SPECTROSCOPIC MODELLING USING PYTHON

COURSE DESCRIPTION

The *Spectroscopic Modelling Using Python* training is a hands-on course designed for individuals aiming to perform spectroscopic model building with custom Python code.

Spectroscopic techniques, such as Near-Infrared (NIR) and Raman spectroscopy, are very valuable tools to non-destructively evaluate a variety of quality attributes both related to the chemical and physical properties of the samples under study. However, adequate processing and model analysis is necessary to obtain the essential information from these rich data sources.

This course guides participants through the critical steps needed to build reliable models in Python, offering flexibility in model construction. The required Python modules will be introduced, with practical demonstrations provided through a case study based on a pharmaceutical manufacturing process. Both theoretical concepts and their practical applications in Python will be thoroughly explained.

COURSE PROGRAM (Day 1)

The course covers (but is not limited to) the following steps:

- Dataset preparation and visualization of the spectra
- Preprocessing evaluation:
  - The evaluation of the most suitable preprocessing techniques (e.g., spectral range trimming, normalization, first derivative, …)
- Model building using Partial least square regression:
  - Determination of the number of principal components
  - Applying cross-validation to avoid under- and overfitting
- Outlier assessment:
  - To detect and flag anomalous data points that may arise due to measurement errors, instrumental noise, or other sources
- Model analysis:
  - Various visualization to interpret the model
  - Calculation of the predictions error

TARGET AUDIENCE

The target audience is professionals or students in chemical, pharmaceutical & healthcare sciences and engineering.

REQUIREMENTS

Basic understanding of the Python programming language is required.

Basic understanding of spectroscopy is recommended.