School for Advanced Residue Analysis in Food
TEACHING MODULE

CON-PRA-054

CONFIRMATORY METHODS
Multi- and Megavariate Data Analysis

• Context

For several years, volumes of raw data generated by analytical systems have been growing exponentially. Some reasons explaining this tendency are for instance the continuous technological improvements in the field of analytical chemistry (high chromatographic/spectrometric resolution and high troughput systems) as well as the introduction of new scientific areas ('omics technologies including the emerging field of metabolomics). One direct consequence of such evolution is the difficulty to manage, analyse, and interpret such large data sets with conventional statistical tools. Then, analysts are more and more confronted to the need of using multi- or megavariate statistical methods to properly handle, describe, and maximise the useful information content of their data. Of particular interest are these techniques for various food safety applications.

• General objective(s)

The goal of this hands-off practical session is first to present briefly some basics of multivariate statistical techniques (principal component analysis, hierachical classification, discriminant analysis,…), and secondly to demonstrate and comment various real case studies in the specific field of residue and contaminant analysis where such techniques have been used. The differenciation of stereoisomer compounds, the comprehensive investigation of global contamination profiles, or the emerging metabolomics approach as new method of characterisation for biological samples, will be especially covered.

• Pedagogical objectives

✓ To know the existence of at least 2 multivariate statistical techniques for descriptive or predictive purpose
✓ To be aware of the potential benefits of such techniques in the field of chemical food safety
✓ To know the main principle and possible applications of metabolomics

• Main items

✓ Brief introduction to multivariate statistics, basic principle of PCA and LDA, application to stereoisomer differentiation, application to contamination profiles analysis, application to metabolomics.

• Pedagogical tools

✓ PowerPoint slide show

• Duration

✓ 1 hour

• Pre-requisite

✓ Basics of mass spectrometry (CON-THE-010, CON-THE-020 and CON-THE-030)
✓ ✓ Basics of descriptive statistics: mean, standard deviation, distribution;…