

School of Chemistry Mass Spectrometry Service

SampleID Ethyl PR
Sample Description
Analysis Name Ethyl PR_137585_GE3_01_13699.d
Method 3a_AccMass_Loop_Positive.m
Instrument maXis impact

Source Type ESI **Ion Polarity** Positive

Submitter

Flora Thorp-Greenwood

Supervisor

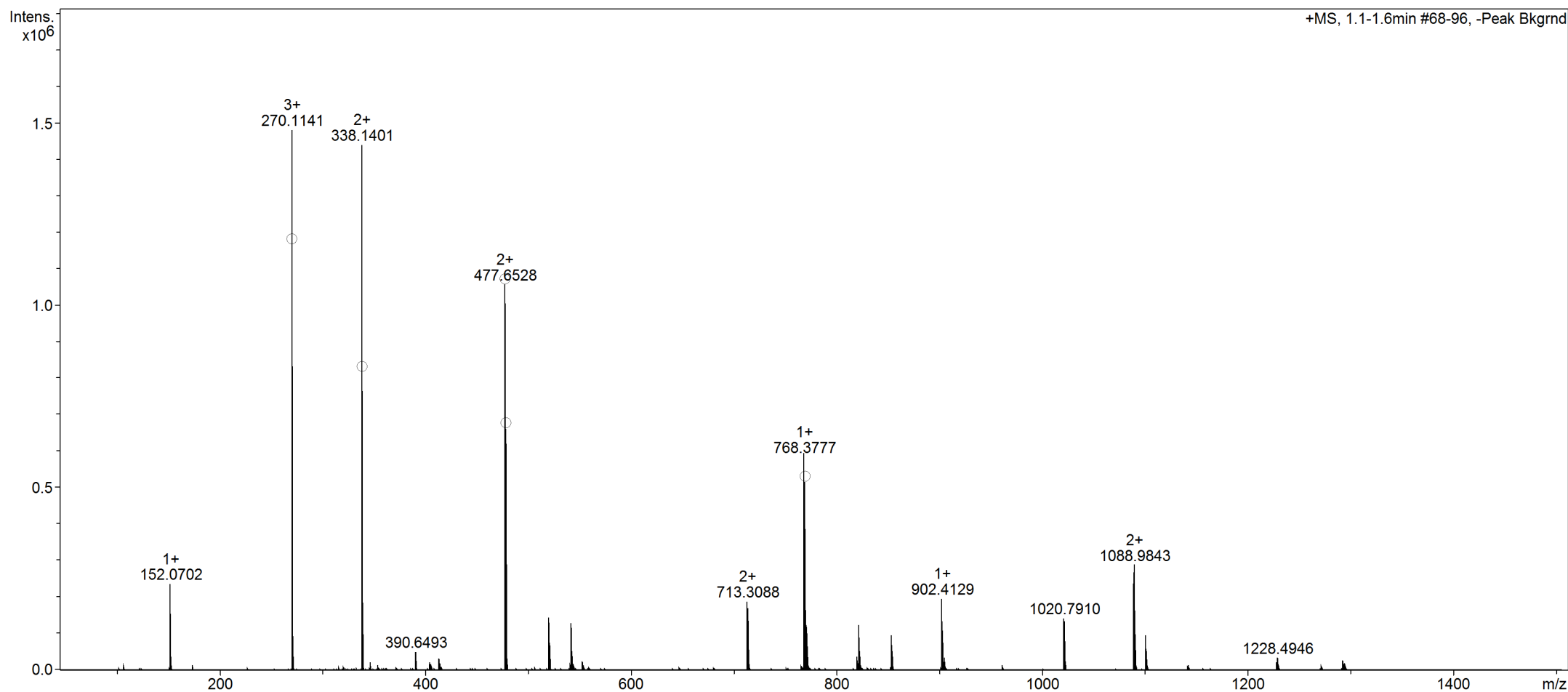
Michael Hardie

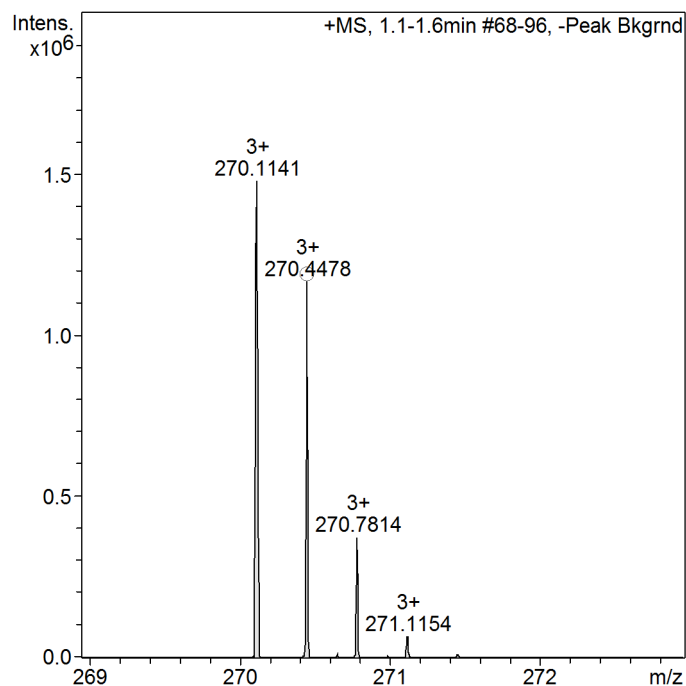
Acquisition Date

13/07/2015 10:18:13

Scan Begin 50 m/z

Scan End 1500 m/z





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

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
270.447757	C19H39N30Na4O2	3+	270.448219	0.5	1.7	1.7	99.23	C19 H36 N30 Na4 O2	M+H
	C22H47N20Na4O8	3+	270.448668	0.9	3.4	5.3	74.21	C22 H44 N20 Na4 O8	M+H
	C18H43N26Na4O6	3+	270.447773	0.0	0.1	12.3	100.00	C18 H40 N26 Na4 O6	M+H
	C15H35N36Na4	3+	270.447324	0.4	1.6	13.6	81.26	C15 H32 N36 Na4	M+H
	C21H51N16Na4O12	3+	270.448223	0.5	1.7	13.9	79.51	C21 H48 N16 Na4 O12	M+H
	C17H47N22Na4O10	3+	270.447327	0.4	1.6	24.0	65.46	C17 H44 N22 Na4 O10	M+H
	C14H39N32Na4O4	3+	270.446878	0.9	3.2	24.2	51.78	C14 H36 N32 Na4 O4	M+H
	C31H55N6Na4O13	3+	270.446714	-1.0	-3.9	30.2	41.01	C31 H52 N6 Na4 O13	M+H
	C29H43N20Na4O3	3+	270.446711	-1.0	-3.9	38.0	33.57	C29 H40 N20 Na4 O3	M+H
	C35H59Na4O15	3+	270.447609	-0.1	-0.5	38.6	64.66	C35 H56 Na4 O15	M+H
	C19H39N30Na4O2	3+	270.448219	0.5	1.7	1.7	99.23	C19 H27 N27 Na4 O2	M+NH4
	C22H47N20Na4O8	3+	270.448668	0.9	3.4	5.3	74.21	C22 H35 N17 Na4 O8	M+NH4
	C18H43N26Na4O6	3+	270.447773	0.0	0.1	12.3	100.00	C18 H31 N23 Na4 O6	M+NH4
	C15H35N36Na4	3+	270.447324	0.4	1.6	13.6	81.26	C15 H23 N33 Na4	M+NH4
	C21H51N16Na4O12	3+	270.448223	0.5	1.7	13.9	79.51	C21 H39 N13 Na4 O12	M+NH4
	C17H47N22Na4O10	3+	270.447327	0.4	1.6	24.0	65.46	C17 H35 N19 Na4 O10	M+NH4
	C14H39N32Na4O4	3+	270.446878	0.9	3.2	24.2	51.78	C14 H27 N29 Na4 O4	M+NH4
	C31H55N6Na4O13	3+	270.446714	-1.0	-3.9	30.2	41.01	C31 H43 N3 Na4 O13	M+NH4
	C29H43N20Na4O3	3+	270.446711	-1.0	-3.9	38.0	33.57	C29 H31 N17 Na4 O3	M+NH4
	C35H59Na4O15	3+	270.447609	-0.1	-0.5	38.6	64.66	C35 H59 Na4 O15	M+NH4
	C23H48N20Na9	3+	270.447786	0.0	0.1	4.0	100.00	C23 H48 N20 Na6	M+Na
	C22H52N16Na9O4	3+	270.447341	0.4	1.5	8.9	77.47	C22 H52 N16 Na6 O4	M+Na
	C27H52N14Na9O2	3+	270.448682	-0.9	-3.4	14.8	53.37	C27 H52 N14 Na6 O2	M+Na
	C22H52N16Na9O4	3+	270.447341	0.4	1.5	8.9	77.47	C11 H26 N8 Na3 O2	2M+Na
338.640937	C23H47N5Na4O12	2+	338.640051	0.9	2.6	29.1	94.62	C23 H45 N5 Na4 O12	M+H
	C21H35N19Na4O2	2+	338.640046	0.9	2.6	38.8	73.57	C21 H33 N19 Na4 O2	M+H
	C24H43N9Na4O8	2+	338.640720	-0.2	-0.6	39.7	100.00	C24 H41 N9 Na4 O8	M+H
	C23H47N5Na4O12	2+	338.640051	0.9	2.6	29.1	94.62	C23 H39 N3 Na4 O12	M+NH4
	C21H35N19Na4O2	2+	338.640046	0.9	2.6	38.8	73.57	C21 H27 N17 Na4 O2	M+NH4
	C24H43N9Na4O8	2+	338.640720	-0.2	-0.6	39.7	100.00	C24 H35 N7 Na4 O8	M+NH4
	C23H47N5Na4O12	2+	338.640051	0.9	2.6	29.1	94.62	C23 H47 N5 Na2 O12	M+Na
	C21H35N19Na4O2	2+	338.640046	0.9	2.6	38.8	73.57	C21 H35 N19 Na2 O2	M+Na
	C24H43N9Na4O8	2+	338.640720	-0.2	-0.6	39.7	100.00	C24 H43 N9 Na2 O8	M+Na
	C51H50N5Na9O	2+	477.654181	1.4	2.9	23.0	87.28	C51 H48 N5 Na9 O	M+H

Smart Formula Parameter	Value
Expected Formula	C189H210N3O39
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
478.153850	C50H54NNa9O5	2+	477.653513	-0.7	-1.5	33.6	100.00	C50 H52 N Na9 O5	M+H
	C51H50N5Na9O	2+	477.654181	1.4	2.9	23.0	87.28	C51 H42 N3 Na9 O	M+NH4
	C50H54NNa9O5	2+	477.653513	-0.7	-1.5	33.6	100.00	C50 H54 N Na9 O5	M+NH4
	C53H41N11Na4O2	2+	477.651225	1.6	3.3	12.3	57.36	C53 H41 N11 Na2 O2	M+Na
	C56H49NNa4O8	2+	477.651899	-0.9	-1.9	18.3	76.89	C56 H49 N Na2 O8	M+Na
	C57H45N5Na4O4	2+	477.652567	-0.2	-0.5	21.4	100.00	C57 H45 N5 Na2 O4	M+Na
	C58H41N9Na4	2+	477.653236	0.4	0.9	28.8	76.30	C58 H41 N9 Na2	M+Na
	C46H45N11Na4O7	2+	477.654161	1.4	2.9	36.7	37.43	C46 H45 N11 Na2 O7	M+Na
	C43H37N21Na4O	2+	477.653487	-0.7	-1.5	37.2	54.49	C43 H37 N21 Na2 O	M+Na
	C59H49NNa8	2+	477.651779	-1.0	-2.1	20.1	100.00	C59 H51 N Na4	M+Na2-H
	C48H49N7Na8O3	2+	477.653373	0.6	1.2	34.3	89.90	C48 H51 N7 Na4 O3	M+Na2-H
	C17H48N22Na4O19	2+	478.152294	1.6	3.3	13.8	59.71	C17 H46 N22 Na4 O19	M+H
	C15H36N36Na4O9	2+	478.152288	1.6	3.3	18.0	54.65	C15 H34 N36 Na4 O9	M+H
	C18H44N26Na4O15	2+	478.152962	0.9	1.9	20.6	78.29	C18 H42 N26 Na4 O15	M+H
	C21H52N16Na4O21	2+	478.153636	-0.2	-0.4	24.5	100.00	C21 H50 N16 Na4 O21	M+H
	C16H32N40Na4O5	2+	478.152957	-0.9	-1.9	29.3	64.01	C16 H30 N40 Na4 O5	M+H
	C19H40N30Na4O11	2+	478.153631	0.2	0.5	30.6	86.34	C19 H38 N30 Na4 O11	M+H
	C25H56N10Na4O23	2+	478.154979	-1.1	-2.4	32.7	64.31	C25 H54 N10 Na4 O23	M+H
	C22H48N20Na4O17	2+	478.154305	0.5	1.0	33.1	72.92	C22 H46 N20 Na4 O17	M+H
	C17H48N22Na4O19	2+	478.152294	1.6	3.3	13.8	59.71	C17 H40 N20 Na4 O19	M+NH4
	C15H36N36Na4O9	2+	478.152288	1.6	3.3	18.0	54.65	C15 H28 N34 Na4 O9	M+NH4
	C18H44N26Na4O15	2+	478.152962	0.9	1.9	20.6	78.29	C18 H36 N24 Na4 O15	M+NH4
	C21H52N16Na4O21	2+	478.153636	-0.2	-0.4	24.5	100.00	C21 H44 N14 Na4 O21	M+NH4
	C16H32N40Na4O5	2+	478.152957	-0.9	-1.9	29.3	64.01	C16 H24 N38 Na4 O5	M+NH4
	C19H40N30Na4O11	2+	478.153631	0.2	0.5	30.6	86.34	C19 H32 N28 Na4 O11	M+NH4
	C25H56N10Na4O23	2+	478.154979	-1.1	-2.4	32.7	64.31	C25 H48 N8 Na4 O23	M+NH4
	C22H48N20Na4O17	2+	478.154305	0.5	1.0	33.1	72.92	C22 H40 N18 Na4 O17	M+NH4
	C17H48N22Na4O19	2+	478.152294	1.6	3.3	13.8	59.71	C17 H48 N22 Na2 O19	M+Na
	C15H36N36Na4O9	2+	478.152288	1.6	3.3	18.0	54.65	C15 H36 N36 Na2 O9	M+Na
	C18H44N26Na4O15	2+	478.152962	0.9	1.9	20.6	78.29	C18 H44 N26 Na2 O15	M+Na
	C21H52N16Na4O21	2+	478.153636	-0.2	-0.4	24.5	100.00	C21 H52 N16 Na2 O21	M+Na
	C16H32N40Na4O5	2+	478.152957	-0.9	-1.9	29.3	64.01	C16 H32 N40 Na2 O5	M+Na
	C19H40N30Na4O11	2+	478.153631	0.2	0.5	30.6	86.34	C19 H40 N30 Na2 O11	M+Na
	C25H56N10Na4O23	2+	478.154979	-1.1	-2.4	32.7	64.31	C25 H56 N10 Na2 O23	M+Na
	C22H48N20Na4O17	2+	478.154305	0.5	1.0	33.1	72.92	C22 H48 N20 Na2 O17	M+Na
	C20H48N22Na8O11	2+	478.152174	-1.7	-3.5	21.4	62.47	C20 H50 N22 Na4 O11	M+Na2-H
	C18H36N36Na8O	2+	478.152169	-1.7	-3.5	31.8	48.85	C18 H38 N36 Na4 O	M+Na2-H
	C21H44N26Na8O7	2+	478.152842	1.0	2.1	32.4	73.95	C21 H46 N26 Na4 O7	M+Na2-H
	C24H52N16Na8O13	2+	478.153516	0.3	0.7	34.1	100.00	C24 H54 N16 Na4 O13	M+Na2-H
769.380327	C13H38N36NaO3	1+	769.381980	1.7	2.1	30.3	100.00	C13 H37 N36 Na O3	M+H
	C16H46N26NaO9	1+	769.383328	3.0	3.9	35.1	28.99	C16 H45 N26 Na O9	M+H
	C23H42N26NaO4	1+	769.377455	2.9	3.7	37.3	30.91	C23 H41 N26 Na O4	M+H

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
	C13H38N36NaO3	1+	769.381980	1.7	2.1	30.3	100.00	C13 H34 N35 Na O3	M+NH4
	C16H46N26NaO9	1+	769.383328	3.0	3.9	35.1	28.99	C16 H42 N25 Na O9	M+NH4
	C23H42N26NaO4	1+	769.377455	2.9	3.7	37.3	30.91	C23 H38 N25 Na O4	M+NH4
	C13H38N36NaO3	1+	769.381980	1.7	2.1	30.3	100.00	C13 H38 N36 O3	M+Na
	C16H46N26NaO9	1+	769.383328	3.0	3.9	35.1	28.99	C16 H46 N26 O9	M+Na
	C23H42N26NaO4	1+	769.377455	2.9	3.7	37.3	30.91	C23 H42 N26 O4	M+Na
	C15H43N30Na2O5	1+	769.382260	-1.9	-2.5	31.5	100.00	C15 H44 N30 O5	M+Na2-H
	C25H47N20Na2O6	1+	769.377734	-2.6	-3.4	39.5	47.38	C25 H48 N20 O6	M+Na2-H