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Machine Learning for Raman Spectroscopy: From Spectra to Robust Industrial Models

Raman spectroscopy has evolved from peak-based molecular identification into a powerful solution for quantitative prediction and process monitoring, driven by advances in chemometrics, Machine Learning (ML) and predictive Artificial Intelligence (AI).

This keynote will present a practical framework for turning Raman spectra into reliable industrial decisions, with particular emphasis on modeling good practices.

Classical and non-linear ML calibration approaches will be benchmarked in terms of predictive performance, development complexity and overfitting risk, together with interpretability strategies for Explainable ML.

Applications will illustrate the breadth of Raman data analytics, from in-line biomanufacturing monitoring of cell culture [1-2] to Raman imaging and continuous chemical-process monitoring.

Calibration robustness, inter-instrument transfer, scale-up from pilot to manufacturing, and multi-sensor data fusion will also be addressed. Drawing on Ondalys' experience across pharma/biotech, chemicals, food and optical-sensor applications, the presentation will show how integrated consulting, proof-of-concept studies, model development and validation, software implementation, transfer, maintenance and training can accelerate the deployment of robust, interpretable and transferable Raman solutions from R&D to routine industrial use.

References

- [1] M. Rubini, A. Berger, T. Saillard, F. Cantais, M. Soucé, J. Poulain, S. Roussel, J. Louet, F. Chauchard-Rios, S. Arnould, I. Chourpa (2025). Monitoring of monoclonal antibody critical quality attributes and free amino acids in CHO bioprocesses using Raman spectroscopy and DUPLEX-based PLS modeling. *Microchemical Journal* 2025, Vol 218 115583A.
- [2] M. Rubini, J. Boyer, J. Poulain, A. Berger, T. Saillard, J. Louet, M. Soucé, S. Roussel, S. Arnould, M. Vergès, F. Chauchard-Rios & I. Chourpa (2025). Monitoring of Nutrients, Metabolites, IgG Titer, and Cell Densities in 10 L Bioreactors Using Raman Spectroscopy and PLS Regression Models. *Pharmaceutics* 2025, Volume 17, Issue 4, 473 (2025)

Figures



Figure 1: inline Raman spectrometer setup at pilot scale for biomanufacturing (CLIMBIN collaborative R&D project)