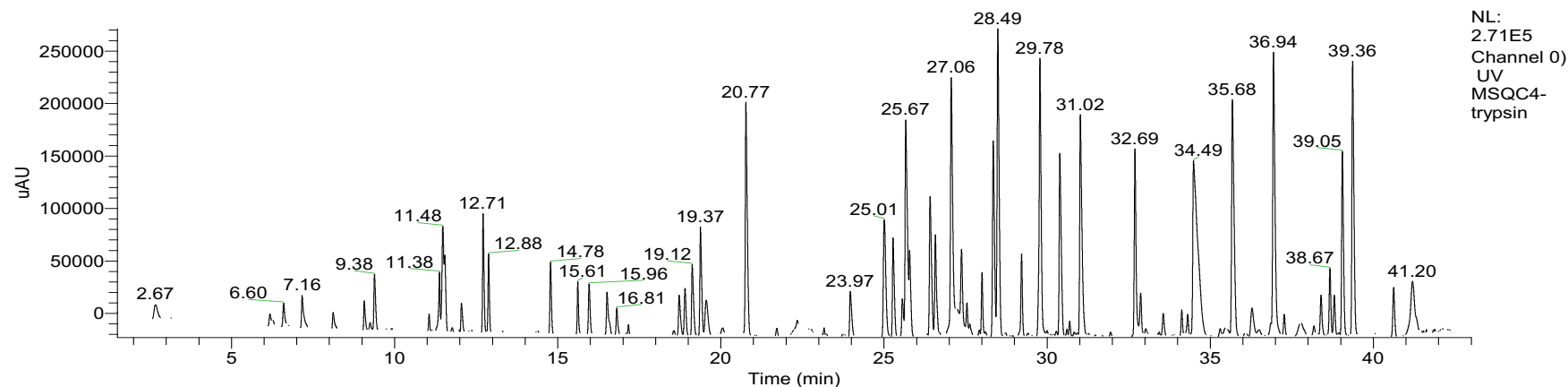
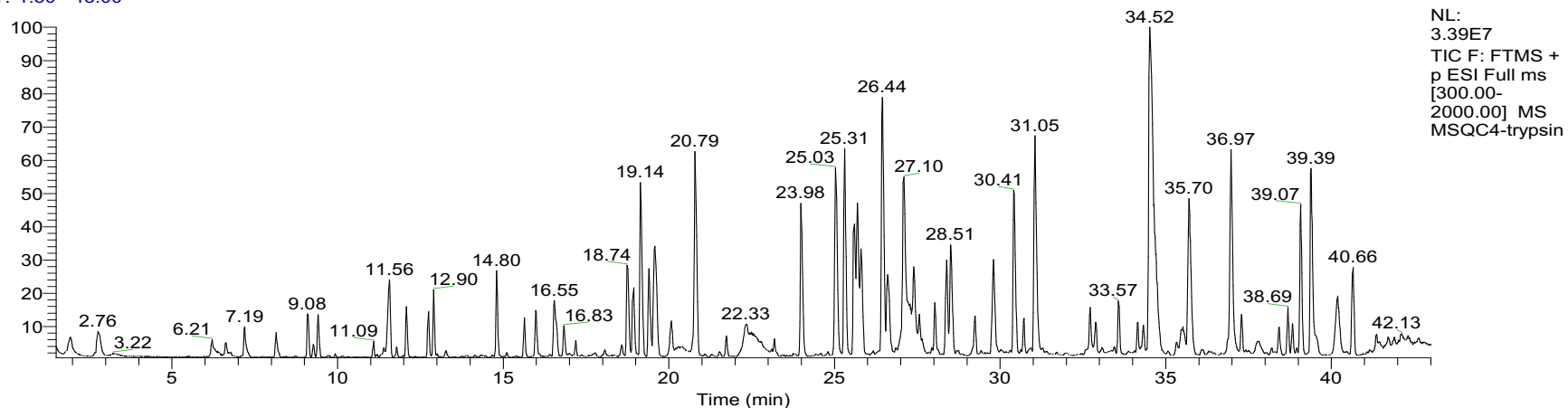


- **Chromatograms worksheet** - shows the LCUV and LCMS chromatograms for the samples.
- **Peptides worksheets** - shows the list of detected peptides and their identity and where they eluted in the chromatogram. The sequence notation, for example: 1:Q1-K18 = 1823.99928m(Q1+NH3 loss) indicates a light chain peptide from residues Q1-K18 with a monoisotopic mass 1823.99928 that has lost NH3 from the Q1 residue (i.e., pyroglutamic acid). Sequences preceded by **1:** are from the light chain, sequences preceded by **2:** are from the heavy chain, and sequences preceded by **3:** are trypsin.
- **Coverage worksheets** - shows a coverage map of the proteins for each sample. The colored bars indicate the intensity level of the peptide and the numbers inside the bars indicate the retention time in the chromatogram. A table at the top right of this sheet shows the % coverage for each protein chain. Warmer colors indicate the most intense peptides red > yellow > green > light blue > dark blue. The color-coded intensity key is at the bottom of the coverage sheet.
- **Modifications summary worksheet** - shows a listing of significant modifications that were detected. Modifications listed were confirmed by accurate mass and MS/MS with a confidence level of 80% or greater.

RT: 1.50 - 43.00



RT: 1.50 - 43.00

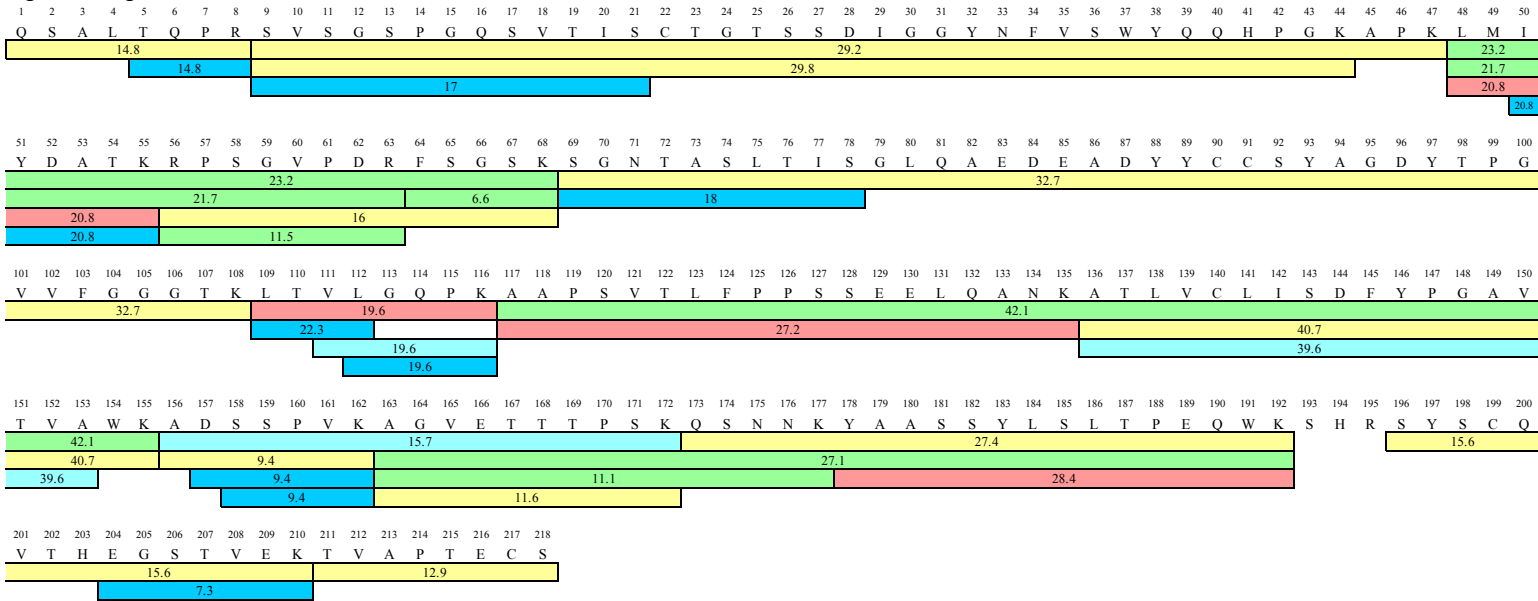


LC/UV, 214 nm (top) and LCMS TIC chromatograms (bottom) of MSQC4 standard tryptic digest.

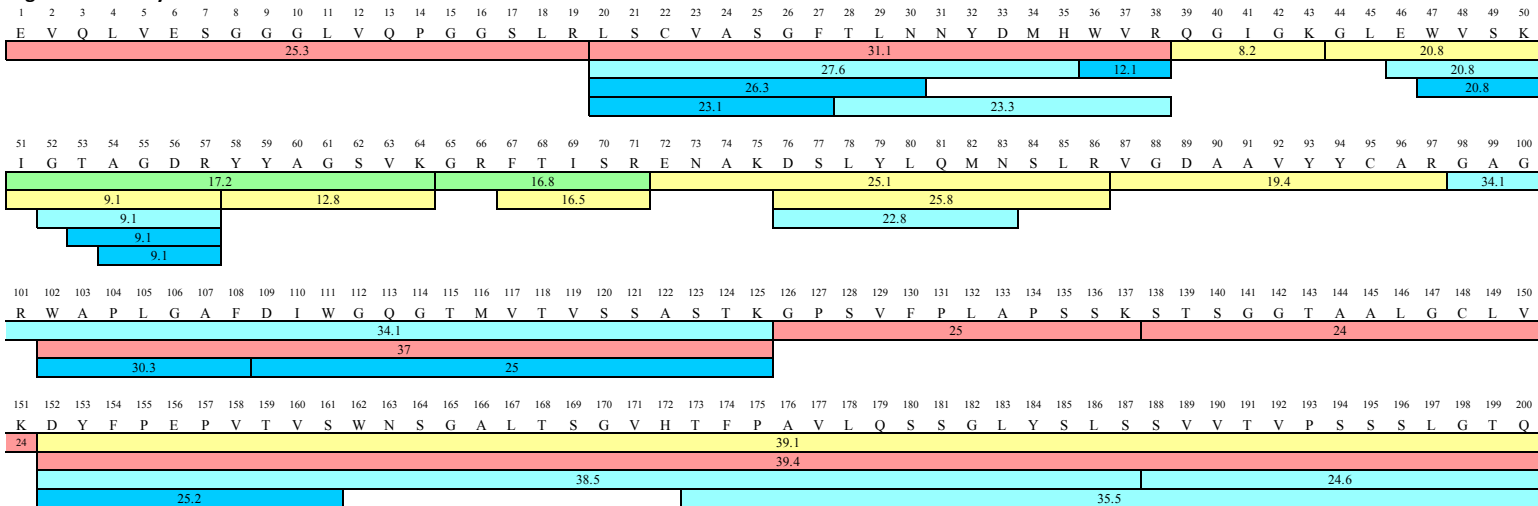
MSQC4 Sequence Coverage Map

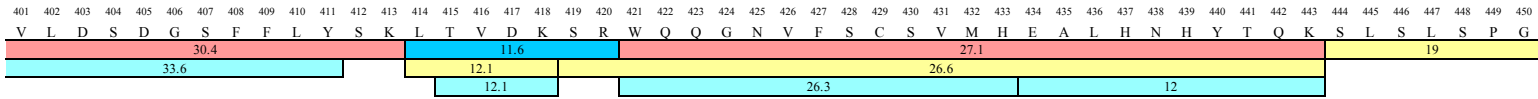
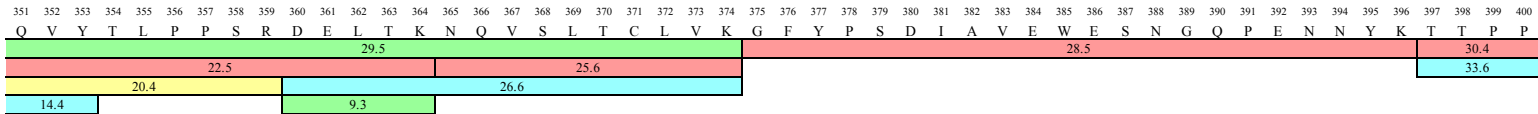
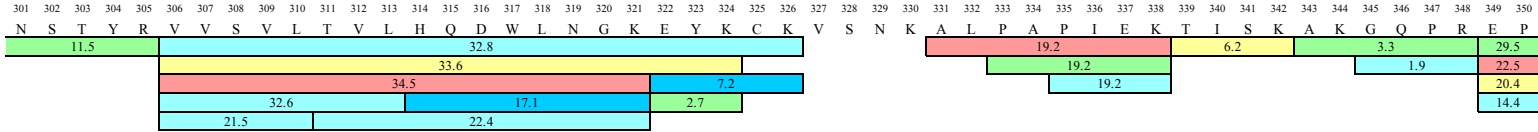
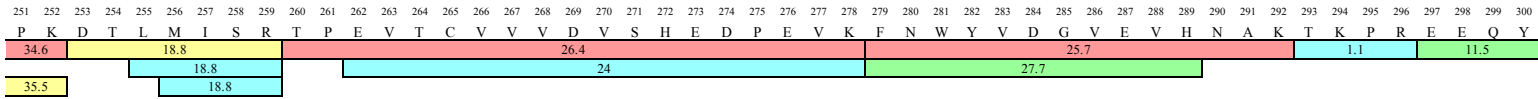
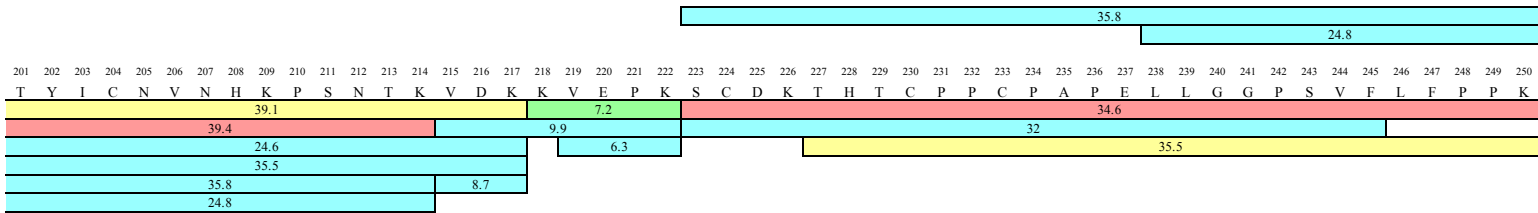
Data File = MSQC4-trypsin.raw
 Protease = Trypsin

SigmaMab Light Chain

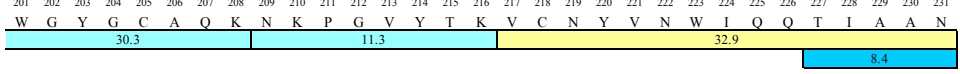
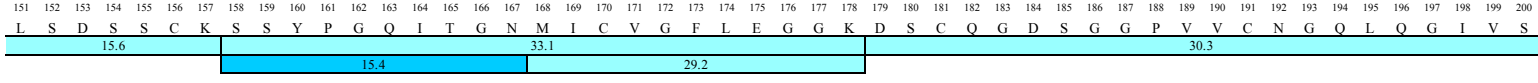
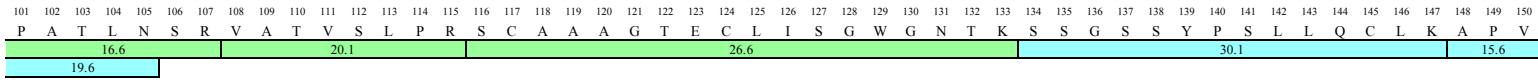
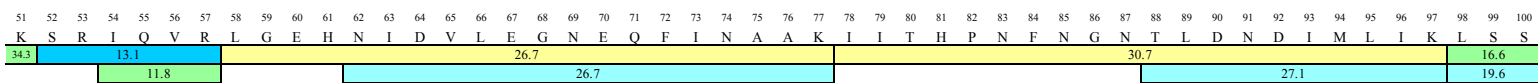


SigmaMab Heavy Chain

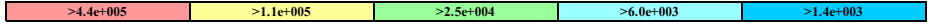




Trypsin



Color Code for Signal Intensity



MSQC4 Sequence Coverage Summary

Proteins	Number of MS Peaks	MS Peak Area	Sequence Coverage	Abundance (mol)
1:SigmaMab Light Chain	80	15.90%	98.60%	38.28%
2:SigmaMab Heavy Chain	226	58.20%	99.10%	56.15%
3:Trypsin	58	2.50%	96.50%	5.57%
Unidentified	797	23.50%		

MS Signal Threshold = 1.4e+003

MSQC4 Modification Summary

Data File = MSQC4-trypsin.raw

Protease = Trypsin

All mods >1% rel. intensity threshold, >80% confidence MS/MS

Protein	Modification	Recovery	Abundance	Comments
SigmaMab Light Chain	Q1+NH3 loss	Good	100.00%	
SigmaMab Light Chain	~N33+NH3 loss	Good	1.80%	
SigmaMab Light Chain	~A73+26.0098	Good	2.67%	?
SigmaMab Heavy Chain	~E1+H2O loss	Good	2.63%	
SigmaMab Heavy Chain	M116+Oxidation	Good	2.98%	
SigmaMab Heavy Chain	M256+Oxidation	Good	4.23%	
SigmaMab Heavy Chain	~D284+H2O loss	Good	3.10%	
SigmaMab Heavy Chain	N301+A2G0	Fair	7.26%	glycosylation
SigmaMab Heavy Chain	N301+A2G0F	Fair	46.89%	glycosylation
SigmaMab Heavy Chain	N301+A2G1	Fair	6.79%	glycosylation
SigmaMab Heavy Chain	N301+A2G1F	Fair	33.80%	glycosylation
SigmaMab Heavy Chain	N301+A2G2F	Fair	5.26%	glycosylation
SigmaMab Heavy Chain	~N319+NH3 loss	Good	0.029366	
SigmaMab Heavy Chain	~N388+NH3 loss	Good	2.68%	
SigmaMab Heavy Chain	~S407+H2O loss	Good	1.82%	
SigmaMab Heavy Chain	~M432+Oxidation	Good	2.06%	
SigmaMab Heavy Chain	G450+Lys	Good	1.43%	C-terminal Lys
SigmaMab Heavy Chain	G450+minus G+amidation	Good	10.94%	-Gly, amide C-terminus

File: E:\Novatia\2019\011619\MSQC4-trypsin.raw

Sample: 50 ug in ~125 uL, 25 uL inj

Comment: 2.1x100 mm Acquity Peptide BEH C18 1.7 um, 50C, 0-35%B in 40 min after 3 min hold, 35-60%B in 5 min, 0.4 mL/min, A=0.05% TFA in water, B=0.05% TFA in ACN, ITMS MS/MS scan

Minimum MS Signal: 20000

List: All ions

Time	m/z	MS Area	Charge	Avg Mass	Mono Mass	Identification	Confidence
14.7951	442.235	60286	2	882.759	882.455	1:Q1-R8 = 899.48248m(Q1+NH3 loss)	0.9999839
14.7951	883.463	215010	1	882.746	882.456	1:Q1-R8 = 899.48248m(Q1+NH3 loss)	0.99626166
14.7951	433.23	1844	2	864.727	864.446	1:Q1-R8 = 899.48248m(Q1+NH3 loss)(~T5-18.0085)	0.95468295
20.7514	622.823	6252	2	1244.24	1243.631	1:Q1-R8 = 899.48248m(Q1+NH3 loss)(~Q1+361.1762)	0.93692136
14.7951	501.278	5368	1	500.445	500.271	1:T5-R8 = 500.27070m[nonspecific]	0.83763611
17.0123	603.304	2708	2	1205.14	1204.594	1:S9-S21 = 1204.59355m[nonspecific]	0.9998194
17.0008	1205.6	3393	1	1205.17	1204.595	1:S9-S21 = 1204.59355m[nonspecific]	0.99832034
29.8125	930.933	83646	4	3719.8	3717.702	1:S9-K44 = 3717.70055m	1
29.8175	744.949	5710	5	3719.81	3717.702	1:S9-K44 = 3717.70055m	1
29.8103	1240.91	406360	3	3719.82	3717.696	1:S9-K44 = 3717.70055m	1
29.8173	1860.85	93745	2	3719.82	3717.689	1:S9-K44 = 3717.70055m	0.99956793
30.8558	1234.9	7454	3	3703.03	3700.681	1:S9-K44 = 3717.70055m(~N33+NH3 loss)	1
29.2403	1339.64	158618	3	4016.15	4013.886	1:S9-K47 = 4013.88539m	1
29.2403	1004.98	60092	4	4016.16	4013.893	1:S9-K47 = 4013.88539m	1
20.8022	477.751	333829	2	953.972	953.488	1:L48-K55 = 953.48920m	0.99999869
20.8018	954.495	467485	1	953.993	953.488	1:L48-K55 = 953.48920m	0.99801439
21.7347	606.988	29788	3	1818.95	1817.944	1:L48-R63 = 1817.94580m	1
21.7346	909.98	64806	2	1818.96	1817.945	1:L48-R63 = 1817.94580m	0.99998456
21.7276	455.744	3654	4	1818.9	1817.945	1:L48-R63 = 1817.94580m	0.9683947
23.1913	776.073	26651	3	2325.43	2324.195	1:L48-K68 = 2324.19470m	1
23.1913	582.307	6960	4	2325.41	2324.194	1:L48-K68 = 2324.19470m	1
23.1913	1163.6	34052	2	2325.42	2324.192	1:L48-K68 = 2324.19470m	0.99998909
20.8026	710.373	3063	1	709.624	709.366	1:I50-K55 = 709.36466m[nonspecific]	0.9122929
11.5414	883.473	23964	1	882.767	882.466	1:R56-R63 = 882.46716m	0.99999475
11.526	442.24	101571	2	882.756	882.466	1:R56-R63 = 882.46716m	0.99991471
15.993	695.366	209117	2	1389.35	1388.717	1:R56-K68 = 1388.71606m	0.99999887
15.993	463.912	74042	3	1389.37	1388.715	1:R56-K68 = 1388.71606m	0.99992633
15.9888	1390.73	8393	1	1389.38	1388.717	1:R56-K68 = 1388.71606m	0.99938715
15.9888	927.153	5669	3	2778.95	2777.434	1:R56-K68 = 1388.71606m[2x]	0.99962443
15.9888	1389.72	9811	2	2778.82	2777.435	1:R56-K68 = 1388.71606m[2x]	0.96837741
6.62922	525.266	69004	1	524.457	524.259	1:F64-K68 = 524.25946m	0.99658251
17.9932	950.479	3424	1	949.785	949.472	1:S69-S78 = 949.47164m[nonspecific]	0.95109975
32.7179	1018.2	27068	4	4069.21	4066.777	1:S69-K108 = 4066.77246m	1
32.718	1357.26	223169	3	4069.09	4066.78	1:S69-K108 = 4066.77246m	0.99999225
33.0465	1365.94	6113	3	4095.11	4092.79	1:S69-K108 = 4066.77246m(~A73+26.0098)	0.99999809
22.3076	445.303	1877	1	444.466	444.295	1:L109-L112 = 444.29479m[nonspecific]	0.89693767
19.5725	428.268	276515	2	854.82	854.522	1:L109-K116 = 854.52255m	0.99999517
19.5726	855.53	458888	1	854.821	854.522	1:L109-K116 = 854.52255m	0.98422801
19.5727	641.398	11614	1	640.626	640.391	1:V111-K116 = 640.39081m[nonspecific]	0.93144614
19.5728	542.33	5441	1	541.513	541.323	1:L112-K116 = 541.32240m[nonspecific]	0.99185485
27.2276	663.012	140858	3	1986.06	1985.011	1:A117-K135 = 1985.01057m	1
27.2387	994.014	1848790	2	1986.06	1985.009	1:A117-K135 = 1985.01057m	0.99999225
27.1125	1987.02	11004	1	1986.04	1985.005	1:A117-K135 = 1985.01057m	0.9993449
27.2361	1325.02	102890	3	3972.22	3970.026	1:A117-K135 = 1985.01057m[2x]	0.99999994
42.0999	1375.05	25211	3	4122.75	4120.135	1:A117-K155 = 4120.12311m	0.99999994
39.5844	920.483	6573	2	1839.99	1838.951	1:A136-A153 = 1838.94882m[nonspecific]	0.99997431
40.6515	719.049	62735	3	2154.31	2153.122	1:A136-K155 = 2153.12310m	1
40.6521	1078.07	420984	2	2154.32	2153.119	1:A136-K155 = 2153.12310m	0.99999225
40.6437	1437.09	26212	3	4308.9	4306.24	1:A136-K155 = 2153.12310m[2x]	0.99881315
40.6586	1089.06	37051	2	2176.3	2175.107	1:A136-K155 = 2153.12310m(Na+)	0.99996215
38.8139	1468.96	10042	4	5872.39	5868.814	1:A136-K155/1:S9-K44 = 5868.808m[1ss]	0.99987775
35.7312	1077.57	6547	2	2153.9	2152.114	1:A136-K155 = 2153.12310m(~L138-1.0044)	0.99996257
40.6645	1102.06	10780	2	2202.43	2201.109	1:A136-K155 = 2153.12310m(~W154+47.9847)	0.99954391
9.41873	352.184	28129	2	702.602	702.353	1:A156-K162 = 702.35482m	0.99993855
9.41876	703.362	137585	1	702.591	702.355	1:A156-K162 = 702.35482m	0.9997015
15.6688	837.932	6035	2	1674.59	1673.849	1:A156-K172 = 1673.84719m	0.99999928
9.41875	632.326	4266	1	631.544	631.318	1:D157-K162 = 631.31771m[nonspecific]	0.99444091
9.41875	517.298	5310	1	516.478	516.291	1:S158-K162 = 516.29076m[nonspecific]	0.98186344
11.5713	495.758	183743	2	989.814	989.502	1:A163-K172 = 989.50294m	0.99998468
11.5714	990.509	219821	1	989.821	989.501	1:A163-K172 = 989.50294m	0.99468547
11.0875	521.265	5828	3	1561.46	1560.773	1:A163-K177 = 1560.77436m	1
11.0875	781.395	50075	2	1561.45	1560.775	1:A163-K177 = 1560.77436m	0.99993539
27.0966	822.663	6500	4	3287.39	3285.622	1:A163-K192 = 3285.61535m	0.99999994
27.0966	1096.55	67078	3	3287.36	3285.615	1:A163-K192 = 3285.61535m	0.99997956
27.0966	1644.31	14098	2	3287.32	3285.609	1:A163-K192 = 3285.61535m	0.99996912
27.398	772.716	92342	3	2315.32	2314.123	1:Q173-K192 = 2314.12298m	1
27.398	1158.57	227451	2	2315.32	2314.12	1:Q173-K192 = 2314.12298m	0.99998909
27.3978	1544.42	7477	3	4630.87	4628.246	1:Q173-K192 = 2314.12298m[2x]	1
28.1414	1150.06	9710	2	2298.44	2297.097	1:Q173-K192 = 2314.12298m(~Q173+NH3 loss)	0.99999934
28.3908	581.957	21571	3	1743.8	1742.849	1:Y178-K192 = 1742.85155m	0.99999994
28.3908	872.432	528832	2	1743.8	1742.85	1:Y178-K192 = 1742.85155m	0.99998909
28.3825	1163.24	38043	3	3487.66	3485.7	1:Y178-K192 = 1742.85155m[2x]	0.99999994
28.3825	1744.86	38081	2	3487.47	3485.692	1:Y178-K192 = 1742.85155m[2x]	0.96837741
28.3965	888.93	8667	2	1775.78	1774.841	1:Y178-K192 = 1742.85155m(GasPhaseDoubleOxidation)	0.91695893
28.391	879.925	7281	2	1757.99	1756.832	1:Y178-K192 = 1742.85155m(~Y183+13.9793)	0.99991554
15.6423	552.25	15062	3	1654.49	1653.729	1:S196-K210 = 1653.73045m	1
15.6423	827.873	119894	2	1654.62	1653.731	1:S196-K210 = 1653.73045m	0.99997109
35.7088	1269.95	982943	3	3807.08	3804.837	1:S196-K210/1:A136-K155 = 3804.838m[1ss]	0.99980669
35.7287	762.377	36351	5	3807.09	3804.843	1:S196-K210/1:A136-K155 = 3804.838m[1ss]	0.99982619
35.715	952.718	202643	4	3807.06	3804.843	1:S196-K210/1:A136-K155 = 3804.838m[1ss]	0.99934912

35.7092	1904.42	106569	2	3807.1	3804.828	1:S196-K210/1:A136-K155 = 3804.838m[1ss]	0.99902469
40.2365	1444.72	53414	4	5775.75	5771.831	1:S196-K210/1:A117-K155 = 5771.838m[1ss]	0.96765238
7.26504	749.368	2594	1	748.615	748.361	1:E204-K210 = 748.36030m[nonspecific]	0.99511719
12.9034	807.356	165919	1	806.609	806.348	1:T211-S218 = 806.34802m	0.99999946
12.9034	404.181	2178	2	806.639	806.348	1:T211-S218 = 806.34802m	0.9996537
12.921	829.338	3172	1	828.616	828.33	1:T211-S218 = 806.34802m(Na+)	0.99825919
25.3045	628.34	200089	3	1881.99	1880.995	2:E1-R19 = 1880.99559m	1
25.3046	941.505	1001130	2	1881.97	1880.996	2:E1-R19 = 1880.99559m	0.99999225
25.3043	1255.67	214079	3	3764.06	3761.996	2:E1-R19 = 1880.99559m[2x]	1
28.0683	932.5	27087	2	1863.97	1862.985	2:E1-R19 = 1880.99559m(~E1+H2O loss)	0.99999988
26.4533	1406.65	9714	3	4218.28	4215.913	2:E1-R19 = 1880.99559m[2x](~G16+453.9170)	0.96014988
23.1101	783.371	3011	1	782.655	782.364	2:L20-F27 = 782.36328m[nonspecific]	0.92859703
26.3384	1111.55	2639	1	1111.1	1110.539	2:L20-N30 = 1110.53795m[nonspecific]	0.99392164
27.5169	886.393	22938	2	1771.77	1770.772	2:L20-H35 = 1770.77054m[nonspecific]	0.99999559
31.054	554.263	4877	4	2213.37	2212.021	2:L20-R38 = 2212.01938m	1
31.054	738.681	432343	3	2213.38	2212.018	2:L20-R38 = 2212.01938m	1
31.054	1107.52	1110100	2	2213.38	2212.014	2:L20-R38 = 2212.01938m	0.99996817
31.054	1476.35	164835	3	4426.76	4424.039	2:L20-R38 = 2212.01938m[2x]	0.99999899
31.0919	1118.51	9144	2	2235.39	2234.004	2:L20-R38 = 2212.01938m(Na+)	0.96913683
31.0736	1123.51	7466	2	2245.19	2244.011	2:L20-R38 = 2212.01938m(GasPhaseDoubleOxidation)	0.93831283
32.6926	1098.51	4341	2	2195.24	2194.011	2:L20-R38 = 2212.01938m(S21+H2O loss)	
32.4657	1099.01	4044	2	2196.21	2194.996	2:L20-R38 = 2212.01938m(~N31+NH3 loss)	0.99999821
23.2594	724.84	7369	2	1448.37	1447.666	2:T28-R38 = 1447.66667m[nonspecific]	0.99998444
12.1062	460.267	2341	1	459.436	459.26	2:W36-R38 = 459.25940m[nonspecific]	0.94735414
8.1512	502.298	109759	1	501.472	501.291	2:Q39-K43 = 501.29110m	0.99979568
10.1395	485.271	3852	1	484.451	484.264	2:Q39-K43 = 501.29110m(Q39+NH3 loss)	0.99444568
8.15119	485.272	3311	1	484.433	484.265	2:Q39-K43 = 501.29110m(Q39+NH3 loss)	0.96640569
20.8023	409.723	85226	2	817.743	817.432	2:G44-K50 = 817.43340m	0.99999499
20.8017	818.44	283634	1	817.732	817.433	2:G44-K50 = 817.43340m	0.99326974
20.8051	425.719	1918	2	849.698	849.423	2:G44-K50 = 817.43340m(W47+Double Oxidation)	0.99997222
20.8139	850.431	4181	1	849.734	849.424	2:G44-K50 = 817.43340m(W47+Double Oxidation)	0.98820114
20.8028	648.336	11747	1	647.585	647.328	2:E46-K50 = 647.32788m[nonspecific]	0.99888325
20.8037	519.293	2683	1	518.484	518.285	2:W47-K50 = 518.28528m[nonspecific]	0.98403519
9.0969	689.358	106833	1	688.577	688.351	2:I51-R57 = 688.35040m	0.99948663
9.0991	345.182	51048	2	688.581	688.35	2:I51-R57 = 688.35040m	0.99872768
9.09943	336.177	2231	2	670.543	670.34	2:I51-R57 = 688.35040m(T53+H2O loss)	0.99697667
17.1921	486.583	8125	3	1457.42	1456.729	2:I51-K64 = 1456.73104m	0.99999994
17.1922	729.373	53338	2	1457.41	1456.731	2:I51-K64 = 1456.73104m	0.9998368
9.09957	576.273	15908	1	575.452	575.266	2:G52-R57 = 575.26634m[nonspecific]	0.9919554
9.09919	519.252	4559	1	518.399	518.245	2:T53-R57 = 518.24487m[nonspecific]	0.86451894
9.0992	418.205	2128	1	417.347	417.197	2:A54-R57 = 417.19720m[nonspecific]	0.92697138
12.7503	394.202	37985	2	786.678	786.39	2:Y58-K64 = 786.39120m	1
12.7543	787.398	109342	1	786.672	786.391	2:Y58-K64 = 786.39120m	0.99782205
16.833	836.472	29642	1	835.764	835.465	2:G65-R71 = 835.46644m	0.99999744
16.8331	418.74	84288	2	835.748	835.466	2:G65-R71 = 835.46644m	0.9998495
16.5342	312.179	55264	2	622.584	622.343	2:F67-R71 = 622.34386m	0.99959493
16.5343	623.351	176824	1	622.574	622.344	2:F67-R71 = 622.34386m	0.9986248
25.0533	891.444	189141	2	1781.84	1780.874	2:E72-R86 = 1780.87778m	0.99999964
22.7931	983.45	7997	1	982.951	982.443	2:D76-N83 = 982.44298m[nonspecific]	0.99993575
25.8124	1339.66	156105	1	1339.32	1338.657	2:D76-R86 = 1338.66019m	0.9999997
25.8119	670.337	439859	2	1339.3	1338.66	2:D76-R86 = 1338.66019m	0.99998111
19.4034	594.279	367523	2	1187.13	1186.544	2:V87-R97 = 1186.54409m	1
19.4034	1187.55	217745	1	1187.15	1186.54	2:V87-R97 = 1186.54409m	0.99996722
29.7645	680.718	4956	5	3398.64	3396.552	2:V87-R97/2:L20-R38 = 3396.548m[1ss]	0.99999845
29.7519	850.645	31938	4	3398.61	3396.551	2:V87-R97/2:L20-R38 = 3396.548m[1ss]	0.99993539
29.7519	1133.86	119559	3	3398.64	3396.546	2:V87-R97/2:L20-R38 = 3396.548m[1ss]	0.99986213
29.7519	1700.28	21560	2	3398.67	3396.543	2:V87-R97/2:L20-R38 = 3396.548m[1ss]	0.99941468
34.142	1434.71	9703	2	2868.03	2866.411	2:G98-K125 = 2850.41230m(W102+Oxidation)	0.9999997
34.1341	956.813	8328	3	2868.02	2866.414	2:G98-K125 = 2850.41230m(W102+Oxidation)	0.99997109
34.3133	1434.71	6991	2	2868.02	2866.412	2:G98-K125 = 2850.41230m(~M116+Oxidation)	
34.3134	956.812	8148	3	2868.03	2866.412	2:G98-K125 = 2850.41230m(~M116+Oxidation)	
30.3071	761.398	3803	1	760.695	760.391	2:W102-F108 = 760.39081m[nonspecific]	0.9999572
36.9701	1256.12	1136640	2	2510.7	2509.225	2:W102-K125 = 2509.23115m	1
36.9701	837.752	222598	3	2510.69	2509.23	2:W102-K125 = 2509.23115m	0.99997956
36.9701	1674.49	152616	3	5021.38	5018.449	2:W102-K125 = 2509.23115m[2x]	1
36.3787	1264.12	10176	2	2526.71	2525.231	2:W102-K125 = 2509.23115m(W102+Oxidation)	0.99999988
36.4529	1258.12	5831	2	2514.7	2513.232	2:W102-K125 = 2509.23115m(W102+Oxidation to kynurenine)	1
36.9917	1248.12	11411	2	2493.79	2492.219	2:W102-K125 = 2509.23115m(~W111-17.0063)	0.89237148
36.9701	848.416	9311	3	2542.62	2541.223	2:W102-K125 = 2509.23115m(W111+Double Oxidation)	0.99999958
36.9817	1272.12	23889	2	2542.68	2541.226	2:W102-K125 = 2509.23115m(W111+Double Oxidation)	0.9996459
36.9699	1263.62	11755	2	2526.09	2524.222	2:W102-K125 = 2509.23115m(~W111+14.9971)	0.9997912
35.3178	1264.12	36899	2	2526.74	2525.229	2:W102-K125 = 2509.23115m(M116+Oxidation)	1
25.0283	884.433	4747	2	1767.77	1766.852	2:D109-K125 = 1766.85090m[nonspecific]	0.99823415
25.0283	593.826	891764	2	1186.23	1185.638	2:G126-K137 = 1185.63937m	0.99999958
25.0283	1186.64	447681	1	1186.24	1185.635	2:G126-K137 = 1185.63937m	0.99978662
25.1003	604.818	6238	2	1208.18	1207.621	2:G126-K137 = 1185.63937m(Na+)	0.99979776
24.0062	422.224	4126	3	1264.22	1263.649	2:S138-K151 = 1263.64929m	1
24.0057	632.832	625243	2	1264.25	1263.65	2:S138-K151 = 1263.64929m	0.99990052
23.9827	1264.65	362712	1	1264.27	1263.646	2:S138-K151 = 1263.64929m	0.99267811
25.1657	1153.54	2887	1	1153.11	1152.536	2:D152-S161 = 1152.53391m[nonspecific]	0.99989903
38.4772	1272.63	8357	3	3815.53	3812.865	2:D152-S187 = 3812.85737m[nonspecific]	0.98469079
39.3938	1332.67	451820	5	6659.29	6655.313	2:D152-K214 = 6655.28571m	1
39.394	952.194	122621	7	6659.32	6655.311	2:D152-K214 = 6655.28571m	1
39.3942	833.296	30736	8	6659.15	6655.301	2:D152-K214 = 6655.28571m	1
39.3939	1665.58	457538	4	6659.27	6655.289	2:D152-K214 = 6655.28571m	1
39.3939	1110.89	294939	6	6659.29	6655.311	2:D152-K214 = 6655.28571m	0.99986665
39.3939	1113.56	13251	6	6676.82	6672.308	2:D152-K214 = 6655.28571m(~T159+16.9966)	0.99960089

39.0726	1401.3	202040	5	7001.62	6997.495	2:D152-K217 = 6997.47603m	1
39.0725	876.194	56009	8	7001.66	6997.492	2:D152-K217 = 6997.47603m	0.99999225
39.0724	1001.22	135981	7	7001.62	6997.496	2:D152-K217 = 6997.47603m	0.99999225
39.0725	1167.92	275614	6	7001.62	6997.495	2:D152-K217 = 6997.47603m	0.99998111
39.0726	778.84	11615	9	7001.69	6997.491	2:D152-K217 = 6997.47603m	0.99997437
39.0724	1751.37	283284	4	7001.6	6997.47	2:D152-K217 = 6997.47603m	0.9980514
38.831	1189.27	41466	6	7129.8	7125.584	2:D152-K218 = 7125.57100m	
38.831	1019.52	27809	7	7129.8	7125.592	2:D152-K218 = 7125.57100m	
38.831	892.206	10625	8	7129.78	7125.58	2:D152-K218 = 7125.57100m	
38.831	1783.4	38486	4	7129.77	7125.564	2:D152-K218 = 7125.57100m	
38.831	1426.92	20471	5	7129.77	7125.58	2:D152-K218 = 7125.57100m	
35.8436	1472.09	22546	3	4413.8	4411.24	2:T173-K214 = 4411.23697m[nonspecific]	0.99999923
35.8328	1104.32	11833	4	4413.81	4411.242	2:T173-K214 = 4411.23697m[nonspecific]	0.99995303
35.46	1190.12	8470	4	4756.17	4753.431	2:T173-K217 = 4753.42729m[nonspecific]	0.9999997
35.46	1586.15	10514	3	4756.14	4753.429	2:T173-K217 = 4753.42729m[nonspecific]	0.9960016
24.8003	954.821	10378	3	2862.02	2860.44	2:S188-K214 = 2860.43891m[nonspecific]	1
24.8002	1431.73	5587	2	2862.03	2860.441	2:S188-K214 = 2860.43891m[nonspecific]	0.99980485
24.5878	1068.88	10117	3	3204.36	3202.631	2:S188-K217 = 3202.62923m[nonspecific]	0.9984715
12.0769	361.208	3189	1	360.201	360.201	2:V215-K217 = 360.20088m	0.97630787
8.7249	328.259	6227	1	327.406	327.252	2:V215-K217 = 360.20088m(K217-32.9492)	0.83085966
9.0484	342.275	2079	1	341.414	341.267	2:V215-K217 = 360.20088m(K217-18.9335)	0.95502144
9.92356	471.784	10374	2	941.882	941.554	2:V215-K222 = 941.55458m	0.99999958
7.19676	300.689	43222	2	599.593	599.364	2:K218-K222 = 599.36426m	0.99964267
7.19673	600.371	99258	1	599.587	599.364	2:K218-K222 = 599.36426m	0.99929267
6.29922	472.276	22613	1	471.456	471.268	2:V219-K222 = 471.26930m	0.99998331
7.19664	472.276	7031	1	471.445	471.269	2:V219-K222 = 471.26930m	0.96516281
18.5306	507.281	4002	1	506.476	506.274	2:V219-K222 = 471.26930m(K222+35.0047)	0.96269274
21.7617	547.312	6216	1	546.538	546.305	2:V219-K222 = 471.26930m(K222+35.0047)(~E220+40.0313)	0.8896035
32.0174	1179.04	8533	2	2356.53	2355.071	2:S223-F245 = 2355.06976m[nonspecific]	0.99992466
34.6239	1055.53	1491630	3	3164.58	3162.567	2:S223-K252 = 3162.57045m	1
34.637	792.151	584933	4	3164.59	3162.573	2:S223-K252 = 3162.57045m	1
34.6363	633.723	80058	5	3164.56	3162.575	2:S223-K252 = 3162.57045m	1
34.6439	1582.79	420399	2	3164.58	3162.571	2:S223-K252 = 3162.57045m	0.99995631
34.2854	791.648	19749	4	3162.58	3160.558	2:S223-K252 = 3160.555m[1ss]	1
33.3199	1055.19	36007	3	3162.58	3160.557	2:S223-K252 = 3160.555m[1ss]	0.99999851
34.6939	1063.19	20295	3	3186.58	3184.562	2:S223-K252 = 3162.57045m(Na+)	0.99999517
36.8814	1582.54	24048	4	6326.91	6323.124	2:S223-K252/2:S223-K252 = 6323.125m[1ss]	0.99217796
34.694	1073.51	14077	3	3218.45	3216.489	2:S223-K252 = 3162.57045m(~A235+53.9224)	0.8134895
35.5143	683.61	27785	4	2731.04	2729.41	2:T227-K252 = 2729.40734m	1
35.5059	1366.21	129525	2	2731.05	2729.409	2:T227-K252 = 2729.40734m	0.99995917
35.5105	911.144	219516	3	2731.05	2729.408	2:T227-K252 = 2729.40734m	0.99890065
35.515	918.472	13527	3	2753.05	2751.392	2:T227-K252 = 2729.40734m(Na+)	0.99308872
18.752	418.22	96010	2	834.712	834.426	2:D253-R259 = 834.42694m	0.99999928
18.7513	835.434	293354	1	834.703	834.427	2:D253-R259 = 834.42694m	0.9999209
18.7507	409.216	2190	2	816.693	816.417	2:D253-R259 = 834.42694m(~T254+H2O loss)	0.99999154
16.6187	851.428	10538	1	850.71	850.421	2:D253-R259 = 834.42694m(M256+Oxidation)	0.99999958
16.6233	426.217	6799	2	850.714	850.42	2:D253-R259 = 834.42694m(M256+Oxidation)	0.99996722
18.7515	619.36	7242	1	618.579	618.353	2:L255-R259 = 618.35232m[nonspecific]	0.98955482
18.751	506.276	7709	1	505.44	505.268	2:M256-R259 = 505.26825m[nonspecific]	0.90649283
26.4461	695.007	471036	3	2082.12	2080.997	2:T260-K278 = 2080.99869m	0.99999994
26.4462	1042.01	1394330	2	2082.1	2080.995	2:T260-K278 = 2080.99869m	0.99997818
26.4456	1389.01	254157	3	4164.48	4161.999	2:T260-K278 = 2080.99869m[2x]	0.99999994
32.6522	1135.83	5978	4	4540.35	4537.292	2:T260-K278/2:V306-K326 = 4537.287m[1ss]	0.99972004
36.0756	1412.38	5767	3	4234.96	4232.11	2:T260-K278/1:A136-K155 = 4232.106m[1ss]	0.99792546
32.6522	1514.11	8387	3	4540.32	4537.291	2:T260-K278/2:V306-K326 = 4537.287m[1ss]	0.97764587
26.3967	1054.51	2355	2	2106.82	2104.987	2:T260-K278 = 2080.99869m(~V266+23.9922)	0.96839893
26.4522	1051.01	10098	2	2099.93	2099.014	2:T260-K278 = 2080.99869m(~S271+18.0190)	0.99947059
26.3782	1079.03	4148	2	2156.14	2155.039	2:T260-K278 = 2080.99869m(~V277+74.0442)	0.99997723
23.9827	942.959	7664	2	1883.94	1882.9	2:E262-K278 = 1882.89824m[nonspecific]	0.99999309
27.6543	682.817	30478	2	1364.3	1363.62	2:F279-H289 = 1363.61970m[nonspecific]	0.99999177
27.6542	1364.63	4558	1	1364.32	1363.622	2:F279-H289 = 1363.61970m[nonspecific]	0.98582971
25.7048	559.938	153570	3	1677.73	1676.792	2:F279-K292 = 1676.79471m	1
25.7048	839.405	948223	2	1677.71	1676.795	2:F279-K292 = 1676.79471m	0.99997437
25.7047	1119.54	76153	3	3355.54	3353.591	2:F279-K292 = 1676.79471m[2x]	0.99999619
25.7052	855.4	9903	2	1709.69	1708.786	2:F279-K292 = 1676.79471m(GasPhaseDoubleOxidation)	0.93014413
25.7051	846.396	11122	2	1691.59	0	2:F279-K292 = 1676.79471m(~Y282+14)	0.99982798
28.1257	830.399	12898	2	1659.71	1658.784	2:F279-K292 = 1676.79471m(D284+H2O loss)	
27.9435	830.399	30733	2	1659.72	1658.783	2:F279-K292 = 1676.79471m(~D284+H2O loss)	0.99999851
1.06135	501.314	20161	1	500.48	500.307	2:T293-R296 = 500.30708m	0.99375486
11.503	1245	8166	2	2488.2	2486.983	2:E297-R305 = 1188.50473m(N301+A2G0)	0.99999702
11.5023	879.022	7620	3	2634.45	2633.041	2:E297-R305 = 1188.50473m(N301+A2G0F)	1
11.5024	1318.03	52733	2	2634.43	2633.035	2:E297-R305 = 1188.50473m(N301+A2G0F)	0.99978602
11.4943	1326.54	7639	2	2651.03	2649.037	2:E297-R305 = 1188.50473m(N301+A2G1)	0.99999997
11.3995	933.039	8089	3	2796.53	2795.093	2:E297-R305 = 1188.50473m(N301+A2G1F)	1
11.3995	1399.05	38020	2	2796.55	2795.088	2:E297-R305 = 1188.50473m(N301+A2G1F)	0.99990642
11.3679	1480.08	5914	2	2958.67	2957.145	2:E297-R305 = 1188.50473m(N301+A2G2F)	0.99999934
21.5291	516.339	15783	1	515.544	515.332	2:V306-L310 = 515.33190m[nonspecific]	0.99477082
32.5926	829.539	21523	1	828.846	828.532	2:V306-L313 = 828.53206m[nonspecific]	0.98239005
34.5191	603.675	462360	3	1807.99	1806.998	2:V306-K321 = 1806.99922m	1
34.5196	905.009	1823020	2	1807.98	1807	2:V306-K321 = 1806.99922m	0.99996549
34.5075	1809.01	67575	1	1807.88	1806.996	2:V306-K321 = 1806.99922m	0.99987864
34.5184	1206.34	242622	3	3616.08	3614.001	2:V306-K321 = 1806.99922m[2x]	1
34.5307	913.514	9354	2	1825.65	0	2:V306-K321 = 1806.99922m(~L313+18)	0.80675507
34.5309	614.339	6826	3	1839.77	1838.99	2:V306-K321 = 1806.99922m(W317+Double Oxidation)	1
34.5203	920.502	28081	2	1839.93	1838.99	2:V306-K321 = 1806.99922m(W317+Double Oxidation)	0.99985069
34.9129	905.001	4105	2	1808.81	1807.987	2:V306-K321 = 1806.99922m(N319+Deamidation)	0.99999905
35.6776	597.999	9689	3	1790.94	1789.974	2:V306-K321 = 1806.99922m(~N319+NH3 loss)	1

35.6649	895.995	56636	2	1790.97	1789.975	2:V306-K321=1806.99922m(~N319+NH3 loss)	0.99982244
34.3138	942.028	7408	2	1882.04	1881.039	2:V306-K321=1806.99922m(~G320+74.0386)	0.99997878
33.5686	743.741	103343	3	2228.39	2227.199	2:V306-K324=2227.20010m	1
33.5686	558.058	10220	4	2228.33	2227.2	2:V306-K324=2227.20010m	1
33.5686	1115.11	127615	2	2228.38	2227.198	2:V306-K324=2227.20010m	0.9999482
33.5686	1486.48	4442	3	4457.02	4454.404	2:V306-K324=2227.20010m[2x]	0.99999732
33.5686	1126.1	5608	2	2250.36	2249.185	2:V306-K324=2227.20010m(Na+)	0.99994433
32.8186	1230.66	4166	2	2459.79	2458.309	2:V306-K326=2458.30425m	0.99999762
32.8186	820.777	6405	3	2459.76	2458.307	2:V306-K326=2458.30425m	0.99948353
22.3572	655.846	23127	2	1310.32	1309.677	2:T311-K321=1309.67788m[nonspecific]	0.99999607
17.1232	499.246	3319	2	996.815	996.477	2:H314-K321=996.47773m[nonspecific]	0.99947792
2.68682	439.218	38614	1	438.389	438.211	2:E322-K324=438.21145m	0.99995834
7.24848	670.323	2994	1	669.564	669.316	2:E322-K326=669.31560m	0.99996811
23.1101	917.442	7897	3	2749.89	2748.302	2:E322-K326/2:T260-K278=2748.299m[1ss]	0.99988759
23.1101	1375.66	5620	2	2749.87	2748.303	2:E322-K326/2:T260-K278=2748.299m[1ss]	0.99852639
19.154	419.755	239352	2	837.798	837.495	2:A331-K338=837.49600m	1
19.1542	838.503	443903	1	837.795	837.496	2:A331-K338=837.49600m	0.9999488
19.1877	860.485	3985	1	859.788	859.478	2:A331-K338=837.49600m(Na+)	0.9999969
19.1543	327.694	29891	2	653.606	653.373	2:P333-K338=653.37483m[nonspecific]	0.99998659
19.1541	654.38	65831	1	653.621	653.373	2:P333-K338=653.37483m[nonspecific]	0.99927521
19.1541	486.292	13957	1	485.46	485.285	2:P335-K338=485.28495m[nonspecific]	0.98829013
6.21731	448.276	117165	1	447.435	447.269	2:T339-K342=447.26930m	0.99920648
11.462	460.313	1584	1	459.488	459.305	2:T339-K342=447.26930m(T339+12.0363)	0.99269319
3.27074	328.695	26720	2	655.61	655.376	2:A343-R348=655.37656m	0.99981081
3.2655	656.383	19028	1	655.608	655.375	2:A343-R348=655.37656m	0.99688399
1.87922	457.252	10397	1	456.395	456.245	2:G345-R348=456.24448m	0.97042674
14.3753	635.303	8436	1	634.545	634.296	2:E349-Y353=634.29624m[nonspecific]	0.98819184
20.3715	1286.68	25911	1	1286.31	1285.669	2:E349-R359=1285.66665m	0.99999714
20.3765	643.841	337352	2	1286.3	1285.667	2:E349-R359=1285.66665m	0.99992758
22.4842	624.995	229070	3	1872.96	1871.962	2:E349-K364=1871.96289m	1
22.4765	936.988	991571	2	1872.96	1871.962	2:E349-K364=1871.96289m	0.99998456
22.4858	1249.65	33887	3	3746.02	3743.934	2:E349-K364=1871.96289m[2x]	1
29.528	987.193	36547	3	2959.19	2957.556	2:E349-K374=2957.55321m	0.9999997
9.27017	303.16	4220	2	604.516	604.306	2:D360-K364=604.30681m	0.99999833
9.26998	605.314	44193	1	604.521	604.307	2:D360-K364=604.30681m	0.99939865
26.6423	845.957	12548	2	1690.81	1689.9	2:D360-K374=1689.89712m	0.99999452
25.6013	552.807	416767	2	1104.14	1103.6	2:N365-K374=1103.60088m	0.99999917
25.6013	1104.61	578394	1	1104.15	1103.598	2:N365-K374=1103.60088m	0.99433517
31.1501	1608.1	6549	3	4822.1	4819.284	2:N365-K374/1:59-K44=4819.286m[1ss]	0.99763942
27.5619	1023.5	22911	4	4090.48	4087.96	2:N365-K374/2:S419-K443=4087.957m[1ss]	0.9983567
27.5619	819.001	4380	5	4090.46	4087.962	2:N365-K374/2:S419-K443=4087.957m[1ss]	0.99738711
28.0329	1283.28	170076	3	3847.1	3844.823	2:N365-K374/2:W421-K443=3844.823m[1ss]	0.99415451
27.5619	1364.33	51840	3	4090.32	4087.962	2:N365-K374/2:S419-K443=4087.957m[1ss]	0.99276227
28.0326	962.714	56149	4	3847.1	3844.826	2:N365-K374/2:W421-K443=3844.823m[1ss]	0.99255437
28.0327	770.374	8696	5	3847.11	3844.827	2:N365-K374/2:W421-K443=3844.823m[1ss]	0.97186899
28.0327	1924.42	8064	2	3847.11	3844.815	2:N365-K374/2:W421-K443=3844.823m[1ss]	0.9684158
28.5151	1273.07	652873	2	2544.54	2543.118	2:G375-K396=2543.12410m	1
28.5151	849.049	105528	3	2544.54	2543.125	2:G375-K396=2543.12410m	1
28.5151	1697.09	86314	3	5089.1	5086.235	2:G375-K396=2543.12410m[2x]	1
28.521	1280.07	10721	2	2558.71	2557.113	2:G375-K396=2543.12410m(~Y377+13.9793)	0.9967283
28.5262	1289.07	7608	2	2576.39	2575.12	2:G375-K396=2543.12410m(W385+Double Oxidation)	0.99959451
28.7385	1273.57	8665	2	2545.55	2544.116	2:G375-K396=2543.12410m(N388+Deamidation)	
29.1865	1264.56	18638	2	2527.53	2526.1	2:G375-K396=2543.12410m(~N388+NH3 loss)	1
30.856	1264.07	5718	2	2526.76	2525.12	2:G375-K396=2543.12410m(~E392+H2O loss)	0.97157156
33.5961	830.404	6951	2	1658.73	1657.79	2:T397-Y411=1657.78755m[nonspecific]	0.99999034
30.4233	937.965	1078950	2	1873.92	1872.911	2:T397-K413=1872.91455m	1
30.4186	625.647	31566	3	1873.91	1872.914	2:T397-K413=1872.91455m	0.99998111
30.423	1874.92	43540	1	1873.96	1872.908	2:T397-K413=1872.91455m	0.99987918
30.4184	1250.29	144278	3	3747.97	3745.831	2:T397-K413=1872.91455m[2x]	0.99998939
30.4653	948.957	9156	2	1895.88	1894.898	2:T397-K413=1872.91455m(Na+)	0.9999705
31.4175	928.962	6691	2	1855.91	1854.905	2:T397-K413=1872.91455m(T397+H2O loss)	
31.2806	928.961	19977	2	1855.93	1854.904	2:T397-K413=1872.91455m(~S407+H2O loss)	1
12.0769	575.34	166237	1	574.542	574.332	2:L414-K418=574.33263m	0.99965954
11.6141	409.74	1638	2	817.737	817.465	2:L414-R420=817.46577m	0.99999148
12.0769	462.255	12348	1	461.412	461.248	2:T415-K418=461.24856m[nonspecific]	0.9829455
16.8839	479.249	4898	1	478.438	478.242	2:T415-K418=461.24856m[nonspecific][D417+16.9941]	0.89509529
26.6017	996.797	310332	3	2988.07	2986.365	2:S419-K443=2986.37151m	0.99999994
26.5923	598.482	10446	5	2988.01	2986.371	2:S419-K443=2986.37151m	0.9998909
26.5922	1494.69	74137	2	2988.07	2986.368	2:S419-K443=2986.37151m	0.99998111
26.5924	747.85	60000	4	2988.05	2986.369	2:S419-K443=2986.37151m	0.99857759
26.6016	1002.8	5313	3	3005.69	3003.372	2:S419-K443=2986.37151m(~N425+17.0068)	0.99886435
26.3384	761.832	7711	2	1522.39	1521.65	2:W421-H433=1521.64930m[nonspecific]	0.99994439
27.0851	687.067	94480	4	2744.81	2743.239	2:W421-K443=2743.23837m	0.99999664
27.0855	549.856	11051	5	2744.89	2743.239	2:W421-K443=2743.23837m	0.99994487
27.0853	1373.13	326885	2	2744.85	2743.236	2:W421-K443=2743.23837m	0.99983209
27.0852	915.754	511773	3	2744.84	2743.236	2:W421-K443=2743.23837m	0.98745275
27.0853	1830.83	17134	3	5489.83	5486.463	2:W421-K443=2743.23837m[2x]	0.99999664
23.7583	921.086	10911	3	2761.09	2759.236	2:W421-K443=2743.23837m(~M432+Oxidation)	0.99570817
27.0849	921.758	7131	3	2762.5	2760.234	2:W421-K443=2743.23837m(~H433+16.9978)	0.95339978
11.9929	620.807	6749	2	1240.21	1239.599	2:E434-K443=1239.59963m[nonspecific]	0.99999905
18.9464	330.682	1847	2	659.593	659.349	2:S444-G450=659.34901m	0.99999022
18.9507	660.356	268080	1	659.579	659.349	2:S444-G450=659.34901m	0.99921346
18.9396	682.338	14263	1	681.571	681.331	2:S444-G450=659.34901m(Na+)	0.93983573
17.7136	394.729	1893	2	787.712	787.443	2:S444-G450=659.34901m(G450+Lys)	0.99996167
17.7136	788.451	2835	1	787.722	787.444	2:S444-G450=659.34901m(G450+Lys)	0.99929875
18.5755	602.351	33272	1	601.57	601.344	2:S444-G450=659.34901m(G450+minus G+amidation)	0.99970734
18.5755	624.333	2124	1	623.55	623.326	2:S444-G450=659.34901m(G450+minus G+amidation)(Na+)	0.91995674

16.2018	968.452	2226	1	967.931	967.444	3:I9-N18 = 967.44332m[nonspecific]	0.99637818
16.5453	996.483	4554	1	995.969	995.476	3:I9-N18 = 967.44332m[nonspecific](~I9+28.0313)	0.99558151
34.332	1497.71	58080	3	4490.81	4488.112	3:I9-K51 = 4488.10895m	1
34.332	899.031	6760	5	4490.84	4488.114	3:I9-K51 = 4488.10895m	1
34.332	1123.54	36989	4	4490.83	4488.116	3:I9-K51 = 4488.10895m	1
34.4415	1502.39	8362	3	4504.9	4502.131	3:I9-K51 = 4488.10895m(~S45+14.0190)	0.99996996
13.1071	379.734	2368	2	757.715	757.454	3:S52-R57 = 757.45587m	0.99992692
11.7834	515.33	33324	1	514.51	514.323	3:I54-R57 = 514.32273m	0.98994756
13.2699	543.361	11448	1	542.562	542.353	3:I54-R57 = 514.32273m(~I54+28.0309)	0.97973806
15.6153	583.392	3028	1	582.609	582.385	3:I54-R57 = 514.32273m(~I54+68.0625)	0.98181576
26.6574	738.04	42439	3	2211.22	2210.096	3:L58-K77 = 2210.09676m	0.99999994
26.6573	1106.56	146599	2	2211.23	2210.095	3:L58-K77 = 2210.09676m	0.99998665
26.8461	742.712	6240	3	2225.23	2224.113	3:L58-K77 = 2210.09676m(~A76+14.0171)	0.99999791
26.8462	1113.56	21735	2	2225.24	2224.111	3:L58-K77 = 2210.09676m(~A76+14.0171)	0.99990052
26.7063	887.953	7436	2	1774.82	1773.891	3:N62-K77 = 1773.88973m[nonspecific]	0.99999446
30.7102	762.065	46214	3	2283.38	2282.172	3:I78-K97 = 2282.17290m	0.99999994
30.7103	1142.59	130079	2	2283.37	2282.169	3:I78-K97 = 2282.17290m	0.99992758
30.9154	1149.6	9768	2	2297.3	2296.189	3:I78-K97 = 2282.17290m(~I96+14.0195)	0.99997878
27.0509	588.32	9832	2	1175.2	1174.626	3:T88-K97 = 1174.62676m[nonspecific]	0.99987739
27.0407	1175.64	2829	1	1175.22	1174.628	3:T88-K97 = 1174.62676m[nonspecific]	0.9760446
29.1602	622.352	8544	2	1243.31	1242.69	3:T88-K97 = 1174.62676m[nonspecific](~I96+68.0635)	0.99795389
16.9774	802.431	1790	1	801.705	801.424	3:L98-N105 = 801.42323m[nonspecific]	0.99586308
18.0526	830.461	9704	1	829.747	829.454	3:L98-N105 = 801.42323m[nonspecific](~L98+28.0297)	0.98106039
19.6276	870.493	12012	1	869.795	869.486	3:L98-N105 = 801.42323m[nonspecific](~L98+68.0620)	0.98644078
16.6175	523.285	104932	2	1045.04	1044.556	3:L98-R107 = 1044.55637m	0.99981368
16.6175	1045.56	29061	1	1045.05	1044.555	3:L98-R107 = 1044.55637m	0.99903101
20.0765	421.758	60708	2	841.795	841.502	3:V108-R115 = 841.50215m	0.99999821
20.0766	842.509	89509	1	841.795	841.502	3:V108-R115 = 841.50215m	0.98616076
20.3875	428.766	6774	2	855.824	855.517	3:V108-R115 = 841.50215m(~V108+14.0154)	0.98592722
20.3875	856.526	4381	1	855.82	855.518	3:V108-R115 = 841.50215m(~V108+14.0154)	0.88274306
20.0717	412.753	3674	2	823.766	823.492	3:V108-R115 = 841.50215m(T110+H2O loss)	0.99298412
26.6338	884.903	53040	2	1768.78	1767.792	3:S116-K133 = 1767.79200m	0.99999994
26.7971	891.911	8594	2	1782.81	1781.808	3:S116-K133 = 1767.79200m(~N131+14.0161)	0.99997598
28.0688	918.936	12489	2	1836.89	1835.857	3:S116-K133 = 1767.79200m(~N131+68.0651)	0.99997526
30.0554	735.369	24181	2	1469.42	1468.723	3:S134-K147 = 1468.72318m	0.99999994
30.2039	749.385	8782	2	1497.46	1496.756	3:S134-K147 = 1468.72318m(~S134+28.0326)	0.99990094
30.8046	769.4	7407	2	1537.5	1536.786	3:S134-K147 = 1468.72318m(~S134+68.0627)	0.99727046
15.6423	503.747	8022	2	1005.81	1005.479	3:A148-K157 = 1005.48010m	0.99999946
15.6423	1006.49	6808	1	1005.96	1005.481	3:A148-K157 = 1005.48010m	0.99973685
37.7898	1055.19	30075	6	6325.43	6322.121	3:A148-K157/3:V108-K133/2:T227-K252 = 6322.140m[2ss]	0.9966954
37.7898	1582.29	68125	4	6325.49	6322.115	3:A148-K157/3:V108-K133/2:T227-K252 = 6322.140m[2ss]	0.99639511
37.7902	1266.03	54506	5	6325.5	6322.125	3:A148-K157/3:V108-K133/2:T227-K252 = 6322.140m[2ss]	0.99342161
15.8757	510.755	3099	2	1019.82	1019.496	3:A148-K157 = 1005.48010m(~A148+14.0164)	0.99354976
18.2669	544.786	2168	2	1088.07	1087.558	3:A148-K157 = 1005.48010m(~A148+14.0164)(~C156+68.0626)	0.99044347
15.9518	1034.52	1896	1	1034.02	1033.513	3:A148-K157 = 1005.48010m(A148+28.0318)	0.99482954
15.9434	517.762	7010	2	1034.01	1033.51	3:A148-K157 = 1005.48010m(A148+28.0318)	0.92816699
15.3926	1023.47	3614	1	1022.96	1022.468	3:S158-N167 = 1022.46689m[nonspecific]	0.99982667
15.6845	1051.51	3214	1	1051.01	1050.499	3:S158-N167 = 1022.46689m[nonspecific](~S158+28.0318)	0.99779558
16.9564	1091.54	3078	1	1091.07	1090.531	3:S158-N167 = 1022.46689m[nonspecific](~S158+68.0634)	0.9918592
33.0799	1080.02	21766	2	2158.2	2157.024	3:S158-K178 = 2157.02346m	1
29.2	577.291	8686	2	1153.15	1152.567	3:M168-K178 = 1152.56714m[nonspecific]	0.99999827
29.2009	1153.58	7621	1	1153.17	1152.568	3:M168-K178 = 1152.56714m[nonspecific]	0.9950043
30.8945	611.322	7064	2	1221.25	1220.63	3:M168-K178 = 1152.56714m[nonspecific](~G177+68.0625)	0.99879199
30.8946	1221.64	3257	1	1221.26	1220.633	3:M168-K178 = 1152.56714m[nonspecific](~G177+68.0625)	0.99220741
31.4023	625.338	4803	2	1249.29	1248.661	3:M168-K178 = 1152.56714m[nonspecific](~G177+68.0625)(~M168+28.031)	0.96285921
30.3189	1507.67	6738	2	3014.01	3012.318	3:D179-K208 = 3012.31642m	0.99999997
30.3189	1005.45	8583	3	3014.15	3012.319	3:D179-K208 = 3012.31642m	0.99997324
11.3164	906.505	3203	1	905.813	905.498	3:N209-K216 = 905.49707m	0.99999005
11.3212	453.755	10645	2	905.818	905.496	3:N209-K216 = 905.49707m	0.98995519
32.881	868.925	137120	2	1736.8	1735.836	3:V217-N231 = 1735.83519m	0.99999869
8.37592	489.266	2654.36	1	488.426	488.259	3:T227-N231 = 488.25946m[nonspecific]	0.99967217