Utilities for Mass Spectrometry Analysis of Proteins

User's Manual

Version 2.1.0

May 2020

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Introduction

Utilities for Mass Spectrometry Analysis of Proteins (UMSAP) is a graphical user interface (GUI) designed to speed up the post-processing of data obtained during mass spectrometry studies involving proteins. The program is not intended to analyze a mass spectrum or a mass chromatogram, neither to identify the peaks in a mass spectrum. The main objective is the fast post-processing of the vast amount of data generated in mass spectrometry experiments involving proteins after peak identification have been performed.

The program is organized in modules with each module performing a single type of data post-processing. The reason for this clear separation is the high dependency between the type of mass spectrometry experiment performed and the way in which the resulting data must be post-processed. The modules are designed in such a way that the required user input is minimized but still users can control every aspect of the analysis. Currently, the software contains four modules but several others are already planned.

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1.2   Acknowledgments

I would like to thank all the persons that have contributed to the development of UMSAP, either by contributing ideas and suggestions or by testing the code. Special thanks goes to: Dr. Farnusch Kaschani, Dr. Juliana Rey and Prof. Dr. Daniel Hoffmann.

In particular, I would like to thank Prof. Dr. Michael Ehrmann for the support and useful discussions during my postdoc stay in his group at the University of Duisburg-Essen.

1.3   Copyrights Notes

UMSAP 2.1.0 is written in Python and uses the following modules and Python version:

Module	Version
Biopython	1.73
Matplotlib	3.0.2
NumPy	1.16.1
PyInstaller	3.4
Python	3.7.1
Requests	2.21.0
wxPython	4.0.4

Table 1.1: List of modules used by UMSAP.

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Chapter 2

Obtaining and Installing Utilities for Mass Spectrometry Analysis of Proteins

2.1 Obtaining Utilities for Mass Spectrometry Analysis of Proteins

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2.2 Installing Utilities for Mass Spectrometry Analysis of Proteins

Windows

Unzip the file you just downloaded from www.umsap.nl. Then, copy the folder UMSAP to the location in your file system where you want to keep it. Finally, create a shortcut to the executable file UMSAP.exe found inside the main folder UMSAP and that is all. You are now ready to use UMSAP.

MacOS X

Unzip the file you just downloaded from www.umsap.nl. Then, just move the UMSAP.app folder to /Applications/. That is all. You are now ready to use UMSAP.

Linux

Currently, there are no precompiled versions of UMSAP for Linux. Therefore, users using a computer running Linux need to install all the required modules before using UMSAP. For UMSAP 2.1.0 the list of required modules is:

Biopython 1.73, Matplotlib 3.0.2, NumPy 1.16.1, PyInstaller 3.4, Python 3.7.1, Requests 2.21.0 and wxPython 4.0.4.

If all these modules are already installed in the computer, then using UMSAP is straightforward. Go to the Downloads page and download the source files for UMSAP 2.1.0. Unzip the files. In the terminal, navigate to the newly created UMSAP folder and type python UMSAP.py. This will launch the GUI.

If the modules are not installed, then it is recommended to use conda to create a virtual environment to install everything and run UMSAP. First, check if the Linux distribution you are using (or a close enough distro) is listed here. If this is the case then you can easily install wxPython with pip as described below. If this is not the case then you have to build wxPython by yourself. Check here for how to do this.

Once you know that you can have a functional wxPython installation do the following.

First, download Miniconda for Linux from here. Then, open a terminal and navigate to the folder containing the Miniconda installer. The installer will have different names depending on which one you choose in the previous step. Once in the folder containing the Miniconda installer, execute the file with the bash command line interpreter by typing:

bash Miniconda-installer-file

and follow the on-screen instruction. After finishing the installation close the terminal and open a new one so the changes done by conda take effect.

In the new terminal window type:

conda create --name umsap
conda activate umsap
conda install python==3.7.1
pip install biopython==1.73
pip install requests==2.21.0
pip install matplotlib==3.0.2

Installing matplotlib should install numpy 1.16.1 or superior, if this is not the case type

pip install numpy==1.16.1

If you found a compatible wheel for wxPython and your Linux distribution here, then install it using pip. You will need to change the gtk version and the linux distribution to suit your case. For example, for gtk3 and ubuntu 16.04 the command line is:

pip install -U -f https://extras.wxpython.org/wxPython4/extras/linux/gtk3/ubuntu-16.04 wxPython

And finally, you are all set. Download the source files for UMSAP 2.1.0 from the Downloads page. Unzip the file and in a terminal navigate to the newly created UMSAP

folder and type python UMSAP.py. This will launch the GUI.

2.3   Uninstalling Utilities for Mass Spectrometry Analysis of Proteins

UMSAP will not create any installation file in your computer. Therefore, the only thing you need to do, to completely uninstall UMSAP, is to delete the folder UMSAP.app in MacOS X or UMSAP in Windows/Linux. In addition, you should delete any shortcut pointing to the executable file of UMSAP. That is all.