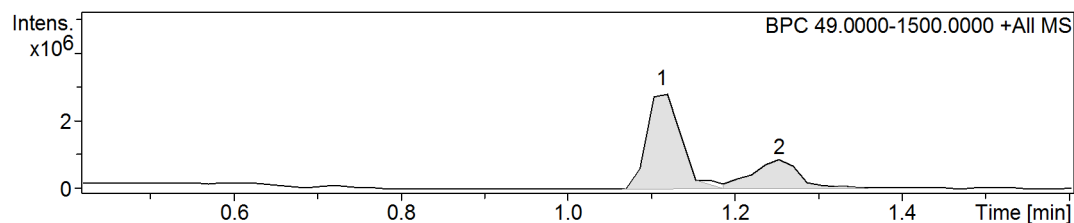


School of Chemistry Mass Spectrometry Service

SampleID bppCOOENBoc
Sample Description
Analysis Name D:\Data\malcolmhalcrow\cmic\bppCOOENBoc_238533_RD4_01_46561.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

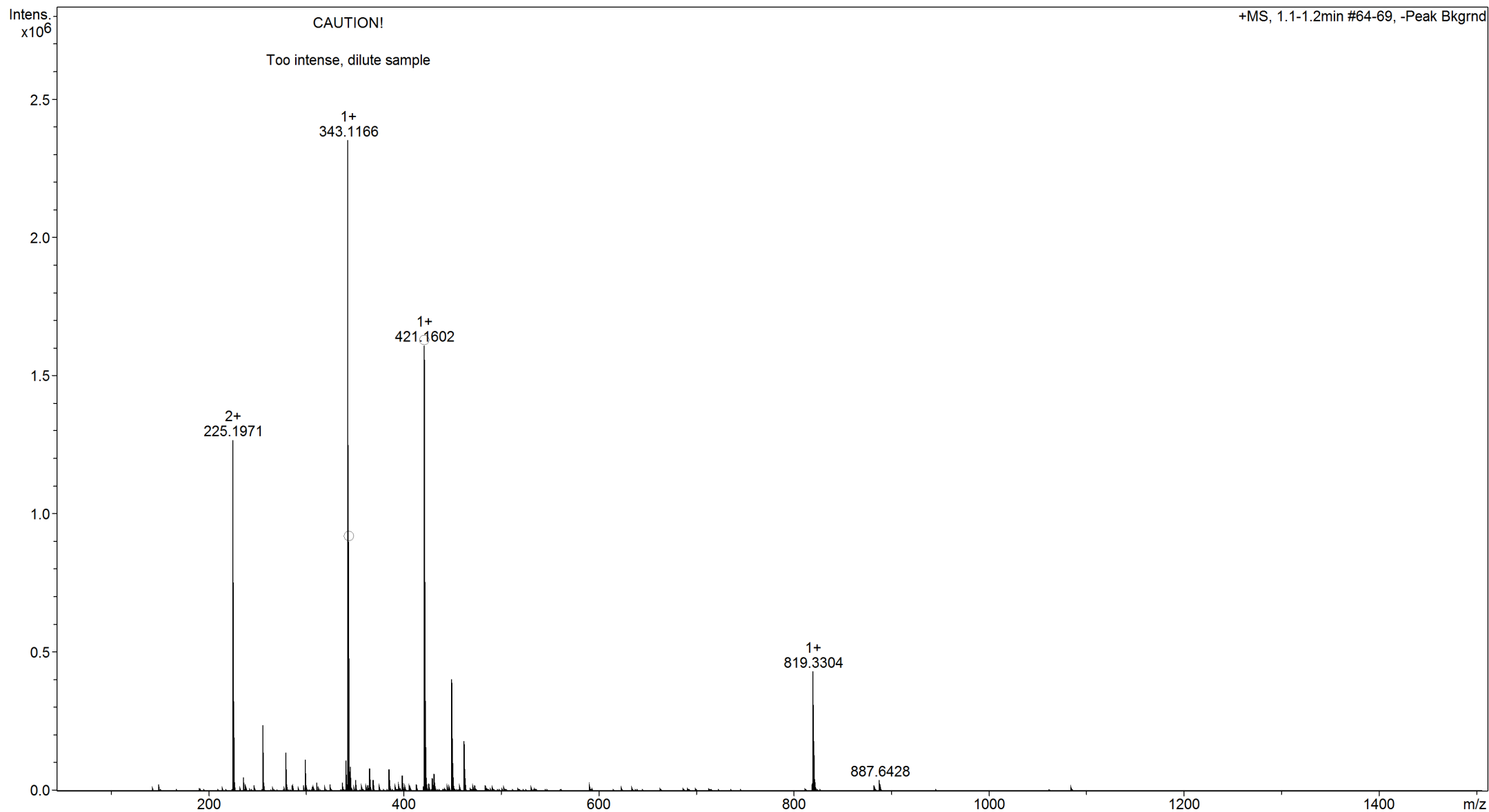
Submitter Izar Capel
Supervisor Malcolm Halcrow
Acquisition Date 30/05/2018 11:45:37
Scan Begin 50 m/z **Scan End** 1500 m/z

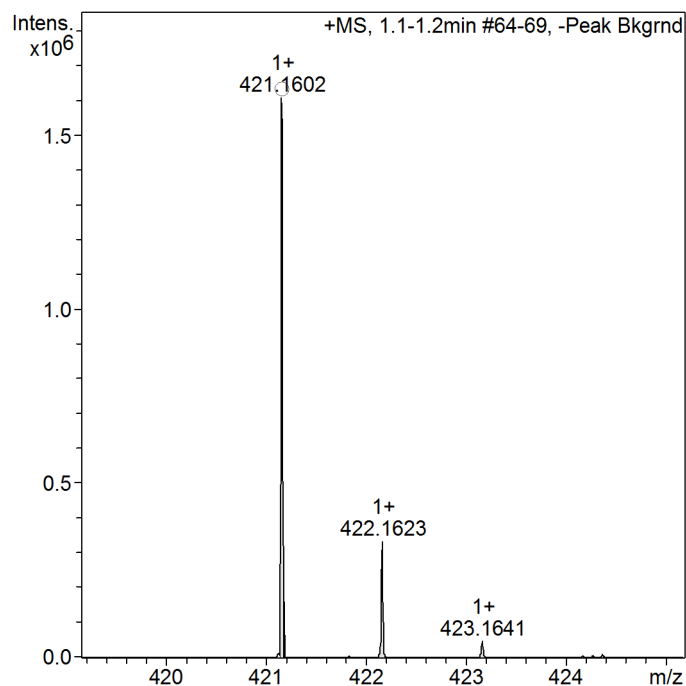


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.1 min	1.11	70.2	no uv	
Cmpd 2, 1.3 min	1.25	29.8	no uv	

Cmpd 1, 1.1 min





Confirm/Find Formula Results

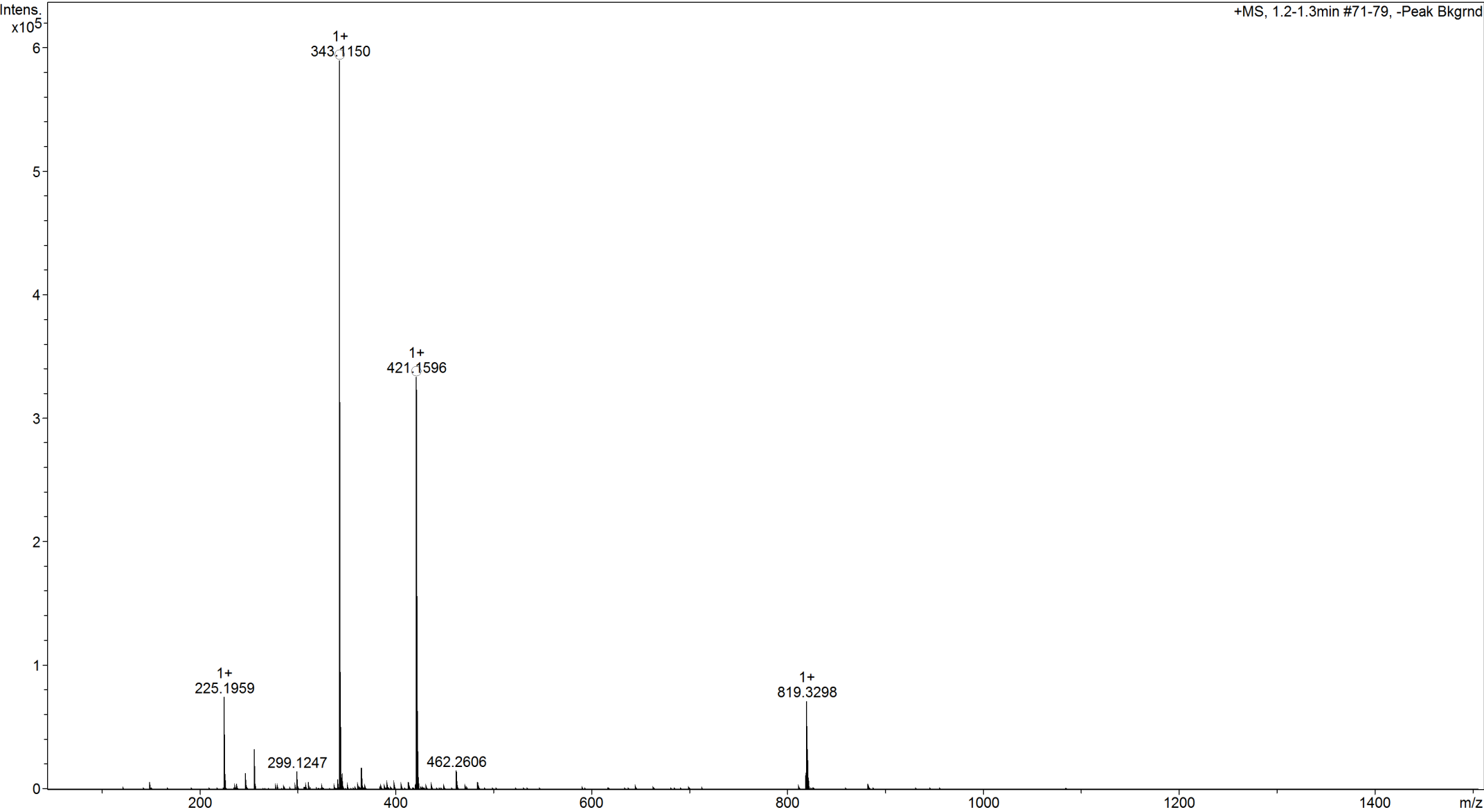
The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

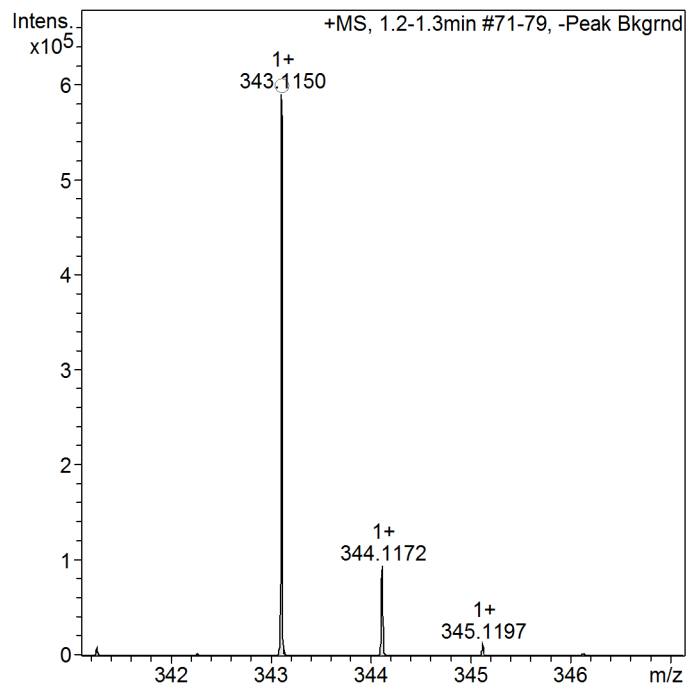
Cmpd 1, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
344.117572	C8H14N11O5	1+	344.117389	-0.2	-0.5	20.2	100.00	C8H13N11O5	M+H
	C11H22NO11	1+	344.118737	1.2	3.4	22.1	58.02	C11H21NO11	M+H
	C9H10N15O	1+	344.118726	1.2	3.4	33.4	44.65	C9H9N15O	M+H
	C8H14N11O5	1+	344.117389	-0.2	-0.5	20.2	100.00	C8H10N10O5	M+NH4
	C11H22NO11	1+	344.118737	1.2	3.4	22.1	58.02	C11H18O11	M+NH4
	C9H10N15O	1+	344.118726	1.2	3.4	33.4	44.65	C9H6N14O	M+NH4
	C7H11N15NaO	1+	344.116321	-1.3	-3.6	21.0	55.68	C7H11N15O	M+Na
	C10H19N5NaO7	1+	344.117669	0.1	0.3	21.3	100.00	C10H19N5O7	M+Na
	C9H16N9Na2O3	1+	344.116600	-1.0	-2.8	21.6	100.00	C9H17N9O3	M+Na2-H
	C17H17N12O2	1+	421.159194	-1.0	-2.3	12.8	74.50	C17H16N12O2	M+H
421.160178	C20H25N2O8	1+	421.160542	0.4	0.9	14.0	100.00	C20H24N2O8	M+H
	C21H21N6O4	1+	421.161880	1.7	4.0	26.3	35.43	C21H20N6O4	M+H
	C17H17N12O2	1+	421.159194	-1.0	-2.3	12.8	74.50	C17H13N11O2	M+NH4
	C20H25N2O8	1+	421.160542	0.4	0.9	14.0	100.00	C20H21N2O8	M+NH4
	C21H21N6O4	1+	421.161880	1.7	4.0	26.3	35.43	C21H17N5O4	M+NH4
	C19H22N6NaO4	1+	421.159474	-0.7	-1.7	13.6	100.00	C19H22N6O4	M+Na
	C20H18N10Na	1+	421.160811	0.6	1.5	27.0	77.85	C20H18N10	M+Na
	C17H22KN100	1+	421.160963	0.8	1.9	35.7	91.10	C17H22N100	M+K
	C16H26KN6O5	1+	421.159626	-0.6	-1.3	36.7	100.00	C16H26N6O5	M+K
	C21H27Na2O6	1+	421.159754	-0.4	-1.0	14.8	100.00	C21H28O6	M+Na2-H
	C22H23N4Na2O2	1+	421.161091	0.9	2.2	27.7	58.79	C22H24N4O2	M+Na2-H
	C20H25N2O8	1+	421.160542	0.4	0.9	14.0	100.00	C10H12N4O4	2M+H
	C20H18N10Na	1+	421.160811	0.6	1.5	27.0	77.85	C10H9N5	2M+Na

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

Cmpd 2, 1.3 min





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

Cmpd 2, 1.3 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
343.114983	C14H19N2O8	1+	343.113592	-1.4	-4.1	5.3	60.49	C14H18N2O8	M+H
	C15H15N6O4	1+	343.114929	-0.1	-0.2	15.7	100.00	C15H14N6O4	M+H
	C16H11N10	1+	343.116267	1.3	3.7	29.1	39.64	C16H10N10	M+H
	C14H19N2O8	1+	343.113592	-1.4	-4.1	5.3	60.49	C14H15N8O8	M+NH4
	C15H15N6O4	1+	343.114929	-0.1	-0.2	15.7	100.00	C15H11N5O4	M+NH4
	C16H11N10	1+	343.116267	1.3	3.7	29.1	39.64	C16H7N9	M+NH4
	C14H12N10Na	1+	343.113861	-1.1	-3.3	16.8	63.32	C14H12N10	M+Na
	C17H20NaO6	1+	343.115209	0.2	0.7	16.9	100.00	C17H20O6	M+Na
	C11H16KN100	1+	343.114013	-1.0	-2.8	33.3	86.08	C11H16N100	M+K
	C14H24KO7	1+	343.115361	0.4	1.1	39.1	100.00	C14H24O7	M+K
	C16H17N4Na2O2	1+	343.114141	-0.8	-2.5	17.2	100.00	C16H18N4O2	M+Na2-H
	C14H19N2O8	1+	343.113592	-1.4	-4.1	5.3	60.49	C7H9NO4	2M+H
	C16H11N10	1+	343.116267	1.3	3.7	29.1	39.64	C8H5N5	2M+H
	C14H12N10Na	1+	343.113861	-1.1	-3.3	16.8	63.32	C7H6N5	2M+Na
421.159627	C16H26KN6O5	1+	421.159626	-0.0	-0.0	36.6	100.00	C16H26N6O5	M+K
	C17H22KN100	1+	421.160963	1.3	3.2	37.7	49.03	C17H22N100	M+K
	C15H30KN2O9	1+	421.158289	-1.3	-3.2	39.5	46.58	C15H30N2O9	M+K
	C21H27Na2O6	1+	421.159754	0.1	0.3	21.8	100.00	C21H28O6	M+Na2-H
	C18H19N10Na2	1+	421.158406	-1.2	-2.9	21.9	56.90	C18H20N10	M+Na2-H
	C22H23N4Na2O2	1+	421.161091	1.5	3.5	35.0	35.71	C22H24N4O2	M+Na2-H
	C20H25N2O8	1+	421.160542	0.9	2.2	20.7	77.07	C10H12NO4	2M+H
	C18H26N2NaO8	1+	421.158137	-1.5	-3.5	8.2	62.38	C9H13NO4	2M+Na
	C20H18N10Na	1+	421.160811	1.2	2.8	34.3	42.95	C10H9N5	2M+Na