CEU MASS MEDIATOR HELP

INTRODUCTION

MassMediator overcomes some limitations of the current metabolomics workflow as follows:

1) The user can introduce data in a single interface that will perform the query in the data coming from different databases (currently METLIN, KEGG and LipidMAPS).

2) As data have been previously uploaded in the server, the query is performed immediately, and results are obtained with no delay.

3) Output data are sorted by the mass, and all the information corresponding to the same entity is grouped.

4) The integrity about the origin of data is conserved by the incorporation of hyperlinks to all the pages referenced, either for compound or pathway.

5) Data can be easily exported to a .xls file, allowing therefore the user to manage the data offline.

HOW TO USE IT

THE INITIAL FORM

The user introduces a list of neutral masses of compounds in the initial form. If (s)he does not have available such masses, (s)he may work with a sample data provided by us pressing the ***Loading of sample data*** button.

The ***tolerance*** is 10 ppm by default, although this number can be changed by the user.

The ***Reset*** button cleans the data of the form.

When the user presses ***Submit for compounds***, the system shows a table that contains a list of masses with the information provided from three public databases, obtained in a single batch-search, grouped by common entities.

THE LIST OF COMPOUNDS

The table is shown in different pages if there are several hundreds of masses in the initial form. The user can navigate from a page to another with the links ***Next*** and ***Previous***.

The table is exported to Excel pressing the button ***Generate Excel***. All the data are exported to a single .xls file, although each page of the table appears in a different sheet of such a file.

The columns of the table are the following:

- *Experimental mass* of the initial form that matches with the compound found by the server.
- *CAS* identifier of the compound.
- *Identifier* in the original dababase (e.g. Lipid Maps identifier). It has a link to the original Web page of the compound.
- *Names* of the compound.

- Its *formula*.
- The original *database* (Metlin, KEGG or Lipid Maps). It has a link to the Web site of the database.
- The pathways where, according to KEGG, the compound is involved. There is a link as well to the original KEGG web page of each pathway.

The ***back to the input data form*** button allows the user to go to the initial form.