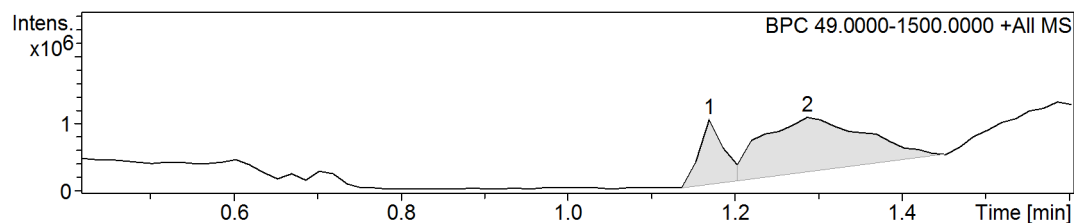


School of Chemistry Mass Spectrometry Service

SampleID Octyl pillar
Sample Description
Analysis Name D:\Data\MichaelHardie\chmft\Octyl pillar_132005_GA3_01_12284.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact **Source Type** ESI **Ion Polarity** Positive

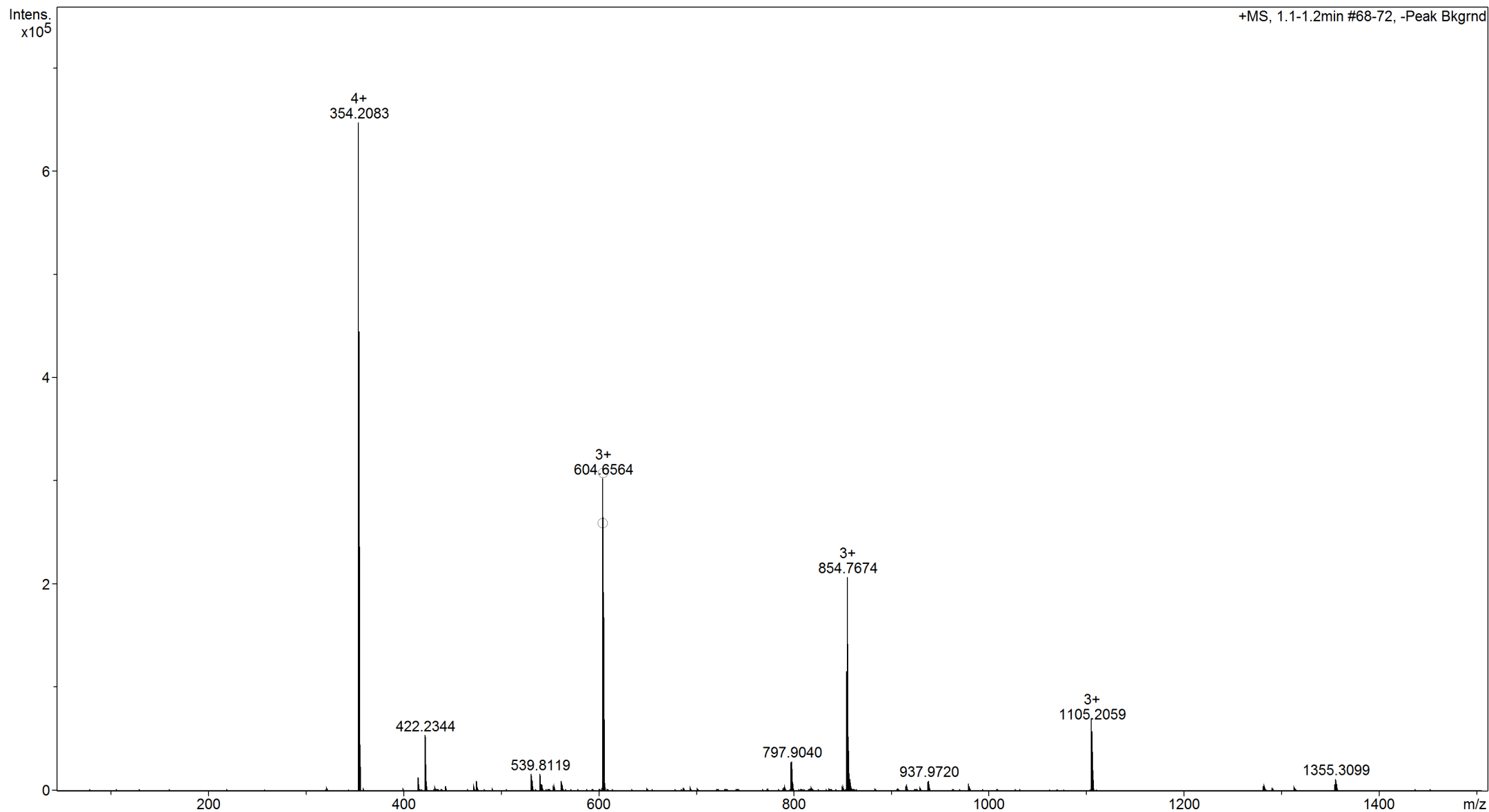
Submitter Flora Thorp-Greenwood
Supervisor Michael Hardie
Acquisition Date 18/05/2015 13:04:05
Scan Begin 50 m/z **Scan End** 1500 m/z

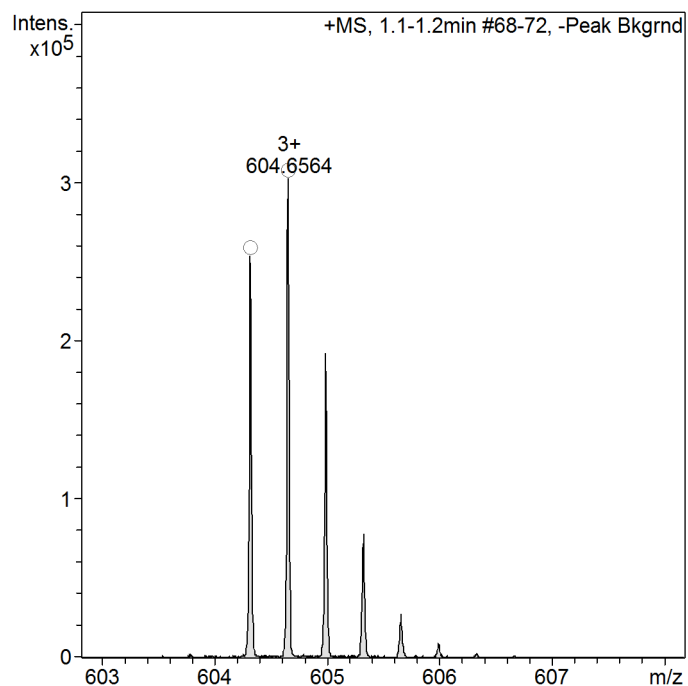


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.2 min	1.17	21.9	no uv	
Cmpd 2, 1.3 min	1.29	78.1	no uv	

Cmpd 1, 1.2 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

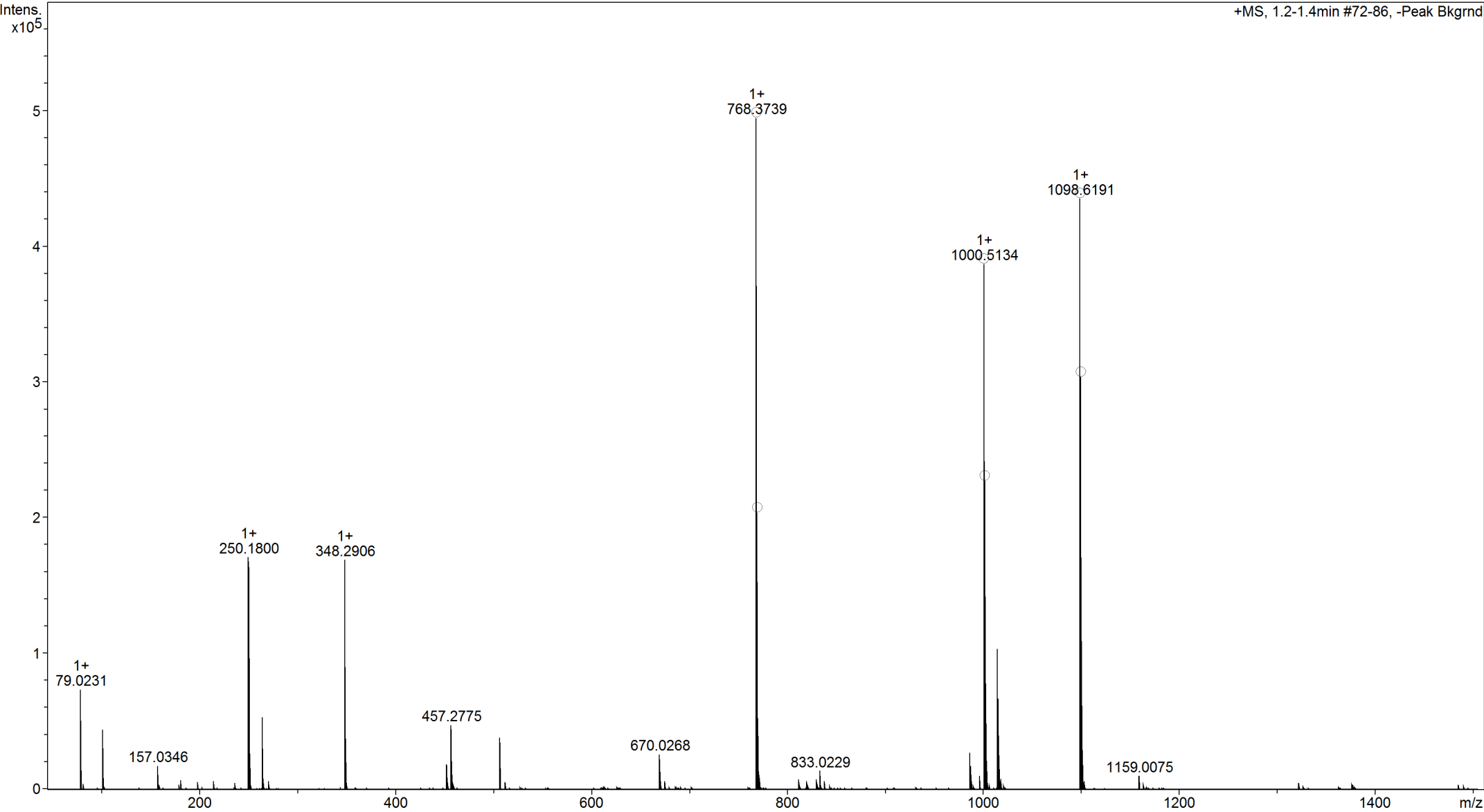
Cmpd 1, 1.2 min

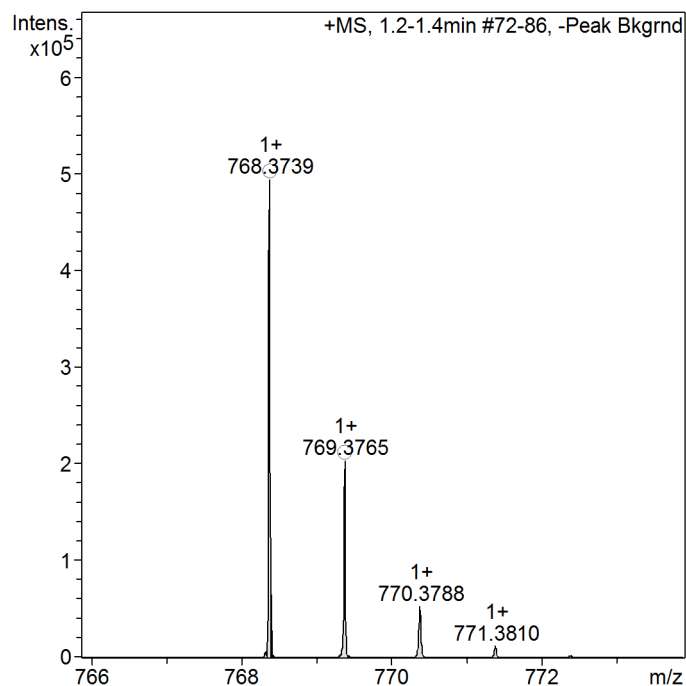
Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
604.321894	C113H139NNa9O6	3+	604.322173	0.3	0.5	14.6	100.00	C113 H136 N Na9 O6	M+H
	C110H131N11Na9	3+	604.321724	0.2	0.3	17.1	99.67	C110 H128 N11 Na9	M+H
	C113H139NNa9O6	3+	604.322173	0.3	0.5	14.6	100.00	C113 H139 N Na9 O6	M+NH4
	C110H131N11Na9	3+	604.321724	0.2	0.3	17.1	99.67	C110 H119 N8 Na9	M+NH4
	C113H139NNa9O6	3+	604.322173	0.3	0.5	14.6	100.00	C113 H139 N Na6 O6	M+Na
	C110H131N11Na9	3+	604.321724	0.2	0.3	17.1	99.67	C110 H131 N11 Na6	M+Na
604.656378	C45H17N35Na9O35	3+	604.656302	-0.1	-0.1	5.7	100.00	C45 H14 N35 Na9 O35	M+H
	C43H5N49Na9O25	3+	604.656298	-0.1	-0.1	9.8	92.74	C43 H2 N49 Na9 O25	M+H
	C46H13N39Na9O31	3+	604.656748	0.4	0.6	9.9	81.69	C46 H10 N39 Na9 O31	M+H
	C47H29N21Na9O45	3+	604.656305	-0.1	-0.1	14.0	85.86	C47 H26 N21 Na9 O45	M+H
	C44HN53Na9O21	3+	604.656744	-0.4	-0.6	18.5	69.02	C44 H N53 Na9 O21	M+H
	C49H41N7Na9O55	3+	604.656309	-0.1	-0.1	24.2	69.31	C49 H38 N7 Na9 O55	M+H
	C45H126N50Na9O15	3+	604.656550	-0.2	-0.3	25.7	53.52	C45 H123 N50 Na9 O15	M+H
	C42H118N60Na9O9	3+	604.656101	-0.3	-0.5	27.5	48.95	C42 H115 N60 Na9 O9	M+H
	C43H114N64Na9O5	3+	604.656547	0.2	0.3	37.0	40.46	C43 H111 N64 Na9 O5	M+H
	C45H17N35Na9O35	3+	604.656302	-0.1	-0.1	5.7	100.00	C45 H5 N32 Na9 O35	M+NH4
	C43H5N49Na9O25	3+	604.656298	-0.1	-0.1	9.8	92.74	C43 H5 N49 Na9 O25	M+NH4
	C46H13N39Na9O31	3+	604.656748	0.4	0.6	9.9	81.69	C46 H N36 Na9 O31	M+NH4
	C47H29N21Na9O45	3+	604.656305	-0.1	-0.1	14.0	85.86	C47 H17 N18 Na9 O45	M+NH4
	C44HN53Na9O21	3+	604.656744	-0.4	-0.6	18.5	69.02	C44 H N53 Na9 O21	M+NH4
	C49H41N7Na9O55	3+	604.656309	-0.1	-0.1	24.2	69.31	C49 H29 N4 Na9 O55	M+NH4
	C45H126N50Na9O15	3+	604.656550	-0.2	-0.3	25.7	53.52	C45 H114 N47 Na9 O15	M+NH4
	C42H118N60Na9O9	3+	604.656101	-0.3	-0.5	27.5	48.95	C42 H106 N57 Na9 O9	M+NH4
	C43H114N64Na9O5	3+	604.656547	0.2	0.3	37.0	40.46	C43 H102 N61 Na9 O5	M+NH4
	C45H17N35Na9O35	3+	604.656302	-0.1	-0.1	5.7	100.00	C45 H17 N35 Na6 O35	M+Na
	C43H5N49Na9O25	3+	604.656298	-0.1	-0.1	9.8	92.74	C43 H5 N49 Na6 O25	M+Na
	C46H13N39Na9O31	3+	604.656748	0.4	0.6	9.9	81.69	C46 H13 N39 Na6 O31	M+Na
	C47H29N21Na9O45	3+	604.656305	-0.1	-0.1	14.0	85.86	C47 H29 N21 Na6 O45	M+Na
	C44HN53Na9O21	3+	604.656744	-0.4	-0.6	18.5	69.02	C44 H N53 Na6 O21	M+Na
	C49H41N7Na9O55	3+	604.656309	-0.1	-0.1	24.2	69.31	C49 H41 N7 Na6 O55	M+Na
	C45H126N50Na9O15	3+	604.656550	-0.2	-0.3	25.7	53.52	C45 H126 N50 Na6 O15	M+Na
	C42H118N60Na9O9	3+	604.656101	-0.3	-0.5	27.5	48.95	C42 H118 N60 Na6 O9	M+Na
	C43H114N64Na9O5	3+	604.656547	0.2	0.3	37.0	40.46	C43 H114 N64 Na6 O5	M+Na
	C57H46NNa18O41	3+	604.656242	-0.1	-0.2	11.7	100.00	C57 H49 N Na12 O41	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
	C55H34N15Na18O31	3+	604.656239	0.1	0.2	15.2	93.09	C55 H37 N15 Na12 O31	M+Na2-H
	C58H42N5Na18O37	3+	604.656688	0.3	0.5	18.4	81.09	C58 H45 N5 Na12 O37	M+Na2-H
	C53H22N29Na18O21	3+	604.656235	-0.1	-0.2	23.6	77.83	C53 H25 N29 Na12 O21	M+Na2-H
	C56H30N19Na18O27	3+	604.656684	0.3	0.5	24.8	70.53	C56 H33 N19 Na12 O27	M+Na2-H
	C37H2N59Na18O8	3+	604.656845	-0.5	-0.8	32.7	45.17	C37 H5 N59 Na12 O8	M+Na2-H
	C39H14N45Na18O18	3+	604.656848	-0.5	-0.8	33.3	44.47	C39 H17 N45 Na12 O18	M+Na2-H
	C54H18N33Na18O17	3+	604.656681	-0.3	-0.5	33.6	57.27	C54 H21 N33 Na12 O17	M+Na2-H
	C51H10N43Na18O11	3+	604.656232	0.1	0.2	36.5	47.32	C51 H13 N43 Na12 O11	M+Na2-H
	C41H26N31Na18O28	3+	604.656852	0.5	0.8	37.7	39.64	C41 H29 N31 Na12 O28	M+Na2-H

Cmpd 2, 1.3 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, 1.3 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
768.373916	C31H46N17O7	1+	768.376063	2.1	2.8	7.9	45.57	C31 H45 N17 O7	M+H
	C28H38N27O	1+	768.374715	-0.8	-1.0	13.8	99.28	C28 H37 N27 O	M+H
	C33H58N3O17	1+	768.376074	2.2	2.8	13.9	50.45	C33 H57 N3 O17	M+H
	C30H50N13O11	1+	768.374726	-0.8	-1.1	16.7	93.17	C30 H49 N13 O11	M+H
	C27H42N23O5	1+	768.373378	-0.5	-0.7	20.0	100.00	C27 H41 N23 O5	M+H
	C29H54N9O15	1+	768.373388	-0.5	-0.7	27.7	84.43	C29 H53 N9 O15	M+H
	C26H46N19O9	1+	768.372041	-1.9	-2.4	29.6	35.50	C26 H45 N19 O9	M+H
	C41H50N7O8	1+	768.371538	2.4	3.1	31.0	28.85	C41 H49 N7 O8	M+H
	C28H58N5O19	1+	768.372051	-1.9	-2.4	39.1	28.04	C28 H57 N5 O19	M+H
	C31H46N17O7	1+	768.376063	2.1	2.8	7.9	45.57	C31 H42 N16 O7	M+NH4
	C28H38N27O	1+	768.374715	-0.8	-1.0	13.8	99.28	C28 H34 N26 O	M+NH4
	C33H58N3O17	1+	768.376074	2.2	2.8	13.9	50.45	C33 H54 N2 O17	M+NH4
	C30H50N13O11	1+	768.374726	-0.8	-1.1	16.7	93.17	C30 H46 N12 O11	M+NH4
	C27H42N23O5	1+	768.373378	-0.5	-0.7	20.0	100.00	C27 H38 N22 O5	M+NH4
	C29H54N9O15	1+	768.373388	-0.5	-0.7	27.7	84.43	C29 H50 N8 O15	M+NH4
	C26H46N19O9	1+	768.372041	-1.9	-2.4	29.6	35.50	C26 H42 N18 O9	M+NH4
	C41H50N7O8	1+	768.371538	2.4	3.1	31.0	28.85	C41 H46 N6 O8	M+NH4
	C28H58N5O19	1+	768.372051	-1.9	-2.4	39.1	28.04	C28 H54 N4 O19	M+NH4
	C33H51N11NaO9	1+	768.376343	-2.4	-3.2	5.6	31.80	C33 H51 N11 O9	M+Na
	C30H43N21NaO3	1+	768.374995	1.1	1.4	11.4	75.01	C30 H43 N21 O3	M+Na
	C32H55N7NaO13	1+	768.375006	1.1	1.4	15.3	69.03	C32 H55 N7 O13	M+Na
	C29H47N17NaO7	1+	768.373658	-0.3	-0.3	18.0	100.00	C29 H47 N17 O7	M+Na
	C26H39N27NaO	1+	768.372310	1.6	2.1	22.3	42.92	C26 H39 N27 O	M+Na
	C31H59N3NaO17	1+	768.373668	0.2	0.3	26.7	82.99	C31 H59 N3 O17	M+Na
	C28H51N13NaO11	1+	768.372320	1.6	2.1	28.1	37.82	C28 H51 N13 O11	M+Na
	C25H43N23NaO5	1+	768.370972	-2.9	-3.8	30.8	11.76	C25 H43 N23 O5	M+Na
	C43H55NNaO10	1+	768.371818	2.1	2.7	32.2	29.65	C43 H55 N O10	M+Na
	C27H55N9NaO15	1+	768.370983	-2.9	-3.8	39.1	9.60	C27 H55 N9 O15	M+Na
	C28H43KN25	1+	768.376485	-2.6	-3.3	21.4	27.58	C28 H43 N25	M+K
	C27H47KN21O4	1+	768.375147	-1.2	-1.6	25.9	67.35	C27 H47 N21 O4	M+K
	C23H43KN27O2	1+	768.372462	-1.5	-1.9	29.9	53.10	C23 H43 N27 O2	M+K
	C30H55KN11O10	1+	768.376495	-2.6	-3.4	30.8	21.97	C30 H55 N11 O10	M+K
	C26H51KN17O8	1+	768.373810	0.1	0.1	33.4	100.00	C26 H51 N17 O8	M+K
	C29H59KN7O14	1+	768.375158	-1.2	-1.6	37.3	50.37	C29 H59 N7 O14	M+K

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
769.376521	C22H47KN23O6	1+	768.371124	-2.8	-3.6	39.5	14.47	C22 H47 N23 O6	M+K
	C35H56N5Na2O11	1+	768.376623	-2.7	-3.5	3.5	22.47	C35 H57 N5 O11	M+Na2-H
	C32H48N15Na2O5	1+	768.375275	-1.4	-1.8	9.0	57.65	C32 H49 N15 O5	M+Na2-H
	C33H44N19Na2O	1+	768.376612	-2.7	-3.5	13.1	19.07	C33 H45 N19 O	M+Na2-H
	C34H60NNa2O15	1+	768.375285	1.4	1.8	14.2	51.80	C34 H61 N O15	M+Na2-H
	C31H52N11Na2O9	1+	768.373937	-0.0	-0.0	16.2	100.00	C31 H53 N11 O9	M+Na2-H
	C28H44N21Na2O3	1+	768.372589	1.3	1.7	20.1	47.13	C28 H45 N21 O3	M+Na2-H
	C30H56N7Na2O13	1+	768.372600	1.3	1.7	26.8	40.87	C30 H57 N7 O13	M+Na2-H
	C27H48N17Na2O7	1+	768.371252	2.7	3.5	29.1	13.85	C27 H49 N17 O7	M+Na2-H
	C29H60N3Na2O17	1+	768.371262	2.7	3.5	38.0	11.16	C29 H61 N3 O17	M+Na2-H
	C21H50N18NaO12	1+	769.374780	1.7	2.3	23.0	60.02	C21 H46 N17 Na O12	M+NH4
	C22H46N22NaO8	1+	769.376117	0.4	0.5	34.4	100.00	C22 H42 N21 Na O8	M+NH4
	C19H38N32NaO2	1+	769.374769	-1.8	-2.3	34.5	45.28	C19 H34 N31 Na O2	M+NH4
	C25H54N12NaO14	1+	769.377465	0.9	1.2	35.4	73.81	C25 H50 N11 Na O14	M+NH4
	C21H50N18NaO12	1+	769.374780	1.7	2.3	23.0	60.02	C21 H50 N18 O12	M+Na
	C22H46N22NaO8	1+	769.376117	0.4	0.5	34.4	100.00	C22 H46 N22 O8	M+Na
	C19H38N32NaO2	1+	769.374769	-1.8	-2.3	34.5	45.28	C19 H38 N32 O2	M+Na
	C25H54N12NaO14	1+	769.377465	0.9	1.2	35.4	73.81	C25 H54 N12 O14	M+Na
	C16H42KN32O3	1+	769.374921	1.6	2.1	33.7	53.40	C16 H42 N32 O3	M+K
	C18H54KN18O13	1+	769.374932	1.6	2.1	36.0	50.72	C18 H54 N18 O13	M+K
	C19H50KN22O9	1+	769.376269	0.3	0.3	38.5	100.00	C19 H50 N22 O9	M+K
	C20H47N22Na2O8	1+	769.373712	-2.8	-3.7	23.3	22.49	C20 H48 N22 O8	M+Na2-H
	C23H55N12Na2O14	1+	769.375059	-1.5	-1.9	24.2	64.09	C23 H56 N12 O14	M+Na2-H
	C21H43N26Na2O4	1+	769.375049	-1.5	-1.9	35.0	48.98	C21 H44 N26 O4	M+Na2-H
	C24H51N16Na2O10	1+	769.376397	-0.1	-0.2	35.3	100.00	C24 H52 N16 O10	M+Na2-H
	C27H59N6Na2O16	1+	769.377745	-1.2	-1.6	36.7	54.83	C27 H60 N6 O16	M+Na2-H
	C20H47N22Na2O8	1+	769.373712	-2.8	-3.7	23.3	22.49	C10 H23 N11 Na O4	2M+H
	C24H51N16Na2O10	1+	769.376397	-0.1	-0.2	35.3	100.00	C12 H25 N8 Na O5	2M+H
	C22H46N22NaO8	1+	769.376117	0.4	0.5	34.4	100.00	C11 H23 N11 O4	2M+Na
	C21H50N18NaO12	1+	769.374780	1.7	2.3	23.0	60.02	C21 H49 N18 Na O12	M+H
	C22H46N22NaO8	1+	769.376117	0.4	0.5	34.4	100.00	C22 H45 N22 Na O8	M+H
	C19H38N32NaO2	1+	769.374769	-1.8	-2.3	34.5	45.28	C19 H37 N32 Na O2	M+H
	C25H54N12NaO14	1+	769.377465	0.9	1.2	35.4	73.81	C25 H53 N12 Na O14	M+H
1000.513395	C53H75N3NaO14	1+	1000.514125	-0.7	-0.7	5.6	98.86	C53 H74 N3 Na O14	M+H
	C50H67N13NaO8	1+	1000.512777	-0.6	-0.6	8.2	100.00	C50 H66 N13 Na O8	M+H
	C49H71N9NaO12	1+	1000.511439	2.0	2.0	9.1	42.59	C49 H70 N9 Na O12	M+H
	C47H59N23NaO2	1+	1000.511429	2.0	2.0	13.4	38.97	C47 H58 N23 Na O2	M+H
	C46H63N19NaO6	1+	1000.510092	-3.3	-3.3	14.5	11.55	C46 H62 N19 Na O6	M+H
	C54H71N7NaO10	1+	1000.515462	-2.1	-2.1	16.3	34.09	C54 H70 N7 Na O10	M+H
	C51H63N17NaO4	1+	1000.514114	-0.7	-0.7	16.8	80.45	C51 H62 N17 Na O4	M+H
	C48H75N5NaO16	1+	1000.510102	-3.3	-3.3	18.1	10.85	C48 H74 N5 Na O16	M+H
	C52H59N21Na	1+	1000.515452	-2.1	-2.1	27.1	27.12	C52 H58 N21 Na	M+H

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
	C55H67N11NaO6	1+	1000.516800	3.4	3.4	27.1	7.91	C55 H66 N11 Na O6	M+H
	C53H75N3NaO14	1+	1000.514125	-0.7	-0.7	5.6	98.86	C53 H71 N2 Na O14	M+NH4
	C50H67N13NaO8	1+	1000.512777	-0.6	-0.6	8.2	100.00	C50 H63 N12 Na O8	M+NH4
	C49H71N9NaO12	1+	1000.511439	2.0	2.0	9.1	42.59	C49 H67 N8 Na O12	M+NH4
	C47H59N23NaO2	1+	1000.511429	2.0	2.0	13.4	38.97	C47 H55 N22 Na O2	M+NH4
	C46H63N19NaO6	1+	1000.510092	-3.3	-3.3	14.5	11.55	C46 H59 N18 Na O6	M+NH4
	C54H71N7NaO10	1+	1000.515462	-2.1	-2.1	16.3	34.09	C54 H67 N6 Na O10	M+NH4
	C51H63N17NaO4	1+	1000.514114	-0.7	-0.7	16.8	80.45	C51 H59 N16 Na O4	M+NH4
	C48H75N5NaO16	1+	1000.510102	-3.3	-3.3	18.1	10.85	C48 H71 N4 Na O16	M+NH4
	C52H59N21Na	1+	1000.515452	-2.1	-2.1	27.1	27.12	C52 H55 N20 Na	M+NH4
	C55H67N11NaO6	1+	1000.516800	3.4	3.4	27.1	7.91	C55 H63 N10 Na O6	M+NH4
	C53H75N3NaO14	1+	1000.514125	-0.7	-0.7	5.6	98.86	C53 H75 N3 O14	M+Na
	C50H67N13NaO8	1+	1000.512777	-0.6	-0.6	8.2	100.00	C50 H67 N13 O8	M+Na
	C49H71N9NaO12	1+	1000.511439	2.0	2.0	9.1	42.59	C49 H71 N9 O12	M+Na
	C47H59N23NaO2	1+	1000.511429	2.0	2.0	13.4	38.97	C47 H59 N23 O2	M+Na
	C46H63N19NaO6	1+	1000.510092	-3.3	-3.3	14.5	11.55	C46 H63 N19 O6	M+Na
	C54H71N7NaO10	1+	1000.515462	-2.1	-2.1	16.3	34.09	C54 H71 N7 O10	M+Na
	C51H63N17NaO4	1+	1000.514114	-0.7	-0.7	16.8	80.45	C51 H63 N17 O4	M+Na
	C48H75N5NaO16	1+	1000.510102	-3.3	-3.3	18.1	10.85	C48 H75 N5 O16	M+Na
	C52H59N21Na	1+	1000.515452	-2.1	-2.1	27.1	27.12	C52 H59 N21	M+Na
	C55H67N11NaO6	1+	1000.516800	3.4	3.4	27.1	7.91	C55 H67 N11 O6	M+Na
	C44H63KN23O3	1+	1000.511581	1.8	1.8	20.4	40.29	C44 H63 N23 O3	M+K
	C47H71KN13O9	1+	1000.512929	0.5	0.5	24.0	100.00	C47 H71 N13 O9	M+K
	C48H67KN17O5	1+	1000.514266	0.9	0.9	24.8	79.85	C48 H67 N17 O5	M+K
	C43H67KN19O7	1+	1000.510244	-3.2	-3.2	25.1	11.47	C43 H67 N19 O7	M+K
	C46H75KN9O13	1+	1000.511592	1.8	1.8	27.1	41.86	C46 H75 N9 O13	M+K
	C50H79KN3O15	1+	1000.514277	0.9	0.9	29.5	71.13	C50 H79 N3 O15	M+K
	C51H75KN7O11	1+	1000.515614	-2.2	-2.2	30.4	28.16	C51 H75 N7 O11	M+K
	C49H63KN21O	1+	1000.515604	-2.2	-2.2	32.0	22.74	C49 H63 N21 O	M+K
	C45H79KN5O17	1+	1000.510254	-3.1	-3.1	33.1	11.47	C45 H79 N5 O17	M+K
	C52H71KN11O7	1+	1000.516952	3.6	3.6	34.5	7.18	C52 H71 N11 O7	M+K
	C51H76N3Na2O14	1+	1000.511719	-1.7	-1.7	7.0	46.59	C51 H77 N3 O14	M+Na2-H
	C52H72N7Na2O10	1+	1000.513057	-0.3	-0.3	7.2	100.00	C52 H73 N7 O10	M+Na2-H
	C49H64N17Na2O4	1+	1000.511709	-1.7	-1.7	11.6	42.49	C49 H65 N17 O4	M+Na2-H
	C48H68N13Na2O8	1+	1000.510371	-3.0	-3.0	12.1	13.77	C48 H69 N13 O8	M+Na2-H
	C53H68N11Na2O6	1+	1000.514394	-1.0	-1.0	16.9	59.18	C53 H69 N11 O6	M+Na2-H
	C56H76NNa2O12	1+	1000.515742	-2.3	-2.3	17.3	22.89	C56 H77 N O12	M+Na2-H
	C50H60N21Na2	1+	1000.513046	-0.3	-0.3	18.8	79.41	C50 H61 N21	M+Na2-H
	C54H64N15Na2O2	1+	1000.515731	-2.3	-2.3	27.6	18.42	C54 H65 N15 O2	M+Na2-H
	C57H72N5Na2O8	1+	1000.517079	-3.7	-3.7	28.1	4.90	C57 H73 N5 O8	M+Na2-H
	C39H60N27Na2O3	1+	1000.516234	-2.8	-2.8	38.8	8.90	C39 H61 N27 O3	M+Na2-H
1001.517219	C24H70KN26O15	1+	1001.514554	2.7	2.7	38.0	100.00	C24 H70 N26 O15	M+K

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
1098.619122	C22H58KN4O05	1+	1001.514543	2.7	2.7	38.3	98.27	C22 H58 N40 O5	M+K
	C18H51N48Na2O	1+	1001.520533	3.3	3.3	21.3	12.93	C18 H52 N48 O	M+Na2-H
	C29H71N20Na2O16	1+	1001.514681	2.5	2.5	27.9	29.18	C29 H72 N20 O16	M+Na2-H
	C26H63N30Na2O10	1+	1001.513333	-3.9	-3.9	30.4	5.59	C26 H64 N30 O10	M+Na2-H
	C30H67N24Na2O12	1+	1001.516019	-1.2	-1.2	38.2	60.39	C30 H68 N24 O12	M+Na2-H
	C33H75N14Na2O18	1+	1001.517367	0.1	0.1	39.5	100.00	C33 H76 N14 O18	M+Na2-H
	C26H63N30Na2O10	1+	1001.513333	-3.9	-3.9	30.4	5.59	C13 H31 N15 Na O5	2M+H
	C30H67N24Na2O12	1+	1001.516019	-1.2	-1.2	38.2	60.39	C15 H33 N12 Na O6	2M+H
	C30H74N16NaO20	1+	1001.515750	1.5	1.5	28.4	62.80	C15 H37 N8 O10	2M+Na
	C27H66N26NaO14	1+	1001.514402	2.8	2.8	26.9	22.34	C27 H65 N26 Na O14	M+H
	C30H74N16NaO20	1+	1001.515750	1.5	1.5	28.4	62.80	C30 H73 N16 Na O20	M+H
	C31H70N20NaO16	1+	1001.517087	-0.1	-0.1	38.3	100.00	C31 H69 N20 Na O16	M+H
	C27H66N26NaO14	1+	1001.514402	2.8	2.8	26.9	22.34	C27 H62 N25 Na O14	M+NH4
	C30H74N16NaO20	1+	1001.515750	1.5	1.5	28.4	62.80	C30 H70 N15 Na O20	M+NH4
	C31H70N20NaO16	1+	1001.517087	-0.1	-0.1	38.3	100.00	C31 H66 N19 Na O16	M+NH4
	C27H66N26NaO14	1+	1001.514402	2.8	2.8	26.9	22.34	C27 H66 N26 O14	M+Na
	C30H74N16NaO20	1+	1001.515750	1.5	1.5	28.4	62.80	C30 H74 N16 O20	M+Na
	C31H70N20NaO16	1+	1001.517087	-0.1	-0.1	38.3	100.00	C31 H70 N20 O16	M+Na
	C57H81N13NaO8	1+	1098.622327	-3.2	-2.9	11.0	18.13	C57 H80 N13 Na O8	M+H
	C54H73N23NaO2	1+	1098.620979	-1.9	-1.7	15.0	54.37	C54 H72 N23 Na O2	M+H
	C63H81N9NaO7	1+	1098.615117	-4.0	-3.6	16.4	6.76	C63 H80 N9 Na O7	M+H
	C56H85N9NaO12	1+	1098.620990	-1.9	-1.7	21.7	46.85	C56 H84 N9 Na O12	M+H
	C53H77N19NaO6	1+	1098.619642	-0.5	-0.5	24.5	100.00	C53 H76 N19 Na O6	M+H
	C64H77N13NaO3	1+	1098.616454	-2.7	-2.4	27.3	21.48	C64 H76 N13 Na O3	M+H
	C50H69N29Na	1+	1098.618294	-0.8	-0.8	28.4	77.93	C50 H68 N29 Na	M+H
	C67H85N3NaO9	1+	1098.617802	-1.3	-1.2	30.6	55.43	C67 H84 N3 Na O9	M+H
	C55H89N5NaO16	1+	1098.619652	0.5	0.5	32.5	82.06	C55 H88 N5 Na O16	M+H
	C52H81N15NaO10	1+	1098.618305	0.8	0.7	34.7	66.98	C52 H80 N15 Na O10	M+H
	C57H81N13NaO8	1+	1098.622327	-3.2	-2.9	11.0	18.13	C57 H77 N12 Na O8	M+NH4
	C54H73N23NaO2	1+	1098.620979	-1.9	-1.7	15.0	54.37	C54 H69 N22 Na O2	M+NH4
	C63H81N9NaO7	1+	1098.615117	-4.0	-3.6	16.4	6.76	C63 H77 N8 Na O7	M+NH4
	C56H85N9NaO12	1+	1098.620990	-1.9	-1.7	21.7	46.85	C56 H81 N8 Na O12	M+NH4
	C53H77N19NaO6	1+	1098.619642	-0.5	-0.5	24.5	100.00	C53 H73 N18 Na O6	M+NH4
	C64H77N13NaO3	1+	1098.616454	-2.7	-2.4	27.3	21.48	C64 H73 N12 Na O3	M+NH4
	C50H69N29Na	1+	1098.618294	-0.8	-0.8	28.4	77.93	C50 H65 N28 Na	M+NH4
	C67H85N3NaO9	1+	1098.617802	-1.3	-1.2	30.6	55.43	C67 H81 N2 Na O9	M+NH4
	C55H89N5NaO16	1+	1098.619652	0.5	0.5	32.5	82.06	C55 H85 N4 Na O16	M+NH4
	C52H81N15NaO10	1+	1098.618305	0.8	0.7	34.7	66.98	C52 H77 N14 Na O10	M+NH4
	C57H81N13NaO8	1+	1098.622327	-3.2	-2.9	11.0	18.13	C57 H81 N13 O8	M+Na
	C54H73N23NaO2	1+	1098.620979	-1.9	-1.7	15.0	54.37	C54 H73 N23 O2	M+Na
	C63H81N9NaO7	1+	1098.615117	-4.0	-3.6	16.4	6.76	C63 H81 N9 O7	M+Na
	C56H85N9NaO12	1+	1098.620990	-1.9	-1.7	21.7	46.85	C56 H85 N9 O12	M+Na

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
	C53H77N19NaO6	1+	1098.619642	-0.5	-0.5	24.5	100.00	C53 H77 N19 O6	M+Na
	C64H77N13NaO3	1+	1098.616454	-2.7	-2.4	27.3	21.48	C64 H77 N13 O3	M+Na
	C50H69N29Na	1+	1098.618294	-0.8	-0.8	28.4	77.93	C50 H69 N29	M+Na
	C67H85N3NaO9	1+	1098.617802	-1.3	-1.2	30.6	55.43	C67 H85 N3 O9	M+Na
	C55H89N5NaO16	1+	1098.619652	0.5	0.5	32.5	82.06	C55 H89 N5 O16	M+Na
	C52H81N15NaO10	1+	1098.618305	0.8	0.7	34.7	66.98	C52 H81 N15 O10	M+Na
	C51H77KN23O3	1+	1098.621132	2.0	1.8	27.6	47.71	C51 H77 N23 O3	M+K
	C54H85KN13O9	1+	1098.622479	-3.4	-3.1	31.8	12.73	C54 H85 N13 O9	M+K
	C47H73KN29O	1+	1098.618446	0.7	0.6	32.0	100.00	C47 H73 N29 O	M+K
	C50H81KN19O7	1+	1098.619794	0.7	0.6	34.4	94.25	C50 H81 N19 O7	M+K
	C60H85KN9O8	1+	1098.615269	3.9	3.5	37.1	6.44	C60 H85 N9 O8	M+K
	C53H89KN9O13	1+	1098.621142	2.0	1.8	37.6	36.79	C53 H89 N9 O13	M+K
	C57H74N21Na2	1+	1098.622596	3.5	3.2	7.1	15.56	C57 H75 N21	M+Na2-H
	C59H86N7Na2O10	1+	1098.622607	3.5	3.2	9.6	14.71	C59 H87 N7 O10	M+Na2-H
	C56H78N17Na2O4	1+	1098.621259	2.1	1.9	12.8	48.54	C56 H79 N17 O4	M+Na2-H
	C65H86N3Na2O9	1+	1098.615396	-3.7	-3.4	18.4	9.48	C65 H87 N3 O9	M+Na2-H
	C58H90N3Na2O14	1+	1098.621270	2.1	2.0	20.5	41.10	C58 H91 N3 O14	M+Na2-H
	C55H82N13Na2O8	1+	1098.619922	0.8	0.7	22.7	95.44	C55 H83 N13 O8	M+Na2-H
	C52H74N23Na2O2	1+	1098.618574	0.5	0.5	26.3	100.00	C52 H75 N23 O2	M+Na2-H
	C66H82N7Na2O5	1+	1098.616734	2.4	2.2	29.0	27.80	C66 H83 N7 O5	M+Na2-H
	C54H86N9Na2O12	1+	1098.618584	0.5	0.5	33.2	85.05	C54 H87 N9 O12	M+Na2-H
	C51H78N19Na2O6	1+	1098.617236	-1.9	-1.7	36.0	34.68	C51 H79 N19 O6	M+Na2-H
1099.621547	C29H80N28NaO16	1+	1099.619929	-1.6	-1.5	34.3	100.00	C29 H79 N28 Na O16	M+H
	C23H64N48NaO4	1+	1099.617233	4.3	3.9	36.5	5.60	C23 H63 N48 Na O4	M+H
	C26H72N38NaO10	1+	1099.618581	-3.0	-2.7	36.9	24.69	C26 H71 N38 Na O10	M+H
	C29H80N28NaO16	1+	1099.619929	-1.6	-1.5	34.3	100.00	C29 H76 N27 Na O16	M+NH4
	C23H64N48NaO4	1+	1099.617233	4.3	3.9	36.5	5.60	C23 H60 N47 Na O4	M+NH4
	C26H72N38NaO10	1+	1099.618581	-3.0	-2.7	36.9	24.69	C26 H68 N37 Na O10	M+NH4
	C27H81N28Na2O16	1+	1099.617524	4.0	3.7	23.8	31.48	C27 H82 N28 O16	M+Na2-H
	C28H77N32Na2O12	1+	1099.618861	2.7	2.4	33.9	100.00	C28 H78 N32 O12	M+Na2-H
	C25H69N42Na2O6	1+	1099.617513	4.0	3.7	37.2	17.93	C25 H70 N42 O6	M+Na2-H
	C28H77N32Na2O12	1+	1099.618861	2.7	2.4	33.9	100.00	C14 H38 N16 Na O6	2M+H
	C26H72N38NaO10	1+	1099.618581	-3.0	-2.7	36.9	24.69	C13 H36 N19 O5	2M+Na
	C29H80N28NaO16	1+	1099.619929	-1.6	-1.5	34.3	100.00	C29 H80 N28 O16	M+Na
	C23H64N48NaO4	1+	1099.617233	4.3	3.9	36.5	5.60	C23 H64 N48 O4	M+Na
	C26H72N38NaO10	1+	1099.618581	-3.0	-2.7	36.9	24.69	C26 H72 N38 O10	M+Na