

## **Application of chemometrics in food chemistry – An overview of statistical tools for classification and modelling, clustering and correlation**

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Concerning the fact that even the simplest food is a complex matrix, the way to investigate its chemistry cannot be other than multivariate. Therefore, chemometrics is a necessary and powerful tool in the field of food analysis and control. Development of efficient and reliable analytical method requires chemometric approach at several levels starting with application of experimental design and optimization techniques for the separation step, followed by data acquisition, and signal manipulation, and finally solving classification and modelling problem, clustering and correlation. Several problems in food analysis which could be solved by chemometrics are traceability (the possibility of verifying the animal/botanical, geographical and/or productive origin of a foodstuff), connection of consumer preferences and sensory attributes with molecular profiling of food, process control and monitoring, etc. This workshop aims to point out to the main chemometrics techniques and their application to different aspects of food science in order to fulfil the knowledge of both, food chemists wanting to learn how these techniques can help in many aspects of their work and chemometricians having to deal with food-related problems. Numerous classification and regression methods such as principal component analysis, hierarchical cluster analysis, linear discriminant analysis, partial least square discriminant analysis, k-nearest neighbours, artificial neural networks, partial least square regression, etc, will be discussed through defining a methodology and practical application of different statistical software such as Statistica, SPSS, NCSS, Matlab, etc.

Keywords: chemometrics, food analysis, statistical techniques, software

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