



# Open-source chemometrics for real-world NIR handheld spectroscopy

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## Introduction

This short and intensive course provides a fast, hands-on introduction to building chemometric pipelines in R for near-infrared (NIR) spectroscopy data. The focus is on making R a practical and accessible tool for developing calibration models within minutes.

Participants will use handheld sensors during the session to generate sample data. They will then combine these measurements with existing training datasets and follow a streamlined workflow covering spectral pre-processing, calibration, validation, rapid prototyping, and deployment. Emphasis is placed on reusable code templates and simple pipeline structures that enable a rapid transition from raw spectra to operational predictive models.

By the end of the session, participants will deploy their model to the handheld device and use it for real measurements, completing the full workflow from data acquisition to operational prediction.

## Objective

Equip participants with hands-on experience in developing chemometric models in R and deploying them directly to handheld NIR devices.

## Pre-requirements

- A laptop with R and RStudio installed
- Basic familiarity with R or a similar programming language (e.g. MATLAB or Python) · A basic understanding of regression methods

## Topics:

- NIR spectroscopy
- Spectral data acquisition and pre-processing
- Chemometric modelling in R
- Exploitation of large training datasets (spectral libraries)
- Model validation and deployment to handheld devices



## Agenda

### Session 1: Foundations of R and chemometric modelling (*1.5 hours*)

- 1.1 Introduction to chemometrics with R for NIR spectroscopy
- 1.2 Overview of the R packages for model building and model deployment
- 1.3 Using core chemometric concepts for NIR data in R (calibration, validation, interpretation)

### Session 2: Chemometric pipeline in R (*1.5 hours*)

- 2.1 Spectral pre-processing and exploratory analysis
- 2.2 Hands-on calibration model development using R
- 2.3 Working with small datasets and spectral libraries

### Session 3: Model testing and deployment (*0.5 hours*)

- 3.1 Exporting models from R for deployment to handheld devices
- 3.2 Collection of independent validation samples
- 3.3 Evaluation of model performance under real-world conditions