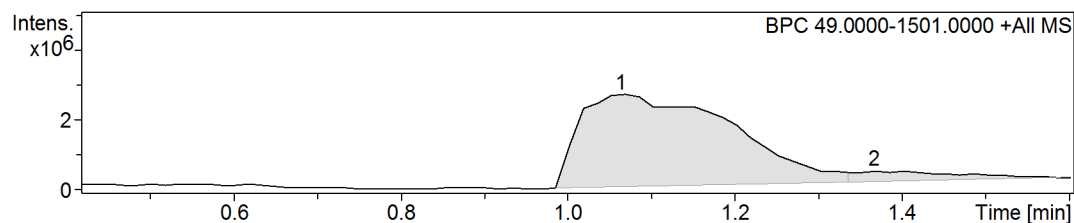


School of Chemistry Mass Spectrometry Service

SampleID ER05 Pure
Sample Description
Analysis Name D:\Data\malcolmhalcrow\cm15esjr\ER05 Pure_261387_BB2_01_54115.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

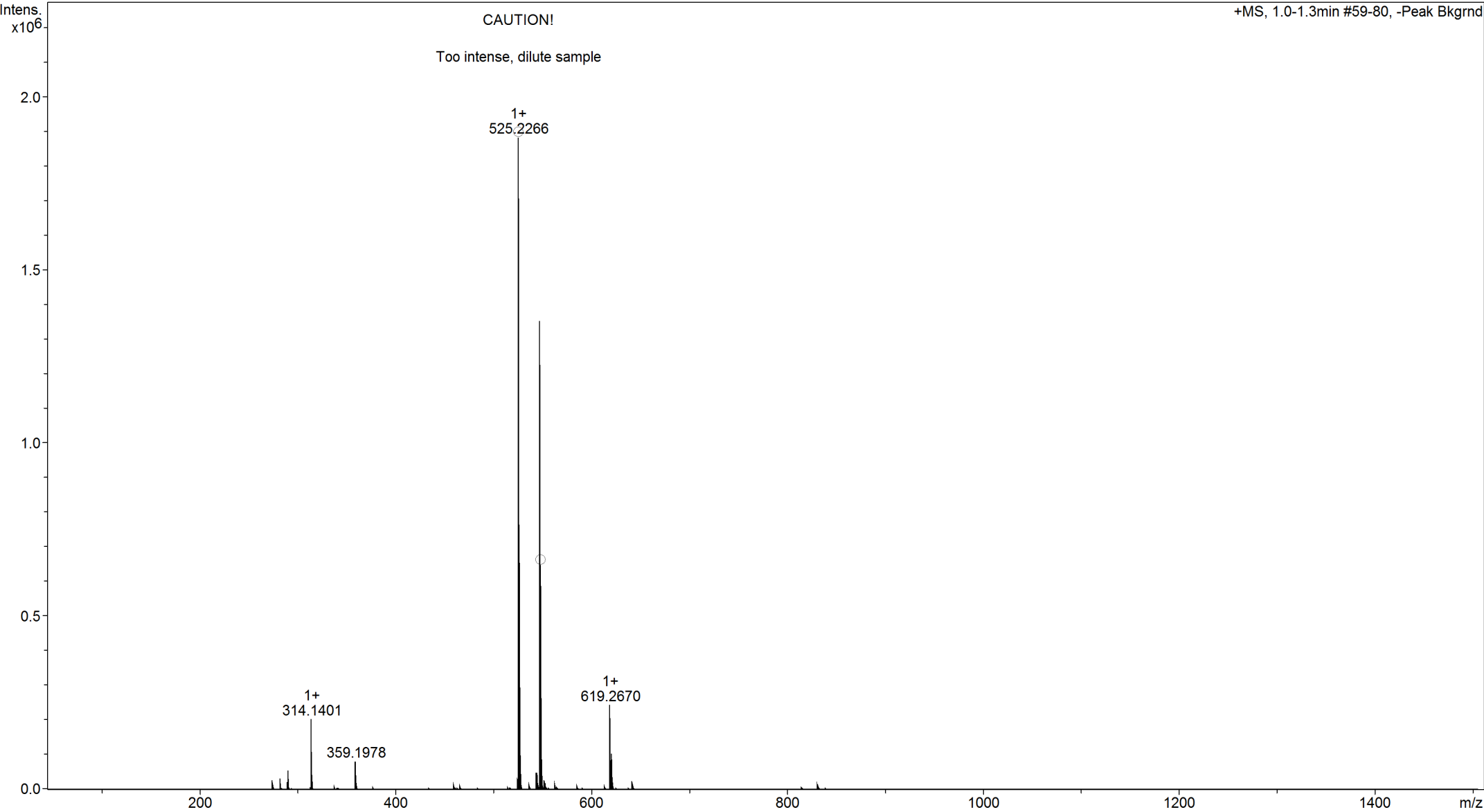
Submitter Emily Ratcliffe
Supervisor Malcolm Halcrow
Acquisition Date 15/02/2019 15:29:58
Scan Begin 50 m/z **Scan End** 1500 m/z

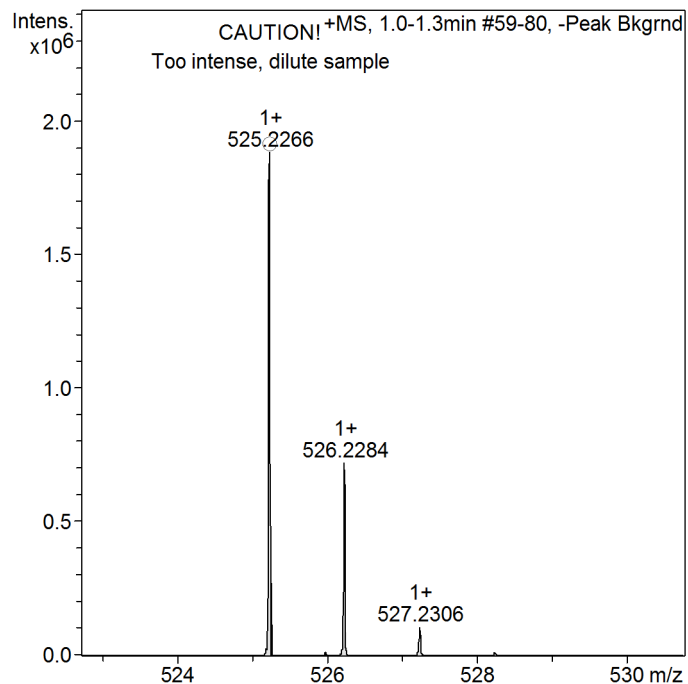


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.1 min	1.06	93.0	no uv	
Cmpd 2, 1.4 min	1.37	7.0	no uv	

Cmpd 1, 1.1 min





Confirm/Find Formula Results

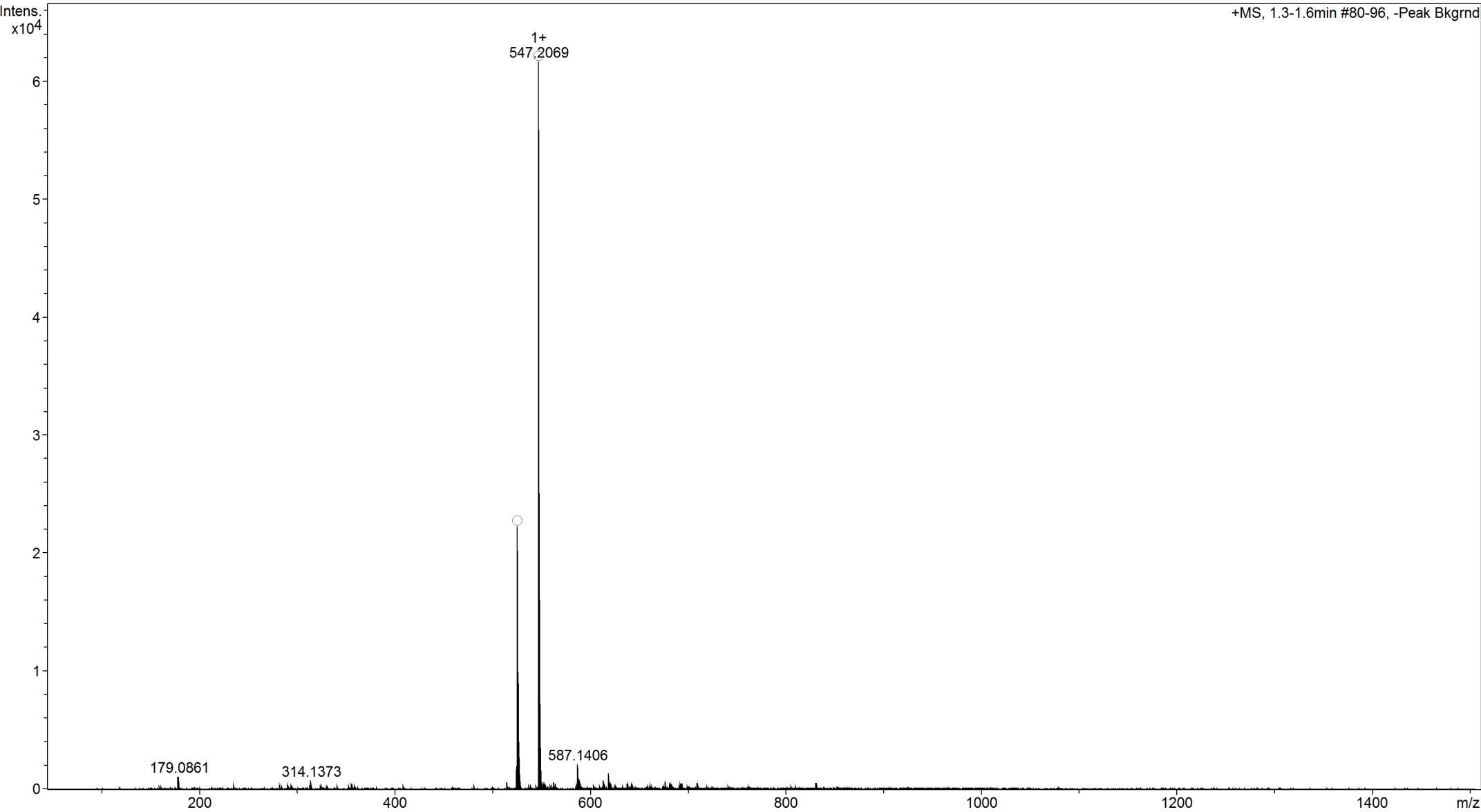
The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

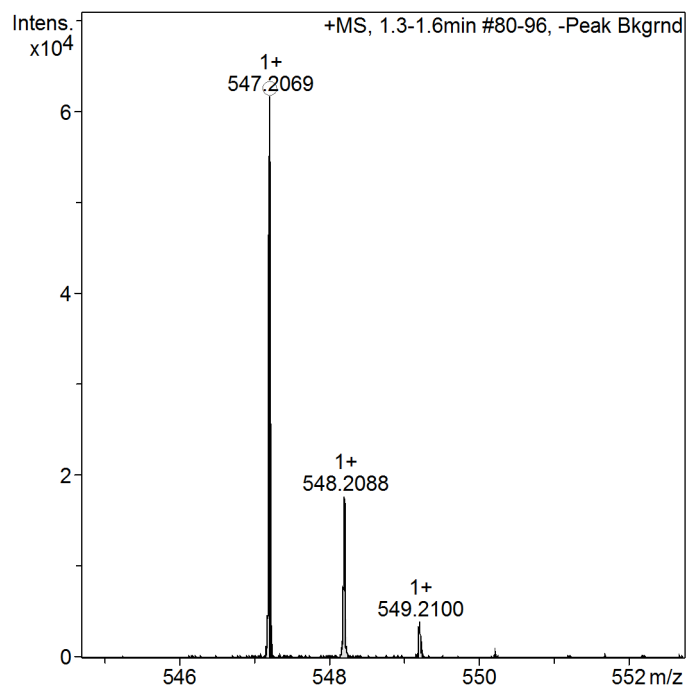
Cmpd 1, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
525.226611	C34H29N4O2	1+	525.228503	1.9	3.6	9.9	47.76	C34H28N4O2	M+H
	C30H25N10	1+	525.225817	-0.8	-1.5	10.5	95.00	C30H24N10	M+H
	C33H33O6	1+	525.227165	0.6	1.1	14.2	100.00	C33H32O6	M+H
	C29H29N6O4	1+	525.224480	-2.1	-4.1	21.9	31.23	C29H28N6O4	M+H
	C34H29N4O2	1+	525.228503	1.9	3.6	9.9	47.76	C34H25N3O2	M+NH4
	C30H25N10	1+	525.225817	-0.8	-1.5	10.5	95.00	C30H21N9	M+NH4
	C29H29N6O4	1+	525.224480	-2.1	-4.1	21.9	31.23	C29H25N5O4	M+NH4
	C32H30N4NaO2	1+	525.226097	-0.5	-1.0	11.0	100.00	C32H30N4O2	M+Na
	C31H34NaO6	1+	525.224760	-1.9	-3.5	21.9	35.62	C31H34O6	M+Na
	C35H31N2Na2	1+	525.227714	1.1	2.1	8.8	100.00	C35H32N2	M+Na2-H
	C34H29N4O2	1+	525.228503	1.9	3.6	9.9	47.76	C17H14N2O	2M+H
	C30H25N10	1+	525.225817	-0.8	-1.5	10.5	95.00	C15H12N5	2M+H
	C32H30N4NaO2	1+	525.226097	-0.5	-1.0	11.0	100.00	C16H15N2O	2M+Na
548.210686	C6H14N33	1+	548.210444	-0.2	-0.4	23.8	100.00	C6H13N33	M+H
	C9H22N23O6	1+	548.211792	1.1	2.0	24.3	63.43	C9H21N23O6	M+H
	C6H14N33	1+	548.210444	-0.2	-0.4	23.8	100.00	C6H10N32	M+NH4
	C9H22N23O6	1+	548.211792	1.1	2.0	24.3	63.43	C9H18N22O6	M+NH4
	C8H19N27NaO2	1+	548.210724	0.0	0.1	24.5	100.00	C8H19N27O2	M+Na
	C11H27N17NaO8	1+	548.212072	1.4	2.5	25.7	48.28	C11H27N17O8	M+Na
	C10H24N21Na2O4	1+	548.211003	0.3	0.6	25.5	100.00	C10H25N21O4	M+Na2-H
	C13H32N11Na2O10	1+	548.212351	1.7	3.0	27.2	44.51	C13H33N11O10	M+Na2-H
	C11H20N25Na2	1+	548.212341	1.7	3.0	38.7	33.62	C11H21N25	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

Cmpd 2, 1.4 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, 1.4 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
525.222508	C24H29N8O6	1+	525.220457	-2.1	-3.9	6.1	47.68	C24H28N8O6	M+H
	C28H33N2O8	1+	525.223142	0.6	1.2	14.7	100.00	C28H32N2O8	M+H
	C25H25N12O2	1+	525.221795	-0.7	-1.4	18.5	66.61	C25H24N12O2	M+H
	C29H29N6O4	1+	525.224480	2.0	3.8	26.4	33.53	C29H28N6O4	M+H
	C24H29N8O6	1+	525.220457	-2.1	-3.9	6.1	47.68	C24H25N7O6	M+NH4
	C28H33N2O8	1+	525.223142	0.6	1.2	14.7	100.00	C28H29N8O8	M+NH4
	C25H25N12O2	1+	525.221795	-0.7	-1.4	18.5	66.61	C25H21N11O2	M+NH4
	C29H29N6O4	1+	525.224480	2.0	3.8	26.4	33.53	C29H25N5O4	M+NH4
	C26H34N2NaO8	1+	525.220737	-1.8	-3.4	4.8	55.96	C26H34N2O8	M+Na
	C27H30N6NaO4	1+	525.222074	-0.4	-0.8	16.0	100.00	C27H30N6O4	M+Na
	C28H26N10Na	1+	525.223412	0.9	1.7	31.8	41.35	C28H26N10	M+Na
	C24H34KN6O5	1+	525.222226	-0.3	-0.5	30.4	100.00	C24H34N6O5	M+K
	C25H30KN10O	1+	525.223564	1.1	2.0	32.0	64.71	C25H30N10O	M+K
	C23H38KN2O9	1+	525.220889	-1.6	-3.1	33.4	43.72	C23H38N2O9	M+K
	C29H35Na2O6	1+	525.222354	-0.2	-0.3	16.2	100.00	C29H36O6	M+Na2-H
	C26H27N10Na2	1+	525.221006	-1.5	-2.9	20.8	32.87	C26H28N10	M+Na2-H
	C30H31N4Na2O2	1+	525.223691	1.2	2.3	27.9	45.63	C30H32N4O2	M+Na2-H
	C24H29N8O6	1+	525.220457	-2.1	-3.9	6.1	47.68	C12H14N4O3	2M+H
	C28H33N2O8	1+	525.223142	0.6	1.2	14.7	100.00	C14H16NO4	2M+H
	C26H34N2NaO8	1+	525.220737	-1.8	-3.4	4.8	55.96	C13H17NO4	2M+Na
547.206920	C28H26N10Na	1+	525.223412	0.9	1.7	31.8	41.35	C14H13N5	2M+Na
	C26H27N8O6	1+	547.204807	-2.1	-3.9	14.2	47.98	C26H26N8O6	M+H
	C30H31N2O8	1+	547.207492	0.6	1.0	25.7	100.00	C30H30N2O8	M+H
	C27H23N12O2	1+	547.206144	-0.8	-1.4	25.9	89.65	C27H22N12O2	M+H
	C31H27N6O4	1+	547.208830	1.9	3.5	37.3	32.88	C31H26N6O4	M+H
	C26H27N8O6	1+	547.204807	-2.1	-3.9	14.2	47.98	C26H23N7O6	M+NH4
	C30H31N2O8	1+	547.207492	0.6	1.0	25.7	100.00	C30H27N8O8	M+NH4
	C27H23N12O2	1+	547.206144	-0.8	-1.4	25.9	89.65	C27H19N11O2	M+NH4
	C31H27N6O4	1+	547.208830	1.9	3.5	37.3	32.88	C31H23N5O4	M+NH4
	C28H32N2NaO8	1+	547.205087	-1.8	-3.3	14.6	57.51	C28H32N2O8	M+Na
	C29H28N6NaO4	1+	547.206424	-0.5	-0.9	26.3	100.00	C29H28N6O4	M+Na
	C15H20N22NaO	1+	547.208264	1.3	2.5	30.9	41.92	C15H20N22O	M+Na
	C17H32N8NaO11	1+	547.208275	1.4	2.5	34.6	50.60	C17H32N8O11	M+Na
	C30H24N10Na	1+	547.207762	0.8	1.5	38.1	62.49	C30H24N10	M+Na

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
	C33H32NaO6	1+	547.209109	2.2	4.0	38.1	25.35	C33H32O6	M+Na
	C25H36KN2O9	1+	547.205239	-1.7	-3.1	34.4	47.64	C25H36N2O9	M+K
	C26H32KN6O5	1+	547.206576	-0.3	-0.6	35.4	100.00	C26H32N6O5	M+K
	C31H33Na2O6	1+	547.206704	-0.2	-0.4	27.0	100.00	C31H34O6	M+Na2-H
	C17H25N16Na2O3	1+	547.208544	1.6	3.0	29.0	32.61	C17H26N16O3	M+Na2-H
	C28H25N10Na2	1+	547.205356	-1.6	-2.9	31.7	31.74	C28H26N10	M+Na2-H
	C19H37N2Na2O13	1+	547.208554	1.6	3.0	33.6	38.52	C19H38N2O13	M+Na2-H
	C32H29N4Na2O2	1+	547.208041	1.1	2.0	38.6	46.87	C32H30N4O2	M+Na2-H
	C26H27N8O6	1+	547.204807	-2.1	-3.9	14.2	47.98	C13H13N4O3	2M+H
	C30H31N2O8	1+	547.207492	0.6	1.0	25.7	100.00	C15H15NO4	2M+H
	C28H32N2NaO8	1+	547.205087	-1.8	-3.3	14.6	57.51	C14H16NO4	2M+Na
	C30H24N10Na	1+	547.207762	0.8	1.5	38.1	62.49	C15H12N5	2M+Na