



## **Chemometrics in Food Chemistry: Chapter 3. Exploratory Data Analysis (Data Handling in Science and Technology)**

*Mario Li Vigni, Caterina Durante, Marina Cocchi*

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In the food research and production field, system complexity is increasing and several new challenges are emerging every day. This implies an urgent necessity to extract information and obtain models capable of inferring the underlying relationships that link all the variability sources which characterize food or its production process (e.g. compositional profile, processing conditions) to very general end properties of foodstuff, such as the healthiness, the consumer perception, the link to a territory and the effect of the production chain itself on food. This makes a ‘deductive’ theory-driven research approach inefficient, as it is often difficult to formulate hypotheses. Explorative multivariate data analysis methods, together with the most recent analytical instrumentation, offer the possibility to come back to an ‘inductive’ data-driven attitude with a minimum of a priori hypotheses, instead helping in formulating new ones from the direct observation of data. The aim of this chapter is to offer the reader an overview of the most significant tools that can be used in a preliminary, exploratory phase, ranging from the most classical descriptive statistics methods, to multivariate analysis methods, with particular attention to projection methods. For all techniques, examples are given so that the main advantage of these techniques, which is a direct, graphical representation of data and their characteristics, can be immediately experienced by the reader.

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