

# School of Chemistry Mass Spectrometry Service

**SampleID** bppCONEOLA  
**Sample Description**  
**Analysis Name** bppCONEOLA\_240544\_BC2\_01\_47422.d  
**Method** 3a\_AccMass\_Loop\_Positive.m  
**Instrument** maXis impact

**Source Type** ESI **Ion Polarity** Positive

**Submitter**

Izar Capel

**Supervisor**

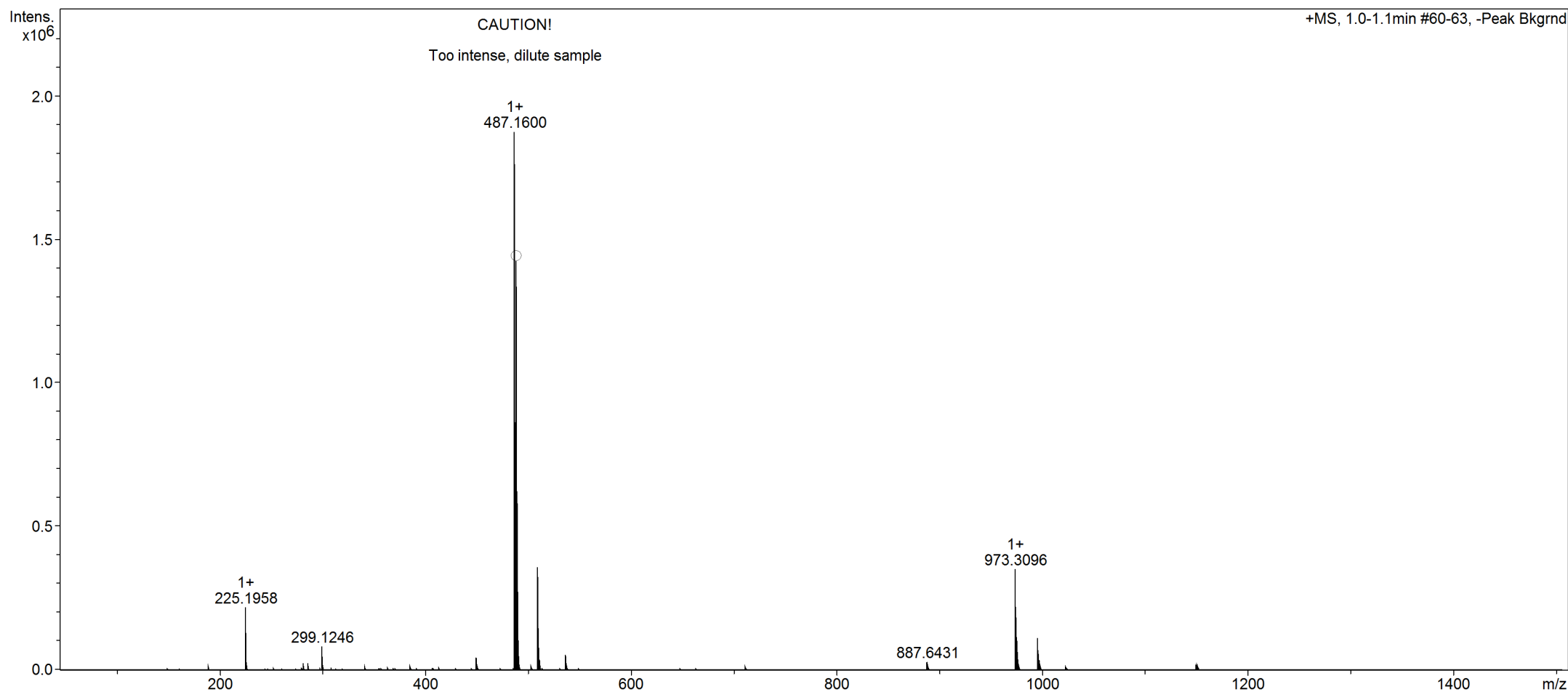
Malcolm Halcrow

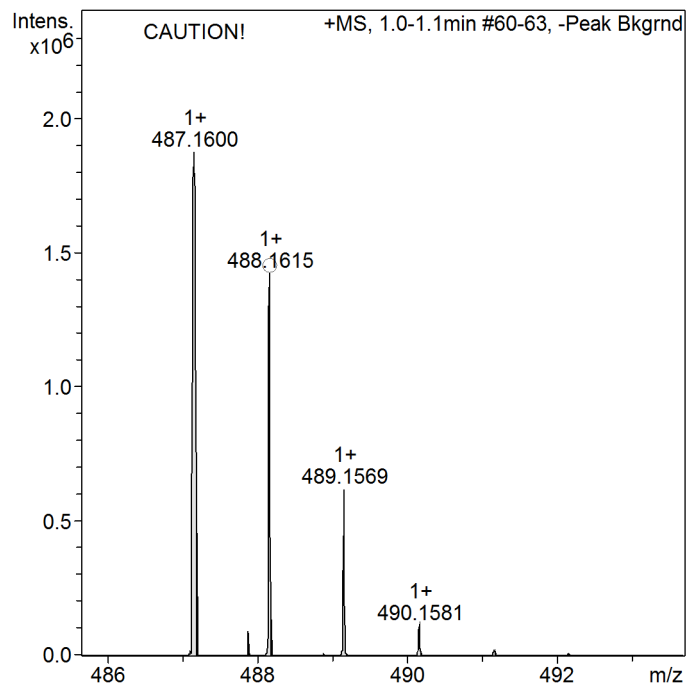
**Acquisition Date**

18/06/2018 15:56:13

**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
488.161528	C31H18N7	1+	488.161820	0.3	0.6	37.5	100.00	C31H17N7	M+H
	C31H18N7	1+	488.161820	0.3	0.6	37.5	100.00	C31H14N6	M+NH4
	C33H23NNaO2	1+	488.162100	0.6	1.2	36.7	100.00	C33H23NO2	M+Na