
Course

# Data analysis for Metabolomics, a practical course

**Metabolomics experiments based on mass spectrometry (MS) or nuclear magnetic resonance (NMR) produce large and complex data sets. This course will introduce approaches to process and analyse data and design high-quality experiments. Through hands-on workshops and lectures highlighting the different concepts you will get a thorough basis for tackling the challenges in metabolomics data analysis.**

## Target group

This course targets professionals working in health and life sciences (e.g., food industry, breeding and seed business, pharmaceutical companies, hospital laboratories, biotech and agro chemical industry). Presumed knowledge: a background in and basic understanding of analytical chemistry or metabolomics by work or education. No prior knowledge of programming, mathematics or statistics is assumed.

## Results

The course provides an overview of the tools and approaches used to design a study, process and analyse the data, avoiding common traps and mistakes. Principles will be explained in a general way, meaning they are valid for all common data acquisition platforms (e.g., NMR and MS) and software packages. The focus is on understanding, correct application and interpretation. After the course, participants are able to design appropriate experiments for typical metabolomics studies, taking into account quality assurance and quality control considerations.

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| **Date** | **7 and 8 April 2022** |
| **Location** | **Wageningen Campus** |
| Course leader | Dr Ron Wehrens, Biometris, Wageningen University & Research |

## Outline and topics

The course is led by experts in the field of metabolomics. They offer interactive tuition with Q&A sessions, hands-on computer practicals using real-world data and the opportunity to discuss case studies submitted by the participants.

This set-up offers participants an ideal mix to learn how to:

- choose pretreatment strategies relevant for the goal of the analysis and the data characteristics;
- select and execute appropriate data analysis methods to link metabolite data to properties of interest;
- interpret and assess the results of these data analysis methods.

## Programme

The programme covers all topics relevant for experimental design and reprocessing, exploratory analysis and modelling.

### Day 1: Thursday 7 April 2022

- **Welcome and introduction**
- **Designing good experiments and avoiding common pitfalls**
- **Preparing your data for analysis:**
  - Data processing: from raw data to a data matrix
  - Data matrix pretreatment: missing values, batch correction and scaling
  - Q&A
- **Fundamentals of metabolomics data analysis:**
  - Exploratory analysis / Visualization
  - Univariate and multivariate analysis
  - Principal Component Analysis (PCA)
- **Q&A: discuss your own research**
- **Networking dinner**

### Day 2: Friday 8 April 2022

- **Linking metabolite data to continuous properties: regression**
  - Linear regression
  - Principal Component Regression (PCR)
  - Validation
  - Partial Least Squares Regression (PLS)
- **Linking metabolite data to discrete properties: classification**
  - Univariate hypothesis testing
  - Linear Discriminant Analysis (LDA)
  - Partial Least Squares Discriminant Analysis (PLSDA)
- **Finding biomarkers**
- **Q&A: discuss your own research**
- **Evaluation and certificates**

## Practical information

€ 1,395.- per person and covers tuition, course materials, networking dinner, lunch and refreshments. Hotel accommodation is not included.

Between 20 and 30 participants.

Based on your attendance you will receive a certificate after the programme is finished.

## Registration

Enrollment is possible until 10 March 2022, or until the maximum number of participants is reached. Register via www.wur.eu/academy.

**Register**

## Wageningen Academy

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