

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

eurac  
research

Philippine Louail<sup>1</sup>, Anna Tagliaferri<sup>2,3</sup>, Vinicius Verri Hernandes<sup>1,4</sup>, Daniel M. S. Silva<sup>5,6</sup>, Johannes Rainer<sup>1</sup>

<sup>1</sup>Institute for Biomedicine, Eurac Research, Italy <sup>2</sup>Sensing Technologies Laboratory (STL), Faculty of Engineering, Free University of Bozen-Bolzano, Italy <sup>3</sup>Faculty of Agricultural, Environmental and Food Sciences, Free University of Bozen-Bolzano, Italy <sup>4</sup>Department of Food Chemistry and Toxicology, University of Vienna, Austria <sup>5</sup>Department of Chemistry, Aristotle University of Thessaloniki, Greece, <sup>6</sup>Biomic\_AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center, Greece

## 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.

Bioconductor  
OPEN SOURCE SOFTWARE FOR BIOINFORMATICS



## 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

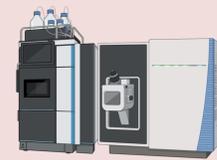
**Do you know of a package that could integrate this workflow ?**



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



SIRUS

Molecular networking



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.

