Data processing: a chemometrics guide for chromatographers

Course Overview

This introductory course covers all main aspects of data analysis of chromatographic data. As data analysis lays at the interface between statistics and chromatography, both backgrounds are necessary. In light of this, I will review the range of techniques that are available for extracting quantitative and qualitative information from chromatography, with emphasis on understanding the principles, along with discussion around the do's and don'ts.

Who Should Attend

This course is addressed to those currently involved in any chromatographic sub-discipline, interested in obtaining the maximum information out of the data generated. The audience should have a basic background in statistical analysis. All those working in disciplines in which the data treatment is critical are specially encouraged to attend. Emphasis will be paid on current methods available for automated data analysis.

Course Outline

1. Introduction.
    1.1. Why do we need statistics to deal with chromatographic data? Some basics of statistics.
2. Pre-processing methods
    2.1. Base-line correction
    2.2. Noise filtering
    2.3. Peak detection (in both one-dimensional and two-dimensional chromatography)
    2.4. Chromatographic alignment
    2.5. Special topics with high-resolution mass spectrometry.
3. Curve resolution methods
    3.1. Raw data vs. peak tables. Which one is best?
    3.2. Second-order methods: AMDIS, MCR-ALS.
    3.3. Third-order methods: PARAFAC, PARAFAC2
    3.4. Advanced methods.
4. Multivariate modelling & pattern recognition
    4.1. Why (and when) should I go multivariate? Let's think about our hypothesis.
    4.2. Exploration: PCA & HCA.
    4.3. Classification: SIMCA, PLS-DA, LDA, SVM.
    4.4. Regression: PLS, RSVM.
5. Applications
    5.1. Food & pharma
    5.2. Oil & gas
    5.3. Forensics
    5.4. Chemicals & polymers
    5.5. Omics
6. Open discussion

Biography

Gabriel Vivó-Truyols (1975) studied analytical chemistry at the University of Balearic Islands (Spain) and graduated in 1998. In 2004 he obtained his PhD with honours from University of Valencia (Spain) on chemometrics methods for optimization and data treatment of HPLC. His PhD dealt with the development of novel methods for optimization and data treatment in HPLC, and was awarded with the D.L. Massart award in chemometrics from the Belgian Chemometrics society in 2006, given every two years to the best PhD thesis in chemometrics, world-wide. In 2004 he joined the team of Peter Schoenmakers (University of Amsterdam), where he developed a research program focused on chemometric techniques for optimization, calibration and data-treatment of two-dimensional chromatographic methods. In 2007 he joined the analytical chemistry team at BP in Sunbury (London area). He worked as chemometric specialist developing algorithms and software for GCxGC analysis of petroleum subproducts, as well as developing chemometrics methods for on-line infra-red analysis. In 2009 he re-joined the analytical-chemistry group of Peter Schoenmakers at University of Amsterdam as assistant professor. He left in 2017, establishing his own consultancy (based in Spain) in data analysis for chromatography and spectroscopy. With 20+ years of teaching experience at 4 different universities in this subject, Gabriel is currently scientific consultant for major multinationals in the area of data analysis, including USP, BP, Castrol, BASF, Merck and Agilent technologies, as well as a collaborator with the university of Pardubice (Holcapek group). Gabriel Vivó-Truyols has co-authored more than 60 papers, besides a book covering the interface of chemometrics & chromatography.