Course Syllabus

Crash Course on LC-MS Based Metabolomics Data Preprocessing

Tu Hu*

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1 Contents

In this crash course, participant(s) will be briefly introduced the principles of LC-MS based metabolomics, principles of data-preprocessing and general procedures. Further, data from participant(s)' project will be used as an example and worked out by MZmine 2 with guidance. Final results will be a feature table including file name (or sample name), retention time, m/z and intensities for further analysis.

2 Learning Outcomes

After completing the course, the student(s) should have:

Knowledge about:

- Principles of LC-MS based untargeted metabolomics
- Principles of data preprocessing of LC-MS based untargeted metabolomics

Skills in/to:

- Explore metabolomics data by MassLynx
- Applying MZmine 2 to preprocess LC-MS based untargeted metabolomics data

Competences in/to:

- Independently handle LC-MS based metabolomics data preprocessing task

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3 Course Structure

	Contents	Time	Location	Duration
Hands-on exercise 0	Explore Data on MassLynx	9 am 29th, Apr	Metabolomics Lab	20 min
Lecture	Principles of LC-MS based Metabolomics and data preprocessing	upon participant's reservation	Local meeting room	20 min
Hands-on exercise 1	Real case work	upon participant's reservation	Local meeting room	1 h
Hands-on exercise 2	Real case work	upon participant's reservation	Local meeting room	1 h
...	Dependent on participant's progress	upon participant's reservation	Local meeting room	...
Q & A	Questions regarding data preprocessing	upon participant's reservation	ad-hoc	1 h

4 Reading Materials and Guides

Reading materials will be delivered to student's email address in pdf. Other formats (such as Mendeley entries, LaTex citation commend or BibTex entry) are available upon request.

1. Yi, L. et al. Chemometric methods in data processing of mass spectrometry-based metabolomics: A review. Anal. Chim. Acta 914, 17–34 (2016).
Only 2.1 (Pre-processing of raw data) is mandatory.

2. Pluskal, T., Castillo, S., Villar-Briones, A. & Orešič, M. MZmine 2: Modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data. BMC Bioinformatics (2010). doi:10.1186/1471-2105-11-395
Only Figure 1 is mandatory.

3. MZmine 2 Downloading Page and Installation Manual: http://mzmine.github.io/download.html
It is recommended to download and familiarize this software before starting the crash course. If installation problems are encountered, they will be troubleshot in hands-on exercise.

4. Karaman, I., Climaco Pinto, R. & Graça, G. Metabolomics Data Preprocessing: From Raw Data to Features for Statistical Analysis. Compr. Anal. Chem. 82, 197–225 (2018).
Following sections are optional:

3. NMR Preprocessing (However, participants should aware that they may be asked about NMR in thesis defence by opponents)
4.1.2.4 LC-MS Preprocessing Example

5. MZmine Instructions by Gözde Gürdeniz
The most important reading material for this crash course. Participant(s) will be guided through this instruction.

6. LC-MS Data Preprocessing lecture slides by Gözde Gürdeniz from PhD course Introduction to Nutitional Metabolomics
This is a very detailed overview of LC-MS Metabolomics data preprocessing.

5 Participant(s)

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6 Remarks

Participant(s) are expected to understand the principles of LC-MS based metabolomics. If not, they will be briefly introduced with a vivid analogy.

This course was developed under the supervision of Lars Ove Dragsted and Natalia Manjarrez.

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