



SCIENCE4U – Pre-Conference Workshop on Chemometrics & AI for Modern Science

Driving Precision, Insight, and Innovation Through Smart Data Analytics

Duration: 1 Day **Date:** 15th January 2026

Target Audience: Pharmaceutical, Food, Agriculture, Environmental, Academia, R&D, QC/QA, and Instrumentation Professionals

Workshop Agenda

Chemometrics Foundations with SCIENCE4U

- Importance of Chemometrics
- Where SCIENCE4U instruments + chemometrics create impact:
 - Food authenticity & adulteration detection
 - Pharma API estimation via NIR
 - Fertilizer & soil nutrient analysis
 - Water and environmental monitoring
 - Rapidly Detect Medical Disease Markers
- Data types (spectral, sensor, chromatographic, process, survey, sensory)

Data Preprocessing for High-Quality Analysis

- Baseline correction for raw sensor outputs
- Smoothing & derivatives (SG) for spectral enhancement
- MSC, SNV, normalization for reducing scatter
- Outlier detection using residuals and leverage
- Benefits for field instruments & portable analyzers
- Ensuring reproducibility and calibration integrity

Exploratory Data Analysis: PCA in Real Problems

- PCA for pattern recognition, anomaly detection, and sample clustering
- Real SCIENCE4U case studies:
 - Differentiating fresh vs degraded food samples
 - Raw material identification in pharma

- Sample classification using spectral fingerprints
- Interpretation of **scores, loadings, Hotelling's T^2 , Q-residuals**
- Understanding sample variability in instrument-based workflows

Calibration & Quantitative Modeling: Building Robust Prediction Models

- PLS regression fundamentals
- Building quantitative prediction models for:
 - Moisture, fat, protein
 - API/assay values
 - Nutrient quantification in fertilizers
- Cross-validation & selecting latent variables
- Preventing overfitting
- Accuracy metrics (RMSEC, RMSECV, RMSEP, R^2)
- Deployment of models into SCIENCE4U instruments

Classification & Discrimination

- Supervised pattern recognition SIMCA, PLS-DA, kNN for class separation
- Real SCIENCE4U examples:
 - Identifying counterfeit drugs
 - Consumer product grading
 - Water quality categorization
- Model validation & regulatory considerations

Chemometrics in PAT, QbD & Industry 4.0

- SCIENCE4U's integrated approach:
 - Real-time monitoring
 - Process sensors
 - Multivariate Statistical Process Control (MSPC)
- Continuous manufacturing with chemometric feedback loops
- Model lifecycle: development → validation → deployment → maintenance
- Transferability across instruments and batches
- Alignment with ICH, WHO, FDA guidelines

Interactive Q&A & Problem-Solving Clinic

- Participants bring their challenges in spectroscopy, sensors, QC/QA
- Discussion on best practices, pitfalls, and advanced strategies
- Suggestions on instrumentation, software, and modeling approaches