

# School of Chemistry Mass Spectrometry Service

**SampleID** 1-4-1  
**Sample Description**  
**Analysis Name** 1-4-1\_171754\_GC5\_01\_24147.d  
**Method** 3a\_AccMass\_Loop\_Positive.m  
**Instrument** maXis impact

**Source Type** ESI **Ion Polarity** Positive

**Submitter**

Izar Capel

**Supervisor**

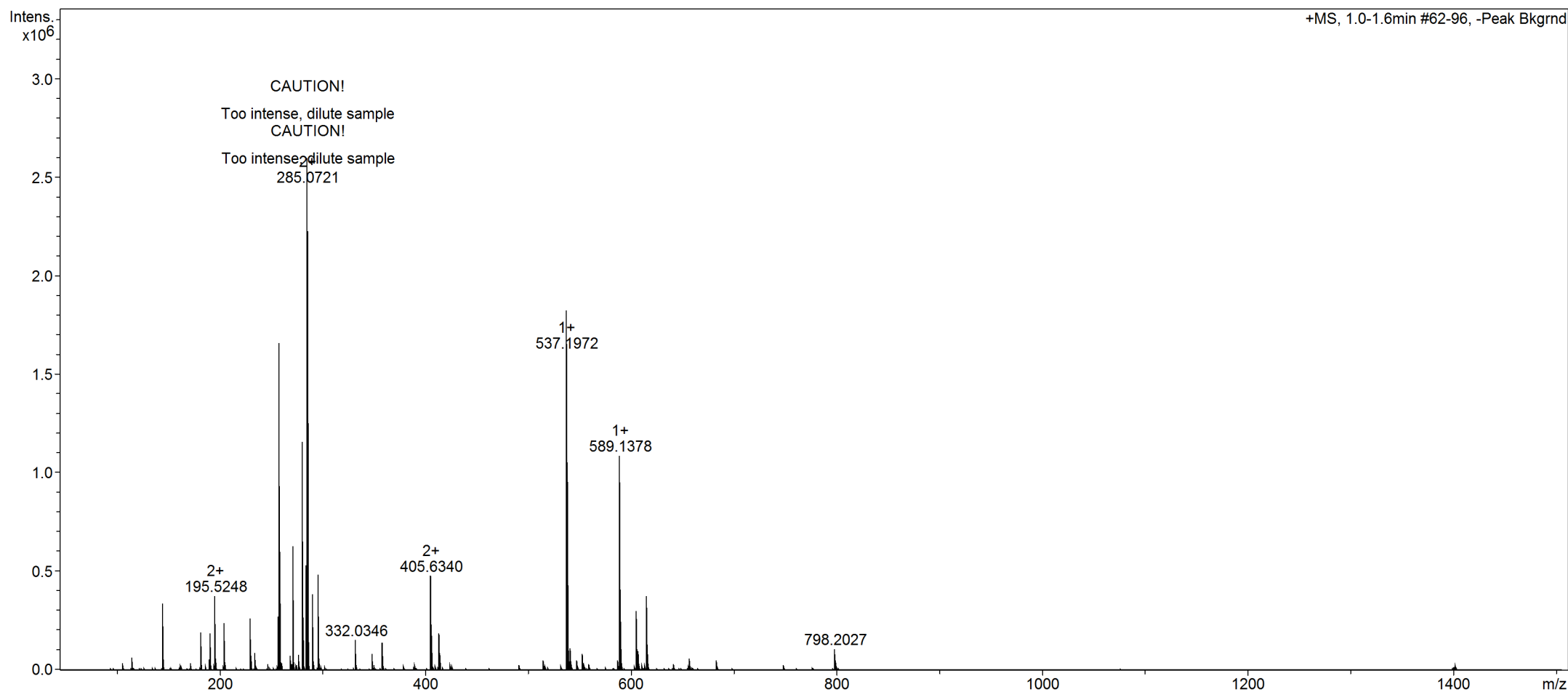
Malcolm Halcrow

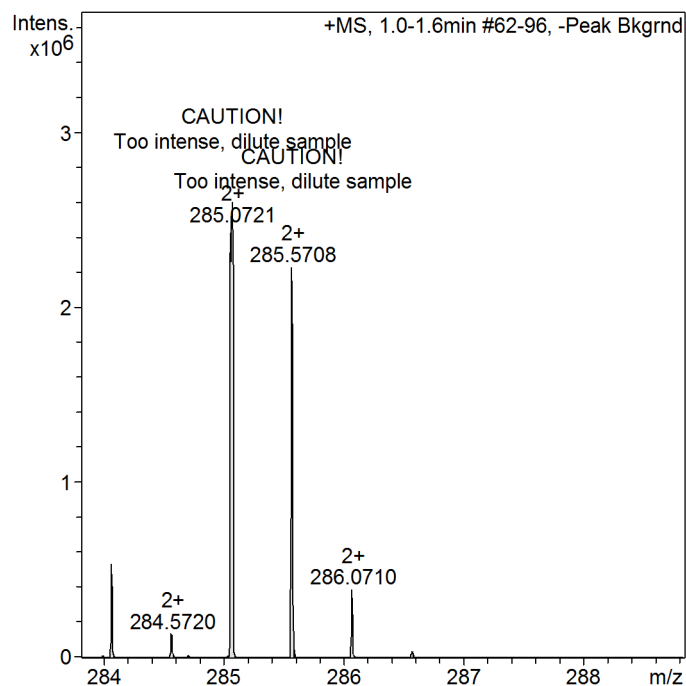
**Acquisition Date**

02/07/2016 23:00:39

**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

Concentration too high. Dilute sample!

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
285.570773	C10H15N22O8	2+	285.571612	0.8	2.9	13.8	78.17	C10 H13 N22 O8	M+H
	C11H21N15O13	2+	285.571614	0.8	2.9	14.2	77.57	C11 H19 N15 O13	M+H
	C10H25N11O17	2+	285.570946	-0.2	-0.6	17.6	100.00	C10 H23 N11 O17	M+H
	C12H27N8O18	2+	285.571617	-0.8	-3.0	17.8	71.89	C12 H25 N8 O18	M+H
	C10H15N22O8	2+	285.571612	0.8	2.9	13.8	78.17	C10 H7 N20 O8	M+NH4
	C11H21N15O13	2+	285.571614	0.8	2.9	14.2	77.57	C11 H13 N13 O13	M+NH4
	C10H25N11O17	2+	285.570946	-0.2	-0.6	17.6	100.00	C10 H17 N9 O17	M+NH4
	C12H27N8O18	2+	285.571617	-0.8	-3.0	17.8	71.89	C12 H19 N6 O18	M+NH4
	C11H23N14Na4O8	2+	285.570154	-0.6	-2.2	8.0	83.47	C11 H23 N14 Na2 O8	M+Na
	C10H17N21Na4O3	2+	285.570152	-0.6	-2.2	9.6	60.76	C10 H17 N21 Na2 O3	M+Na
	C13H25N11Na4O9	2+	285.570826	0.1	0.2	12.1	100.00	C13 H25 N11 Na2 O9	M+Na
	C12H29N7Na4O13	2+	285.570157	-0.6	-2.2	13.0	76.15	C12 H29 N7 Na2 O13	M+Na
	C12H19N18Na4O4	2+	285.570823	-0.1	-0.2	16.5	68.87	C12 H19 N18 Na2 O4	M+Na
	C15H27N8Na4O10	2+	285.571497	-0.7	-2.5	17.4	65.95	C15 H27 N8 Na2 O10	M+Na
	C14H21N15Na4O5	2+	285.571494	-0.7	-2.5	20.3	62.11	C14 H21 N15 Na2 O5	M+Na
	C13H15N22Na4	2+	285.571492	-0.7	-2.5	29.0	38.33	C13 H15 N22 Na2	M+Na
	C15H29N7Na8O5	2+	285.570037	0.7	2.6	13.5	59.67	C15 H31 N7 Na4 O5	M+Na2-H
	C17H31N4Na8O6	2+	285.570708	-0.1	-0.2	17.7	100.00	C17 H33 N4 Na4 O6	M+Na2-H
	C14H23N14Na8	2+	285.570034	0.7	2.6	18.6	53.71	C14 H25 N14 Na4	M+Na2-H
	C19H33NNa8O7	2+	285.571380	0.6	2.1	23.7	68.65	C19 H35 N Na4 O7	M+Na2-H
	C16H25N11Na8O	2+	285.570706	-0.1	-0.2	25.5	63.15	C16 H27 N11 Na4 O	M+Na2-H
	C18H27N8Na8O2	2+	285.571377	0.6	2.1	32.4	41.91	C18 H29 N8 Na4 O2	M+Na2-H
589.137821	C17H17N16O9	1+	589.135893	1.9	3.3	6.7	44.55	C17 H16 N16 O9	M+H
	C19H19N13O10	1+	589.137235	0.6	1.0	8.0	100.00	C19 H18 N13 O10	M+H
	C18H13N20O5	1+	589.137230	0.6	1.0	8.8	98.35	C18 H12 N20 O5	M+H
	C20H25N6O15	1+	589.137241	0.6	1.0	12.4	92.41	C20 H24 N6 O15	M+H
	C21H21N10O11	1+	589.138578	0.8	1.3	12.7	83.94	C21 H20 N10 O11	M+H
	C18H23N9O14	1+	589.135898	1.9	3.3	13.6	39.32	C18 H22 N9 O14	M+H
	C22H27N3O16	1+	589.138583	0.8	1.3	14.1	81.44	C22 H26 N3 O16	M+H
	C20H15N17O6	1+	589.138573	0.8	1.3	15.0	80.44	C20 H14 N17 O6	M+H
	C17H7N27	1+	589.137225	0.6	1.0	15.9	64.08	C17 H6 N27	M+H
	C24H29O17	1+	589.139926	-2.1	-3.6	17.9	31.34	C24 H28 O17	M+H
	C17H17N16O9	1+	589.135893	1.9	3.3	6.7	44.55	C17 H13 N15 O9	M+NH4
	C19H19N13O10	1+	589.137235	0.6	1.0	8.0	100.00	C19 H15 N12 O10	M+NH4

Smart Formula Parameter	Value
Expected Formula	C22H22N14O2Fe
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	Fe 2
Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	both
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
	C18H13N2O05	1+	589.137230	0.6	1.0	8.8	98.35	C18 H9 N19 O5	M+NH4
	C20H25N6O15	1+	589.137241	0.6	1.0	12.4	92.41	C20 H21 N5 O15	M+NH4
	C21H21N10O11	1+	589.138578	0.8	1.3	12.7	83.94	C21 H17 N9 O11	M+NH4
	C18H23N9O14	1+	589.135898	1.9	3.3	13.6	39.32	C18 H19 N8 O14	M+NH4
	C22H27N3O16	1+	589.138583	0.8	1.3	14.1	81.44	C22 H23 N2 O16	M+NH4
	C20H15N17O6	1+	589.138573	0.8	1.3	15.0	80.44	C20 H11 N16 O6	M+NH4
	C17H7N27	1+	589.137225	0.6	1.0	15.9	64.08	C17 H3 N26	M+NH4
	C24H29O17	1+	589.139926	-2.1	-3.6	17.9	31.34	C24 H29 O17	M+NH4
	C18H16N17NaO6	1+	589.136167	1.7	2.8	4.7	51.41	C18 H16 N17 O6	M+Na
	C19H22N10NaO11	1+	589.136172	1.6	2.8	8.3	48.35	C19 H22 N10 O11	M+Na
	C17H10N24NaO	1+	589.136162	1.7	2.8	8.7	47.68	C17 H10 N24 O	M+Na
	C21H24N7NaO12	1+	589.137515	-0.3	-0.5	10.3	100.00	C21 H24 N7 O12	M+Na
	C20H18N14NaO7	1+	589.137510	-0.3	-0.5	10.4	99.48	C20 H18 N14 O7	M+Na
	C17H32FeN7NaO11	1+	589.140165	-2.3	-4.0	11.7	40.07	C17 H32 Fe N7 O11	M+Na
	C22H30NaO17	1+	589.137520	0.3	0.5	14.3	92.78	C22 H30 O17	M+Na
	C19H12N21NaO2	1+	589.137504	-0.3	-0.5	14.6	91.58	C19 H12 N21 O2	M+Na
	C23H26N4NaO13	1+	589.138858	1.0	1.8	14.8	63.01	C23 H26 N4 O13	M+Na
	C20H28N3NaO16	1+	589.136178	1.6	2.8	14.8	42.88	C20 H28 N3 O16	M+Na
	C17H22KN14O8	1+	589.137662	0.2	0.3	36.9	100.00	C17 H22 N14 O8	M+K
	C19H24KN11O9	1+	589.139004	1.2	2.0	38.6	56.56	C19 H24 N11 O9	M+K
	C18H18KN18O4	1+	589.138999	1.2	2.0	39.7	44.02	C18 H18 N18 O4	M+K
	C22H28FeKN11O3	1+	589.135794	-2.0	-3.4	39.9	42.86	C22 H28 Fe N11 O3	M+K
	C20H21N11Na2O8	1+	589.136447	-1.4	-2.3	6.8	55.12	C20 H22 N11 O8	M+Na2-H
	C19H15N18Na2O3	1+	589.136441	-1.4	-2.3	9.5	52.33	C19 H16 N18 O3	M+Na2-H
	C21H27N4Na2O13	1+	589.136452	-1.4	-2.3	10.2	52.00	C21 H28 N4 O13	M+Na2-H
	C22H23N8Na2O9	1+	589.137789	-0.0	-0.1	12.3	100.00	C22 H24 N8 O9	M+Na2-H
	C23H29NNa2O14	1+	589.137795	0.0	0.0	12.6	99.70	C23 H30 N O14	M+Na2-H
	C17H35FeN4Na2O12	1+	589.139103	1.3	2.2	14.3	76.12	C17 H36 Fe N4 O12	M+Na2-H
	C21H17N15Na2O4	1+	589.137784	-0.0	-0.1	15.7	93.36	C21 H18 N15 O4	M+Na2-H
	C24H25N5Na2O10	1+	589.139132	-1.3	-2.2	18.3	46.00	C24 H26 N5 O10	M+Na2-H
	C23H19N12Na2O5	1+	589.139127	-1.3	-2.2	21.9	42.71	C23 H20 N12 O5	M+Na2-H
	C22H13N19Na2	1+	589.139121	-1.3	-2.2	26.9	38.24	C22 H14 N19	M+Na2-H
	C20H33Fe2N10O4	1+	589.138006	-0.2	-0.3	37.5	93.70	C10 H16 Fe N5 O2	2M+H
	C18H34Fe2N10NaO4	1+	589.135593	-2.2	-3.8	33.7	27.10	C9 H17 Fe N5 O2	2M+Na
	C22H38Fe2N4NaO6	1+	589.138296	0.5	0.8	38.1	73.94	C11 H19 Fe N2 O3	2M+Na