

PeptideMassCalculator – HELP

1. The Overview

“PeptideMassCalculator” is an application that helps you to calculate peptide mass.

- To calculate peptide mass you have to:
 - a) choose an amino acid type,
 - b) choose N- and C-terminus,
 - c) provide peptide sequence.

2. The Sequence

- The sequence can contain only an standard amino acid.
Example: peptide "AC", "A" means "Alanina", "C" means "Cysteina" - the sequence can be of any length.
- The sequence can contain both standard amino acid and an unusual amino acids. If you would like to provide such a sequence you need to use brackets (to mark unusual amino acids). Put three letters long abbreviation between them.
Example: "AC(Cit)QV" where "A", "C", "Q", "V" means a standard amino acid and "Cit" is unusual amino acid - "Citrulline"

3. The Menu - "Show"

"Show" function will display accordingly all available "Unusual Amino Acids", "Standard Amino Acids", "Protected Amino Acids" and Terminus (N and C)

4. Add Unusual Amino Acid

This function allows you to add your own unusual amino acid to the data base.

To add it, you need to provide Amino acid name, 3-letter abbreviation and molecular weight. Amino acid - any name, 3 letter abbreviation – anything- only condition is that it is 3 character long, Molecular weight - you need to use "." not ",",

Example: 111,1 - incorrect, 111.1 – correct.

If an unusual amino acid has been added to the data base, you will get the message.

5. Delete an Unusual Amino Acid

This function allows you to remove any unusual amino acid.

Amino acid and 3-letter abbreviation, have to be the same as shown by "Show" function. Molecular weight in "Show" function has 5 decimal places, if last digit is 0 please leave it empty.

Example: Show: "111.100" please write "111.1", show: "111.000" please write "111.0" .

If for some reason, you just cannot remove an unusual amino acid, you can open the file "unusual_amino.csv" and remove it (whole row) manually. Please note that the file "unusual_amino.csv" contains all your unusual amino acids. File should not be modify manually, unless it is really necessary (in such case please remember to remove a whole row, otherwise program can work incorrectly).

6. logo.ico

The file contains program icon, and is needed for the proper application functioning

7. unusual_amino.csv

The application creates the file with unusual amino acids. This file is required if you would like to calculate Peptide Mass with an unusual amino acid or show an unusual amino acid. If file doesn't exist, you can create it simply by adding an unusual amino acid.

