

Intact Mass Analysis

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Introduction

This document outlines how to use this software for Intact Mass Analysis. Given three inputs - a modifications file, an observed masses file, and an integer error range - the program will calculate all possible combinations of modifications that could have lead to the observed mass within the specified error range, and write out these results in a csv file.

Running

To run - navigate to 192.168.50.69\D:Mass\ and double click IntactMassAnalysis.exe and a gui will pop up. Input the required files and error range. Make sure the files are in the form specified in [Inputs](#) then hit run.

Inputs

Modification file

Name

The name of the modification file should be the following: {YOUR_NAME}_modifications.csv. The {YOUR_NAME} prefix will be used for the ouput file so make sure it is something indicative i.e (240718HeLaDigest)

File Format

The modifications file should have the following columns:

1. Name
Name of the modification
2. ShortName
Short hand name of the modification - this is what will be used in the output file
3. Experiment
Experiment(s) in which to search for this modification - if you want to search for that modification in all experiments simply put "All", else list the specific experiments with a comma separating different ones
4. Mass
Mass of the modification
5. From
Minimum amount of the modification

- 6. To
Maximum amount of the modification

Example

Name	ShortName	Experiment	Mass	From	To
L43 Heavy chain	L43HC	L43, Intact, L43, Reduced	49214	1	2
L43 Light chain	L43LC	L43, Intact, L43, Reduced	22,915	1	2
RS43 Heavy chain	RS43HC	RS43, Intact, RS43, Reduced	49214	1	2
RS43 Light chain	RS43LC	RS43, Intact, RS43, Reduced	22,915	1	2
RS1326 Heavy chain	RS1326HC	RS1326 Intact, RS1326, Reduced	36,708	1	2
RS1326 Light chain	RS1326LCS	RS1326 Intact, RS1326, Reduced	49,324	1	2
PyroGln	pyroGln	All	-17	1	4
Disulfide	Dis	All	-2	1	10
Bodipy	By	All	414	1	4
Lysine Clip	Lys	All	-128	1	2
G0F Glycosylation	G0F	All	1,462	1	2
Hexose	Hex	All	162	1	3
Fucose	Fuc	All	146	1	3

Observed Mass file

Name

The name of the observed mass file should be the following: {YOUR_NAME}_observed_masses.csv. The {YOUR_NAME} prefix will be used for the ouput file so make sure it is something indicative i.e (240718HeLaDigest)

File Format

This file should have the experiments as the column names and the masses observed in that experiment as the column values.

Example

L43, Intact	L43, Reduced	RS43, Intact	RS43, Reduced	RS1326, Intact	RS1326, Reduced
170,261	22,910	23,029	22,910	36,819	36,701
170,387	62,239	42,568	62,240	73,399	50,633
	62,365	45,820	62,368	87,327	50,794
		170,265	23,029	174,659	
		172,954	23,215	174,819	
		175,646		174,985	

Ouput

Location

The program will write the output to the same directory that the Modification file is in as {YOUR_NAME}_results.csv where YOUR_NAME is the prefix of the modification file.

Format

The output file is a .csv file where each row corresponds to a possible combination of modifications corresponding to a specific observed mass. The columns are:

1. Experiment
- The experiement in which this mass was observed
2. Masses Observed
- The mass that was observed
3. Matched Mass
- A possible combination of modifications for this mass. Represented as a string of the short name of the modifications where Mod[xn]_ indicates that Mod is present n times in this particular match
4. Num_Mods
- The number of modifications in this match (not including proteins and drugs)
5. Delta Mass
- The difference between the Matched Mass and the Observed Mass (within the error range)

Example

Experiment	Masses Observed	Matched Mass	Num_Mods	Delta Mass
L43, Intact	170261	By[x3]_Dis[x4]_Fuc[x3]_G0F[x1]_Hex[x0]_L43HC[x2]_L43LC[x3]_Lys[x0]_pyroGln[x3]	14	-5
L43, Intact	170261	By[x0]_Dis[x10]_Fuc[x0]_G0F[x2]_Hex[x3]_L43HC[x2]_L43LC[x3]_Lys[x2]_pyroGln[x3]	20	-5
L43, Intact	170261	By[x0]_Dis[x10]_Fuc[x0]_G0F[x2]_Hex[x2]_L43HC[x2]_L43LC[x3]_Lys[x1]_pyroGln[x1]	16	-5
L43, Intact	170261	By[x0]_Dis[x2]_Fuc[x1]_G0F[x2]_Hex[x1]_L43HC[x2]_L43LC[x3]_Lys[x1]_pyroGln[x1]	8	-5
L43, Intact	170261	By[x0]_Dis[x2]_Fuc[x1]_G0F[x2]_Hex[x2]_L43HC[x2]_L43LC[x3]_Lys[x2]_pyroGln[x3]	12	-5
L43, Intact	170261	By[x4]_Dis[x10]_Fuc[x2]_G0F[x1]_Hex[x0]_L43HC[x2]_L43LC[x3]_Lys[x2]_pyroGln[x3]	22	-5
L43, Intact	170261	By[x4]_Dis[x9]_Fuc[x0]_G0F[x1]_Hex[x0]_L43HC[x2]_L43LC[x3]_Lys[x0]_pyroGln[x1]	15	-5
L43, Intact	170261	By[x4]_Dis[x1]_Fuc[x1]_G0F[x1]_Hex[x0]_L43HC[x2]_L43LC[x3]_Lys[x1]_pyroGln[x3]	11	-5
L43, Intact	170261	By[x0]_Dis[x3]_Fuc[x3]_G0F[x2]_Hex[x0]_L43HC[x2]_L43LC[x3]_Lys[x2]_pyroGln[x1]	11	-5
L43, Intact	170261	By[x4]_Dis[x9]_Fuc[x0]_G0F[x1]_Hex[x1]_L43HC[x2]_L43LC[x3]_Lys[x1]_pyroGln[x3]	19	-5
L43, Intact	170261	By[x0]_Dis[x1]_Fuc[x0]_G0F[x2]_Hex[x2]_L43HC[x2]_L43LC[x3]_Lys[x1]_pyroGln[x2]	8	-4
L43, Intact	170261	By[x0]_Dis[x1]_Fuc[x0]_G0F[x2]_Hex[x1]_L43HC[x2]_L43LC[x3]_Lys[x0]_pyroGln[x0]	4	-4
L43, Intact	170261	By[x4]_Dis[x9]_Fuc[x1]_G0F[x1]_Hex[x1]_L43HC[x2]_L43LC[x3]_Lys[x2]_pyroGln[x4]	22	-4
L43, Intact	170261	By[x0]_Dis[x2]_Fuc[x2]_G0F[x2]_Hex[x0]_L43HC[x2]_L43LC[x3]_Lys[x1]_pyroGln[x0]	7	-4
L43, Intact	170261	By[x4]_Dis[x1]_Fuc[x2]_G0F[x1]_Hex[x0]_L43HC[x2]_L43LC[x3]_Lys[x2]_pyroGln[x4]	14	-4
L43, Intact	170261	By[x4]_Dis[x0]_Fuc[x0]_G0F[x1]_Hex[x1]_L43HC[x2]_L43LC[x3]_Lys[x1]_pyroGln[x4]	11	-4