

School of Chemistry Mass Spectrometry Service

SampleID bppSENL

Sample Description

Analysis Name D:\Data\malcolmhalcrow\cmic\bppSENL_245255_GE5_01_49725.d

Method 3a_AccMass_Loop_Positive.m

Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

Submitter

Izar Capel

Supervisor

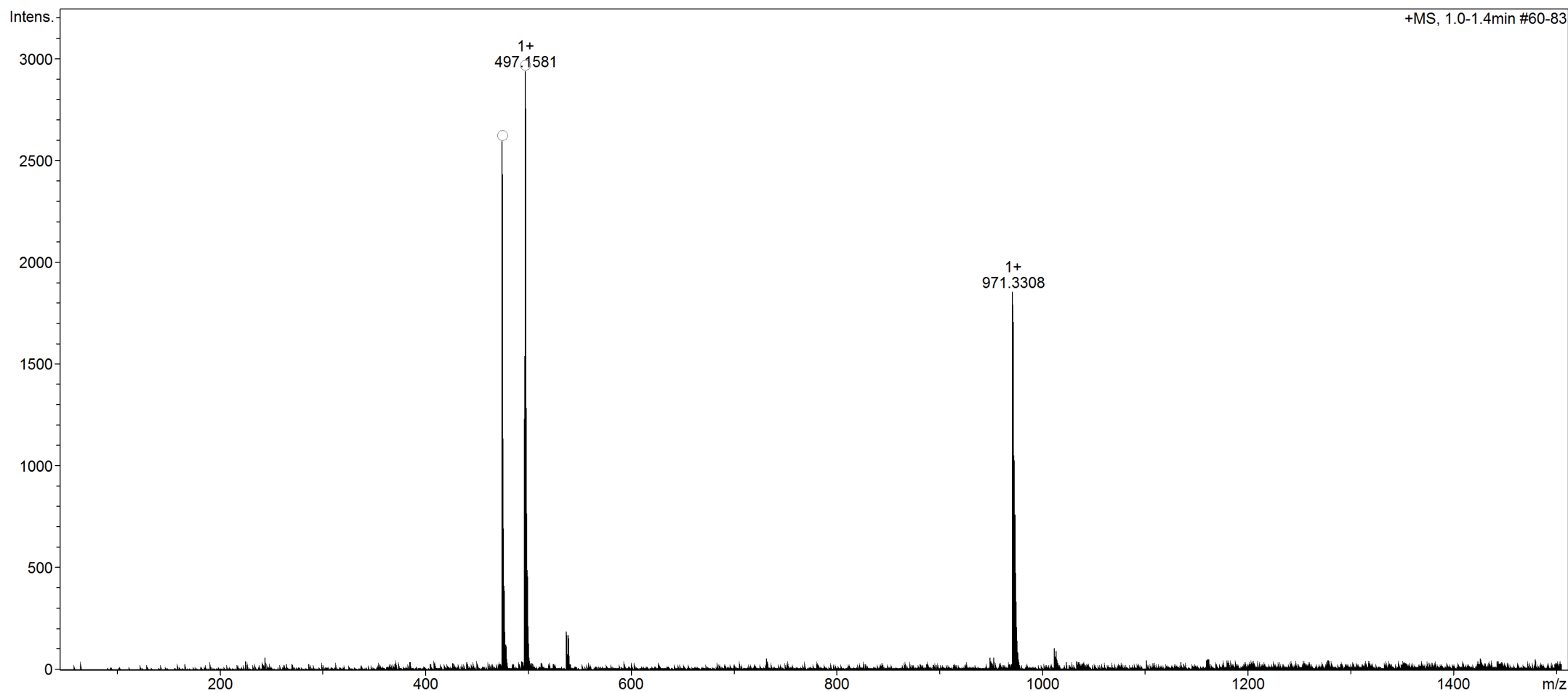
Malcolm Halcrow

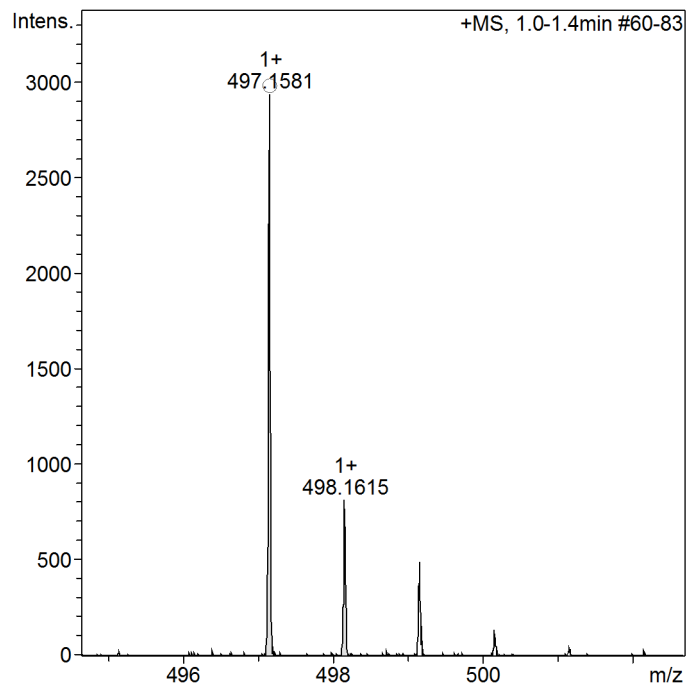
Acquisition Date

31/08/2018 14:12:36

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

Calibration failed!

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
475.174998	C25H19N10O	1+	475.173782	-1.2	-2.6	33.3	43.88	C25H18N10O	M+H
	C28H27O7	1+	475.175130	0.1	0.3	34.1	100.00	C28H26O7	M+H
	C25H19N10O	1+	475.173782	-1.2	-2.6	33.3	43.88	C25H15N9O	M+NH4
	C27H24N4NaO3	1+	475.174061	-0.9	-2.0	35.8	100.00	C27H24N4O3	M+Na
	C13H16N20Na	1+	475.175901	0.9	1.9	38.4	95.00	C13H16N20	M+Na
	C15H21N14Na2O2	1+	475.176181	1.2	2.5	38.7	86.99	C15H22N14O2	M+Na2-H
497.158131	C26H21N6O5	1+	497.156794	-1.3	-2.7	31.8	93.25	C26H20N6O5	M+H
	C26H21N6O5	1+	497.156794	-1.3	-2.7	31.8	93.25	C26H17N5O5	M+NH4
	C28H26NaO7	1+	497.157074	-1.1	-2.1	34.1	79.31	C28H26O7	M+Na
	C13H15N20Na2	1+	497.157846	-0.3	-0.6	38.4	100.00	C13H16N20	M+Na2-H

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