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Importance of Statistical Techniques in Food Science: Chemical Analysis Data

Mercedes Bertotto*

University of Buenos Aires, Argentina

***Corresponding author:** Mercedes Bertotto, University of Buenos Aires, Paroissien 2548 5A, Argentina, Tel no: 1544442272; Email: mbertotto@hotmail.com

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Abstract

There is an interest in developing fast, accurate, easy to use and low-cost analytical methods to detect adulteration in food products. Fourier transform infrared spectroscopy, in combination with multivariate statistical techniques such as chemometrics, makes possible to obtain specific information about different parameters simultaneously in a direct, reliable, and rapid way.

Keywords: Chemometrics; Spectroscopy

Editorial

"Food practitioners encounter data interpretation and dissemination tasks on a daily basis. Data comes not only from laboratory experiments, but also via surveys on consumers, as the users and receivers of the end products. Understanding such diverse information demands an ability to be, at least, aware of the process of analysing data and interpreting results. This knowledge and ability gives undeniable advantages in the increasingly numerate world of food science, but it requires that the practitioner have some experience with statistical methods" (Muredzi, 2013). In recent years, analytical chemistry has undergone significant changes due to a variety of causes, including the need for component measurements at increasingly lower concentrations, and for measurements of highly complex samples, such as natural or biological samples. Another reason for the changes undergone is the advance in scientific instruments, including the progress of computer sciences, which provide methodological and technical tools to achieve the aforementioned objectives. At the same time, the information that can be registered with such equipment has become more complex, because of its volume and mathematical structure, which makes it necessary to have more complex calculation and interpretation tools. These tools belong to a relatively new discipline known as chemometrics.

"Chemometrics is the chemical discipline that uses mathematics and statistics to design or select optimal experimental procedures, to provide significant chemical information by analyzing chemical data, and to gain insight into chemical systems" (D. L. Massart). The science of chemometrics provides spectroscopists with many different ways of solving the calibration problem for spectral data analysis. Some are very simple to

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understand, while others require a solid training in linear algebra. This discipline has set new ground for analytical chemistry and has defined new areas of research in three important aspects:

i. The design and optimization of experiments
ii. Descriptive analysis
iii. Predictive analysis

The objective of the design and the optimization of experiments are to find optimal conditions for carrying out a chemical analysis.

On the one hand, a descriptive analysis attempts to draw up mathematical models of the properties of a chemical system in order to understand relationships that may be hidden. It deals with what is commonly called classification problems, since the result of this type of analysis is the ability to assign different samples to different classes. On the other hand, in predictive studies, the goal is to model the properties of a system to predict its behavior in new situations. This can be used to detect adulteration in food products.

Food authentication is of concern to food processors who don't want to suffer unfair competition from unscrupulous processors who would gain an economic advantage with the misrepresentation of the food they are selling. Many foods have the potential to be deliberately adulterated, but those that are expensive, and that are produced under wide changes in weather and harvesting conditions are particularly susceptible, honey, for example, is one of such material. The addition of syrups allows the dishonest producers to maintain the sweet taste without any noticeable difference in the product. Honey can be consumed directly or used as an ingredient in various processed food products. Due to its high nutritional value, unique flavour, natural provenance and antiseptic properties, the price of natural bee honey is higher than any other natural sweetener, and is susceptible to be adulterated by these other sweeteners. Detection of adulteration in honey is done using different techniques, such as isotopic, trace element analysis, thermal analysis, chromatographic. Carbon isotope ratio is the standard method used for many years. The utility of these methods has been demonstrated. Nevertheless, they are destructive, expensive, and time-consuming to carry out. Consequently here is an interest in developing fast, accurate, easy to use and low cost analytical methods to detect adulteration in honey.

Fourier transform infrared spectroscopy, in combination with multivariate statistical techniques such as chemo metrics, makes possible to obtain specific information about different parameters simultaneously in a direct, reliable, and rapid way. A mathematical model of the relationship between the near-infrared spectra of honey samples with known adulterant content would allow prediction of this content in new samples of honey. The near infrared, represented by NIR (near infrared), is one of the three bands in which the infrared radiation zone of the spectrum is usually divided, with wavelengths between 0.7 and 2.5micrometers (thousandths of a millimeter). These applications play a dominant role in analytical chemistry, since one of the objectives of greater interest for it is the quantification of the analytes of the samples that it studies, and one of the most interesting challenges of the discipline is to quantify components of complex samples, usually in the presence of a multitude of other substances that can produce a response similar to that of the analyte in the instruments of analysis.

In many cases, experimental approaches may be inadequate, for cost or time reasons, or simply because the selectivity of the system cannot be increased in these ways. Chemometrics provides an alternative pathway to these procedures, which consists of mathematically processing instrumental data that are inherently slightly selective, in order to isolate the contribution of the desired analyte from the total signal. Multivariate calibration (another way of referring to chemometrics) was conceived for this purpose. It is a set of mathematical-statistical techniques capable of modeling the relationship between the concentration of the components in a sample and the instrumental information that can be recorded for said sample in the form of multiple variables (wavelengths in spectroscopy, for example).

In my opinion, scientists and food technologists should investigate and develop efficient data analysis methods, in order to obtain more information about their food products, which are always, very complex systems.