Streamlining LC-MS/MS Data Analysis in R with Open-Source xcms and RforMassSpectrometry: An End-to-End Workflow

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INTRODUCTION

We present a detailed step-by-step analysis of an untargeted metabolomics dataset:

- Identifying differences between individuals with cardiovascular disease and healthy control.
- Workflow includes **preprocessing, feature detection, alignment, normalization, statistical analysis and annotation** within a unified framework.
- Presents branching points for integrations with external tools and software.
- Emphasizes proper quality management for LC-MS data analysis.

Aims

Keeping it user-friendly

Facilitate open access through software solutions

Step-by-step guide to establish reproducible LC-MS(/MS) analysis workflows

Adaptable and scalable to custom LC-MS/MS setups

Creating a dynamic workflow

Will be updated to incorporate future developments

Integrate with external softwares

Do you know of a package that could integrate this workflow ?

Contact us

RESULTS

Raw data

Preprocessing
Chromatographic peak detection
Retention time alignment
Correspondence analysis

mzmine

Normalisation
Median scaling

Quality control
Dratio, Rsd, Contamination

Differential abundance analysis
Linear models

Annotation
At different confidence level
Multiple libraries support

SIRIUS

Molecular networking

GNPS

The figure above presents the main steps described in detail in the workflow and the software/tools used.

We strive towards **integration and interoperability** of our method, allowing the user to integrate external tools and software into the workflow at any time. The alternative tools shown above (dotted lines) are mentioned in our workflow.

To learn more about the RforMassSpectrometry Ecosystem see this poster: https://doi.org/10.5281/zenodo.11370345 and this website : www.rformassspectrometry.org

To contact me and see my current work: https://linktr.ee/philippinelouail

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