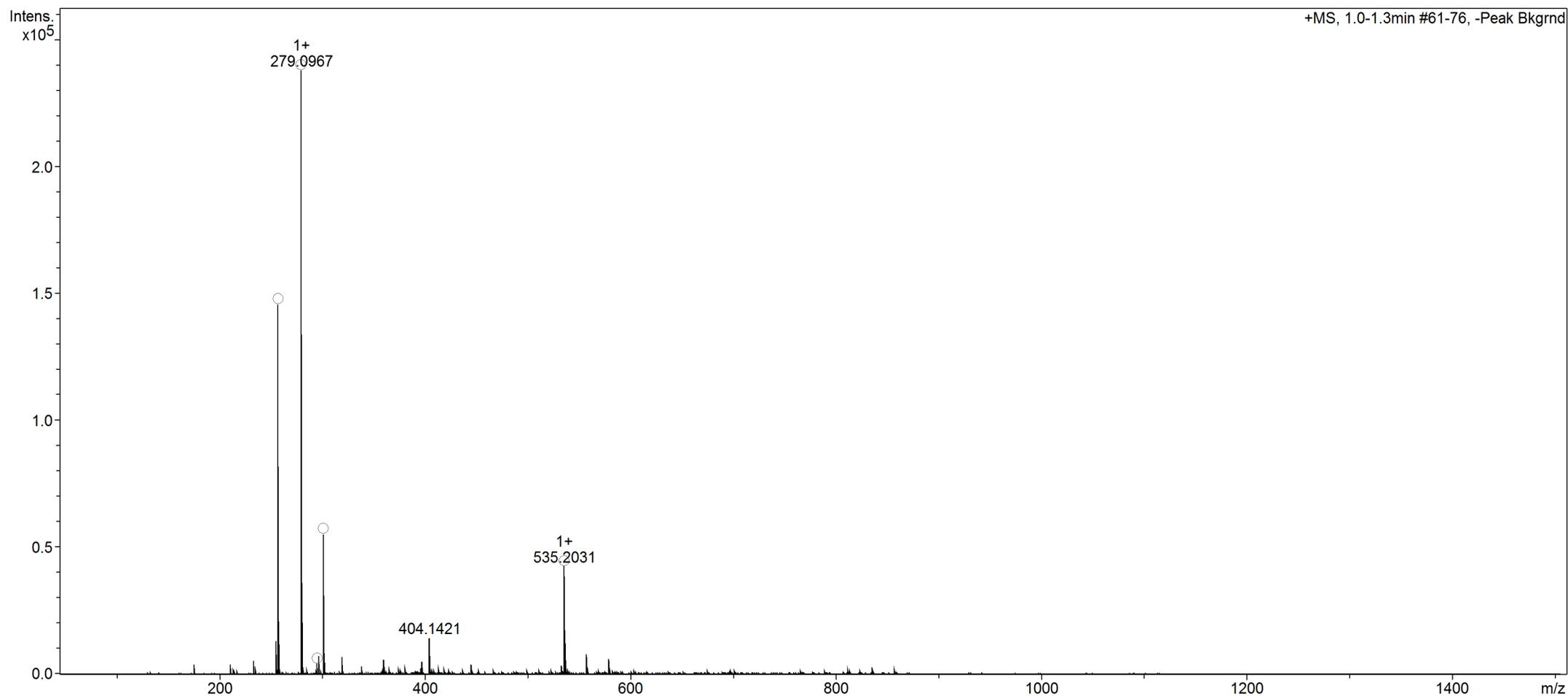
Malcolm Halcrow

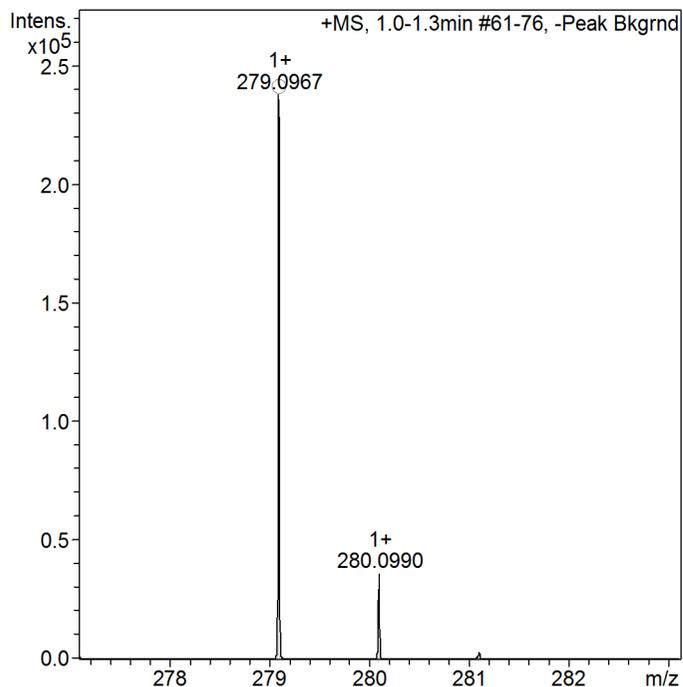
Acquisition Date

12/02/2019 09:55:59

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

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
257.114570	C12H13N6O	1+	257.114535	-0.0	-0.1	6.8	100.00	C12H12N6O	M+H
279.096658	C12H12N6NaO	1+	279.096480	-0.2	-0.6	1.8	100.00		M+Na
295.070286	C12H12KN6O	1+	295.070417	0.1	0.4	40.0	100.00		M+K
301.078477	C12H11N6Na2O	1+	301.078424	-0.1	-0.2	3.8	100.00		M+Na2-H
535.203078	C24H24N12NaO2	1+	535.203739	0.7	1.2	4.6	100.00		2M+Na

Smart Formula Parameter Value
 Expected Formula C12H12N6O
 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