

# School of Chemistry Mass Spectrometry Service

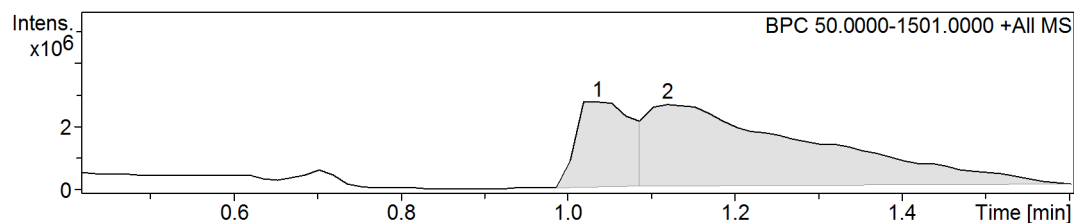
**SampleID** Butyl PR3  
**Sample Description**  
**Analysis Name** D:\Data\michaelehardie\chmft\Butyl PR3\_137403\_BB3\_01\_13634.d  
**Method** 3a\_AccMass\_Loop\_Positive.m  
**Instrument** maXis impact      **Source Type** ESI      **Ion Polarity** Positive

**Submitter** Flora Thorp-Greenwood

**Supervisor** Michael Hardie

**Acquisition Date** 10/07/2015 13:00:50

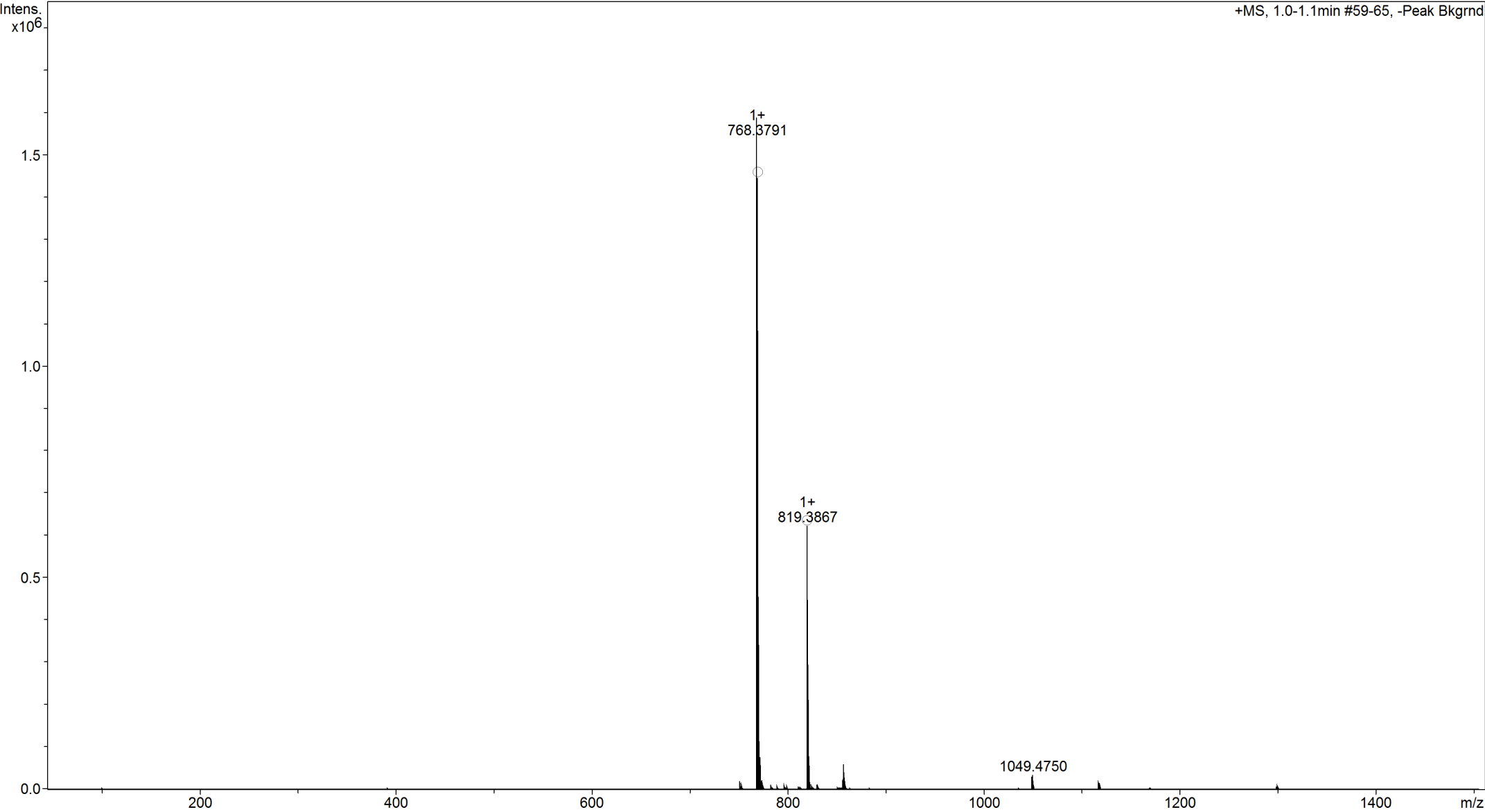
**Scan Begin** 50 m/z      **Scan End** 1500 m/z

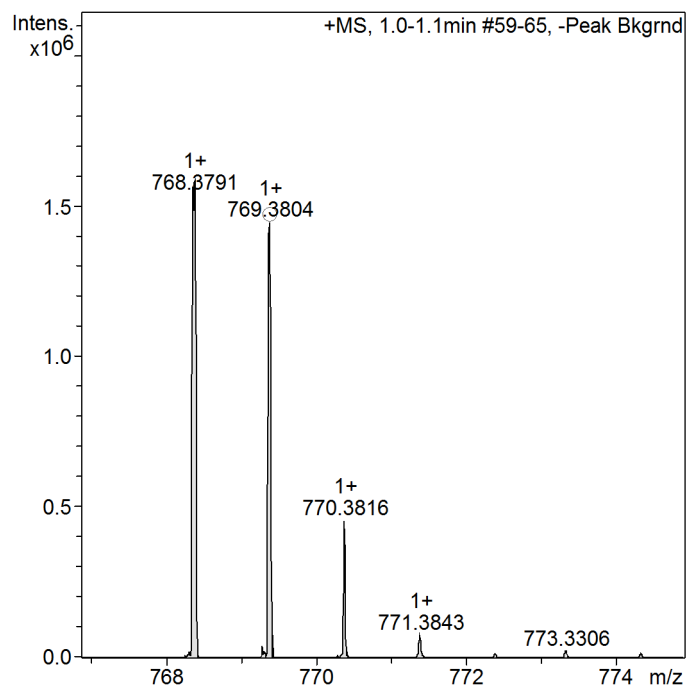


## Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.0 min	1.04	26.4	no uv	
Cmpd 2, 1.1 min	1.12	73.6	no uv	

Cmpd 1, 1.0 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, 1.0 min

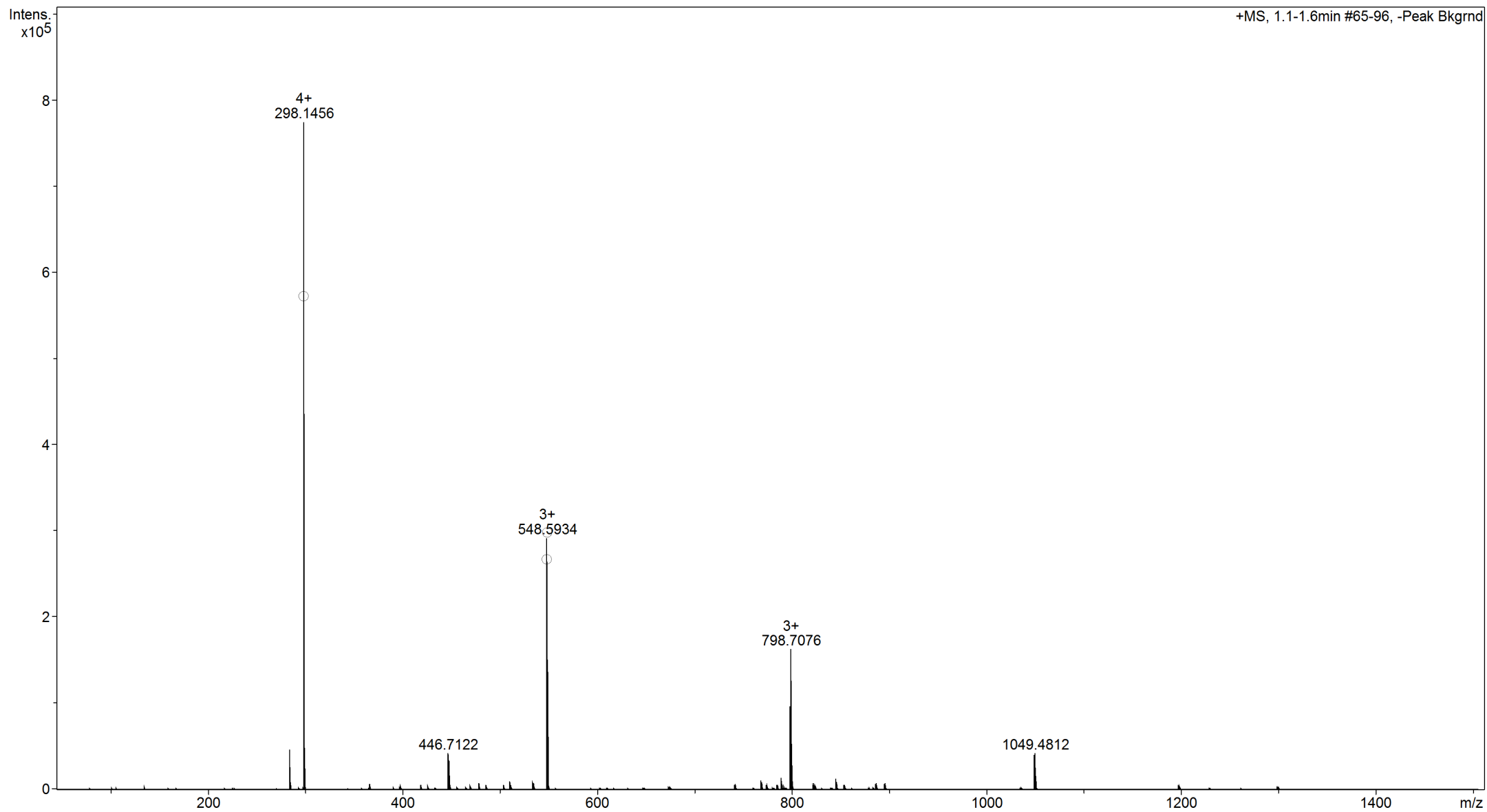
Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
769.380369	C25H54N12NaO14	1+	769.377465	-2.9	-3.8	15.3	20.33	C25 H53 N12 Na O14	M+H
	C23H42N26NaO4	1+	769.377455	-2.9	-3.8	19.2	18.57	C23 H41 N26 Na O4	M+H
	C16H46N26NaO9	1+	769.383328	-3.0	-3.8	19.3	17.76	C16 H45 N26 Na O9	M+H
	C13H38N36NaO3	1+	769.381980	1.6	2.1	19.3	53.67	C13 H37 N36 Na O3	M+H
	C26H50N16NaO10	1+	769.378803	1.6	2.0	22.1	52.13	C26 H49 N16 Na O10	M+H
	C29H58N6NaO16	1+	769.380151	0.2	0.3	26.2	100.00	C29 H57 N6 Na O16	M+H
	C24H38N30Na	1+	769.378792	1.6	2.0	30.3	42.80	C24 H37 N30 Na	M+H
	C27H46N20NaO6	1+	769.380140	-0.2	-0.3	32.0	86.61	C27 H45 N20 Na O6	M+H
	C33H62NaO18	1+	769.382836	-2.5	-3.2	34.5	19.46	C33 H61 Na O18	M+H
	C30H54N10NaO12	1+	769.381488	1.1	1.5	34.8	51.09	C30 H53 N10 Na O12	M+H
	C25H54N12NaO14	1+	769.377465	-2.9	-3.8	15.3	20.33	C25 H50 N11 Na O14	M+NH4
	C23H42N26NaO4	1+	769.377455	-2.9	-3.8	19.2	18.57	C23 H38 N25 Na O4	M+NH4
	C16H46N26NaO9	1+	769.383328	-3.0	-3.8	19.3	17.76	C16 H42 N25 Na O9	M+NH4
	C13H38N36NaO3	1+	769.381980	1.6	2.1	19.3	53.67	C13 H34 N35 Na O3	M+NH4
	C26H50N16NaO10	1+	769.378803	1.6	2.0	22.1	52.13	C26 H46 N15 Na O10	M+NH4
	C29H58N6NaO16	1+	769.380151	0.2	0.3	26.2	100.00	C29 H54 N5 Na O16	M+NH4
	C24H38N30Na	1+	769.378792	1.6	2.0	30.3	42.80	C24 H34 N29 Na	M+NH4
	C27H46N20NaO6	1+	769.380140	-0.2	-0.3	32.0	86.61	C27 H42 N19 Na O6	M+NH4
	C33H62NaO18	1+	769.382836	-2.5	-3.2	34.5	19.46	C33 H62 Na O18	M+NH4
	C30H54N10NaO12	1+	769.381488	1.1	1.5	34.8	51.09	C30 H50 N9 Na O12	M+NH4
	C25H54N12NaO14	1+	769.377465	-2.9	-3.8	15.3	20.33	C25 H54 N12 O14	M+Na
	C23H42N26NaO4	1+	769.377455	-2.9	-3.8	19.2	18.57	C23 H42 N26 O4	M+Na
	C16H46N26NaO9	1+	769.383328	-3.0	-3.8	19.3	17.76	C16 H46 N26 O9	M+Na
	C13H38N36NaO3	1+	769.381980	1.6	2.1	19.3	53.67	C13 H38 N36 O3	M+Na
	C26H50N16NaO10	1+	769.378803	1.6	2.0	22.1	52.13	C26 H50 N16 O10	M+Na
	C29H58N6NaO16	1+	769.380151	0.2	0.3	26.2	100.00	C29 H58 N6 O16	M+Na
	C24H38N30Na	1+	769.378792	1.6	2.0	30.3	42.80	C24 H38 N30	M+Na
	C27H46N20NaO6	1+	769.380140	-0.2	-0.3	32.0	86.61	C27 H46 N20 O6	M+Na
	C33H62NaO18	1+	769.382836	-2.5	-3.2	34.5	19.46	C33 H62 O18	M+Na
	C30H54N10NaO12	1+	769.381488	1.1	1.5	34.8	51.09	C30 H54 N10 O12	M+Na
	C20H46KN26O5	1+	769.377607	-2.8	-3.6	37.1	36.73	C20 H46 N26 O5	M+K
	C21H42KN30O	1+	769.378944	1.4	1.9	38.8	100.00	C21 H42 N30 O	M+K
	C27H59N6Na2O16	1+	769.377745	-2.6	-3.4	17.6	27.91	C27 H60 N6 O16	M+Na2-H
	C15H43N30Na2O5	1+	769.382260	-1.9	-2.5	18.4	49.90	C15 H44 N30 O5	M+Na2-H

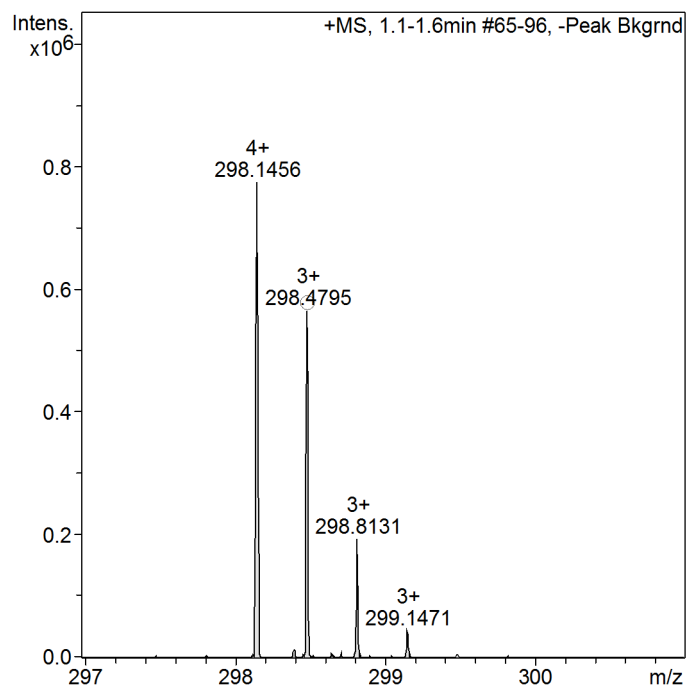
Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;
Smart Formula Search Parameters	
CHNO and adducts considered implicitly	
Formula Search Minimum	
Formula Search Maximum	
Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	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

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
819.386687	C25H47N20Na2O6	1+	769.377734	-2.6	-3.4	20.7	25.91	C25 H48 N20 O6	M+Na2-H
	C28H55N10Na2O12	1+	769.379082	-1.3	-1.7	24.0	66.70	C28 H56 N10 O12	M+Na2-H
	C26H43N24Na2O2	1+	769.379072	-1.3	-1.7	31.4	55.58	C26 H44 N24 O2	M+Na2-H
	C29H51N14Na2O8	1+	769.380420	0.1	0.1	33.6	100.00	C29 H52 N14 O8	M+Na2-H
	C32H59N4Na2O14	1+	769.381768	-1.4	-1.8	36.7	45.62	C32 H60 N4 O14	M+Na2-H
	C28H55N10Na2O12	1+	769.379082	-1.3	-1.7	24.0	66.70	C14 H27 N5 Na O6	2M+H
	C26H43N24Na2O2	1+	769.379072	-1.3	-1.7	31.4	55.58	C13 H21 N12 Na O	2M+H
	C32H59N4Na2O14	1+	769.381768	-1.4	-1.8	36.7	45.62	C16 H29 N2 Na O7	2M+H
	C26H50N16NaO10	1+	769.378803	1.6	2.0	22.1	52.13	C13 H25 N8 O5	2M+Na
	C24H38N30Na	1+	769.378792	1.6	2.0	30.3	42.80	C12 H19 N15	2M+Na
	C30H54N10NaO12	1+	769.381488	1.1	1.5	34.8	51.09	C15 H27 N5 O6	2M+Na
	C40H56N6NaO11	1+	819.389927	3.2	4.0	3.1	21.27	C40 H55 N6 Na O11	M+H
	C37H48N16NaO5	1+	819.388579	-1.9	-2.3	6.3	52.69	C37 H47 N16 Na O5	M+H
	C38H44N20NaO	1+	819.389917	3.2	3.9	10.3	15.14	C38 H43 N20 Na O	M+H
	C39H60N2NaO15	1+	819.388590	-1.9	-2.3	13.3	57.36	C39 H59 N2 Na O15	M+H
	C36H52N12NaO9	1+	819.387242	0.6	0.7	15.8	100.00	C36 H51 N12 Na O9	M+H
	C33H44N22NaO3	1+	819.385894	0.8	1.0	19.1	82.69	C33 H43 N22 Na O3	M+H
	C35H56N8NaO13	1+	819.385905	0.8	1.0	24.2	92.84	C35 H55 N8 Na O13	M+H
	C32H48N18NaO7	1+	819.384557	2.1	2.6	29.1	27.36	C32 H47 N18 Na O7	M+H
	C47H52N6NaO6	1+	819.384054	2.6	3.2	32.7	20.52	C47 H51 N6 Na O6	M+H
	C34H60N4NaO17	1+	819.384567	2.1	2.6	34.5	30.09	C34 H59 N4 Na O17	M+H
	C40H56N6NaO11	1+	819.389927	3.2	4.0	3.1	21.27	C40 H52 N5 Na O11	M+NH4
	C37H48N16NaO5	1+	819.388579	-1.9	-2.3	6.3	52.69	C37 H44 N15 Na O5	M+NH4
	C38H44N20NaO	1+	819.389917	3.2	3.9	10.3	15.14	C38 H40 N19 Na O	M+NH4
	C39H60N2NaO15	1+	819.388590	-1.9	-2.3	13.3	57.36	C39 H56 N Na O15	M+NH4
	C36H52N12NaO9	1+	819.387242	0.6	0.7	15.8	100.00	C36 H48 N11 Na O9	M+NH4
	C33H44N22NaO3	1+	819.385894	0.8	1.0	19.1	82.69	C33 H40 N21 Na O3	M+NH4
	C35H56N8NaO13	1+	819.385905	0.8	1.0	24.2	92.84	C35 H52 N7 Na O13	M+NH4
	C32H48N18NaO7	1+	819.384557	2.1	2.6	29.1	27.36	C32 H44 N17 Na O7	M+NH4
	C47H52N6NaO6	1+	819.384054	2.6	3.2	32.7	20.52	C47 H48 N5 Na O6	M+NH4
	C34H60N4NaO17	1+	819.384567	2.1	2.6	34.5	30.09	C34 H56 N3 Na O17	M+NH4
	C40H56N6NaO11	1+	819.389927	3.2	4.0	3.1	21.27	C40 H56 N6 O11	M+Na
	C37H48N16NaO5	1+	819.388579	-1.9	-2.3	6.3	52.69	C37 H48 N16 O5	M+Na
	C38H44N20NaO	1+	819.389917	3.2	3.9	10.3	15.14	C38 H44 N20 O	M+Na
	C39H60N2NaO15	1+	819.388590	-1.9	-2.3	13.3	57.36	C39 H60 N2 O15	M+Na
	C36H52N12NaO9	1+	819.387242	0.6	0.7	15.8	100.00	C36 H52 N12 O9	M+Na
	C33H44N22NaO3	1+	819.385894	0.8	1.0	19.1	82.69	C33 H44 N22 O3	M+Na
	C35H56N8NaO13	1+	819.385905	0.8	1.0	24.2	92.84	C35 H56 N8 O13	M+Na
	C32H48N18NaO7	1+	819.384557	2.1	2.6	29.1	27.36	C32 H48 N18 O7	M+Na
	C47H52N6NaO6	1+	819.384054	2.6	3.2	32.7	20.52	C47 H52 N6 O6	M+Na
	C34H60N4NaO17	1+	819.384567	2.1	2.6	34.5	30.09	C34 H60 N4 O17	M+Na
	C31H44KN26	1+	819.387384	-0.7	-0.8	25.0	100.00	C31 H44 N26	M+K

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
	C34H52KN16O6	1+	819.388732	-2.0	-2.5	30.0	37.52	C34 H52 N16 O6	M+K
	C30H48KN22O4	1+	819.386046	-0.6	-0.8	32.4	86.32	C30 H48 N22 O4	M+K
	C33H56KN12O10	1+	819.387394	-0.7	-0.9	36.3	75.50	C33 H56 N12 O10	M+K
	C39H53N10Na2O7	1+	819.388859	-2.2	-2.7	3.9	38.70	C39 H54 N10 O7	M+Na2-H
	C36H45N20Na2O	1+	819.387511	0.8	1.0	9.9	85.23	C36 H46 N20 O	M+Na2-H
	C38H57N6Na2O11	1+	819.387522	-0.8	-1.0	12.9	100.00	C38 H58 N6 O11	M+Na2-H
	C35H49N16Na2O5	1+	819.386174	-0.5	-0.6	17.1	86.81	C35 H50 N16 O5	M+Na2-H
	C37H61N2Na2O15	1+	819.386184	-0.5	-0.6	23.3	95.43	C37 H62 N2 O15	M+Na2-H
	C34H53N12Na2O9	1+	819.384836	1.9	2.3	27.5	30.67	C34 H54 N12 O9	M+Na2-H
	C31H45N22Na2O3	1+	819.383488	3.2	3.9	30.4	8.86	C31 H46 N22 O3	M+Na2-H
	C49H57Na2O8	1+	819.384334	-2.4	-2.9	34.1	17.62	C49 H58 O8	M+Na2-H
	C33H57N8Na2O13	1+	819.383499	3.2	3.9	38.7	7.24	C33 H58 N8 O13	M+Na2-H

Cmpd 2, 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 2, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
298.479475	C28H64N16Na9O4	3+	298.478641	0.8	2.8	14.2	100.00	C28 H64 N16 Na6 O4	M+Na
	C29H60N20Na9	3+	298.479087	0.4	1.3	25.9	97.40	C29 H60 N20 Na6	M+Na
	C33H64N14Na9O2	3+	298.479982	0.5	1.7	37.7	68.68	C33 H64 N14 Na6 O2	M+Na
	C28H64N16Na9O4	3+	298.478641	0.8	2.8	14.2	100.00	C14 H32 N8 Na3 O2	2M+Na
548.258814	C98H107N11Na9	3+	548.259123	0.3	0.6	15.4	95.28	C98 H104 N11 Na9	M+H
	C97H111N7Na9O4	3+	548.258678	0.1	0.2	16.7	100.00	C97 H108 N7 Na9 O4	M+H
	C96H115N3Na9O8	3+	548.258232	-0.6	-1.1	21.7	73.43	C96 H112 N3 Na9 O8	M+H
	C98H107N11Na9	3+	548.259123	0.3	0.6	15.4	95.28	C98 H95 N8 Na9	M+NH4
	C97H111N7Na9O4	3+	548.258678	0.1	0.2	16.7	100.00	C97 H99 N4 Na9 O4	M+NH4
	C96H115N3Na9O8	3+	548.258232	-0.6	-1.1	21.7	73.43	C96 H103 Na9 O8	M+NH4
	C98H107N11Na9	3+	548.259123	0.3	0.6	15.4	95.28	C98 H107 N11 Na6	M+Na
	C97H111N7Na9O4	3+	548.258678	0.1	0.2	16.7	100.00	C97 H111 N7 Na6 O4	M+Na
	C96H115N3Na9O8	3+	548.258232	-0.6	-1.1	21.7	73.43	C96 H115 N3 Na6 O8	M+Na
	C35H5N21Na9O45	3+	548.593705	-0.3	-0.6	18.1	100.00	C35 H2 N21 Na9 O45	M+H
548.593367	C34H9N17Na9O49	3+	548.593259	0.1	0.2	27.3	90.14	C34 H6 N17 Na9 O49	M+H
	C37H17N7Na9O55	3+	548.593708	0.3	0.6	28.8	78.67	C37 H14 N7 Na9 O55	M+H
	C31HN27Na9O43	3+	548.592810	0.6	1.0	29.5	58.20	C31 H N27 Na9 O43	M+H
	C31H90N64Na9O5	3+	548.593947	0.6	1.1	32.1	53.99	C31 H87 N64 Na9 O5	M+H
	C49H13N5Na9O48	3+	548.593092	-0.3	-0.5	35.9	67.77	C49 H10 N5 Na9 O48	M+H
	C33H13N13Na9O53	3+	548.592813	0.6	1.0	36.8	58.20	C33 H10 N13 Na9 O53	M+H
	C36H21N3Na9O59	3+	548.593263	0.1	0.2	37.8	69.38	C36 H18 N3 Na9 O59	M+H
	C35H5N21Na9O45	3+	548.593705	-0.3	-0.6	18.1	100.00	C35 H5 N21 Na9 O45	M+NH4
	C34H9N17Na9O49	3+	548.593259	0.1	0.2	27.3	90.14	C34 H9 N17 Na9 O49	M+NH4
	C37H17N7Na9O55	3+	548.593708	0.3	0.6	28.8	78.67	C37 H5 N4 Na9 O55	M+NH4
	C31HN27Na9O43	3+	548.592810	0.6	1.0	29.5	58.20	C31 H N27 Na9 O43	M+NH4
	C31H90N64Na9O5	3+	548.593947	0.6	1.1	32.1	53.99	C31 H78 N61 Na9 O5	M+NH4
	C49H13N5Na9O48	3+	548.593092	-0.3	-0.5	35.9	67.77	C49 H N2 Na9 O48	M+NH4
	C33H13N13Na9O53	3+	548.592813	0.6	1.0	36.8	58.20	C33 H N10 Na9 O53	M+NH4
	C36H21N3Na9O59	3+	548.593263	0.1	0.2	37.8	69.38	C36 H9 Na9 O59	M+NH4
	C35H5N21Na9O45	3+	548.593705	-0.3	-0.6	18.1	100.00	C35 H5 N21 Na6 O45	M+Na
	C34H9N17Na9O49	3+	548.593259	0.1	0.2	27.3	90.14	C34 H9 N17 Na6 O49	M+Na
	C37H17N7Na9O55	3+	548.593708	0.3	0.6	28.8	78.67	C37 H17 N7 Na6 O55	M+Na
	C31HN27Na9O43	3+	548.592810	0.6	1.0	29.5	58.20	C31 H N27 Na6 O43	M+Na
	C31H90N64Na9O5	3+	548.593947	0.6	1.1	32.1	53.99	C31 H90 N64 Na6 O5	M+Na

Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;
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

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
	C49H13N5Na9O48	3+	548.593092	-0.3	-0.5	35.9	67.77	C49 H13 N5 Na6 O48	M+Na
	C33H13N13Na9O53	3+	548.592813	0.6	1.0	36.8	58.20	C33 H13 N13 Na6 O53	M+Na
	C36H21N3Na9O59	3+	548.593263	0.1	0.2	37.8	69.38	C36 H21 N3 Na6 O59	M+Na
	C42H14N11Na18O35	3+	548.593193	-0.2	-0.3	5.1	92.96	C42 H17 N11 Na12 O35	M+Na2-H
	C39H6N21Na18O29	3+	548.592743	0.6	1.1	5.7	74.73	C39 H9 N21 Na12 O29	M+Na2-H
	C45H22NNa18O41	3+	548.593642	-0.3	-0.5	8.8	100.00	C45 H25 N Na12 O41	M+Na2-H
	C40H2N25Na18O25	3+	548.593189	-0.2	-0.3	9.4	86.06	C40 H5 N25 Na12 O25	M+Na2-H
	C43H10N15Na18O31	3+	548.593638	-0.3	-0.5	9.6	82.31	C43 H13 N15 Na12 O31	M+Na2-H
	C46H18N5Na18O37	3+	548.594088	-0.7	-1.3	11.9	76.19	C46 H21 N5 Na12 O37	M+Na2-H
	C41H18N7Na18O39	3+	548.592747	-0.6	-1.1	13.7	64.48	C41 H21 N7 Na12 O39	M+Na2-H
	C44H6N19Na18O27	3+	548.594084	0.7	1.3	19.7	54.35	C44 H9 N19 Na12 O27	M+Na2-H