

School of Chemistry Mass Spectrometry Service

SampleID bppCOOEN-mb
Sample Description
Analysis Name bppCOOEN-mb_238600_BA8_01_46581.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Izar Capel

Supervisor

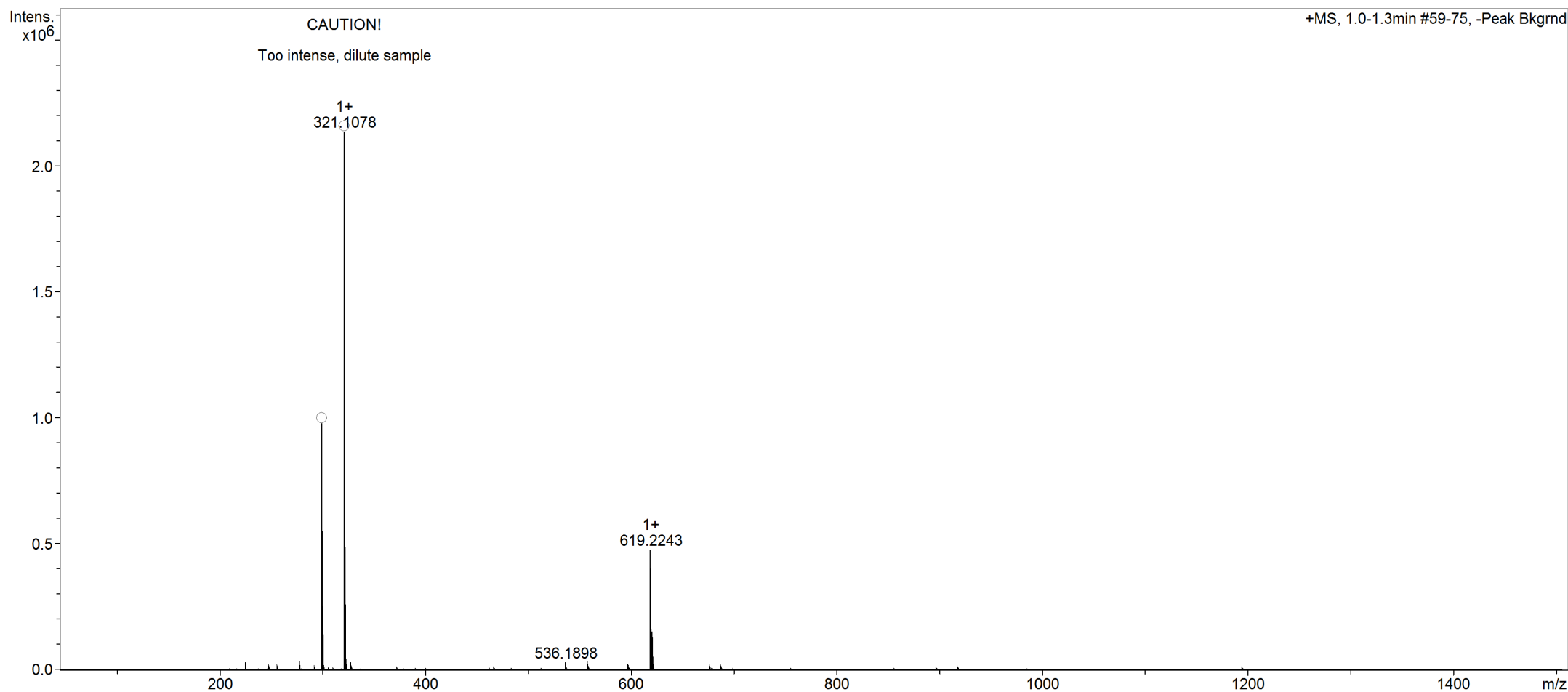
Malcolm Halcrow

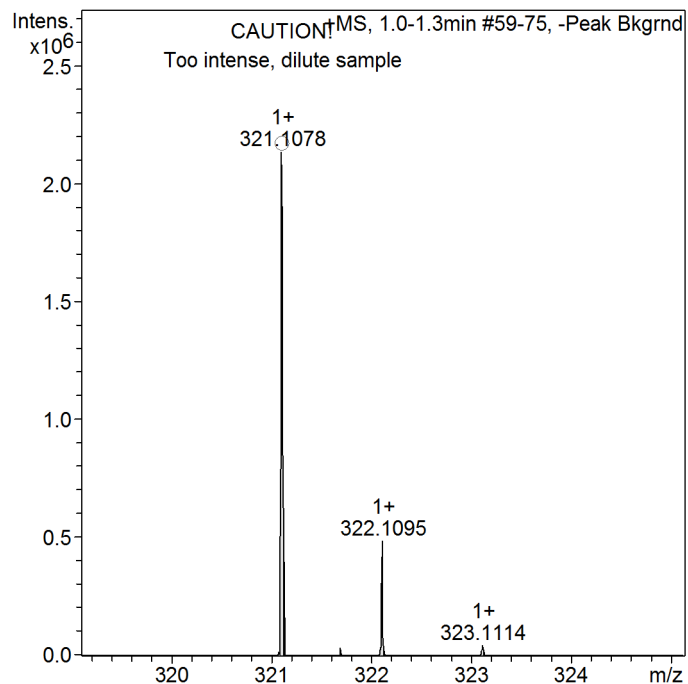
Acquisition Date

30/05/2018 17:16:38

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
299.125921	C17H16N4Na	1+	299.126717	0.8	2.7	33.9	100.00	C17H16N4	M+Na
321.107850	C12H9N12	1+	321.106765	-1.1	-3.4	30.8	66.39	C12H8N12	M+H
	C15H17N2O6	1+	321.108113	0.3	0.8	31.3	100.00	C15H16N2O6	M+H
	C12H9N12	1+	321.106765	-1.1	-3.4	30.8	66.39	C12H5N11	M+NH4
	C15H17N2O6	1+	321.108113	0.3	0.8	31.3	100.00	C15H13NO6	M+NH4
	C14H14N6NaO2	1+	321.107044	-0.8	-2.5	30.0	100.00	C14H14N6O2	M+Na
	C17H15N4Na2	1+	321.108661	0.8	2.5	15.9	100.00	C17H16N4	M+Na2-H
	C16H19Na2O4	1+	321.107324	-0.5	-1.6	29.4	85.76	C16H20O4	M+Na2-H
	C12H9N12	1+	321.106765	-1.1	-3.4	30.8	66.39	C6H4N6	2M+H
	C14H14N6NaO2	1+	321.107044	-0.8	-2.5	30.0	100.00	C7H7N3O	2M+Na