

Special Issue “Application of Spectroscopy in Food Analysis”

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1. Introduction

“Man is what he eats”: food represents one of the fundamental needs for human beings, and, therefore, food analysis is a field of utmost importance. At the same time, given its inherent complexity, this subject encompasses multiple aspects, e.g., safety of use, health requirements, compliance to laws, organoleptic characteristics, and consumers' acceptance, and they are often intertwined.

In this context, spectroscopy serves as a suitable tool, as it is versatile, relatively rapid, non-destructive (or, at least, micro-destructive), and, in many cases, it requires minimum sample manipulation or pretreatment, thus representing a green alternative to other state-of-the-art methods.

The present special issue has been proposed with the aim of collecting studies describing interesting/relevant problems in food analysis and, ideally, suggesting strategies for solving/handling them. Among the 15 submitted manuscript, 10 were published (66.6% publication rate), indicating the high scientific level of the authors who decided to contribute. The published papers encompass different aspects and scopes: authenticating and/or characterizing foodstuffs, detecting frauds, and ensuring law/sanitary compliance. In particular, of these, three papers present diverse methodologies for quality assessment of food products by means of quantification of specific constituents, two are focused on the employment of classification tools for tracing high-valued foodstuffs, one aims at proposing a strategy for detecting frauds and, eventually, two are reviews, one about the most widely used chemometric tools in food analysis, and the other one focalized on authentication and traceability of seafood products.

2. Detection of Sensitizing Agents/Contaminants in Food

As above-mentioned, it is important to check the presence/absence of harmful compounds in foodstuff, ensuring law/sanitary compliance. In the present special issue, three papers have been published on this regard. Of these, chronologically speaking, the first one is the paper published by Solorzano et al. [1]. In their valuable work, the authors exploited liquid chromatography-diode array detection-quadrupole-time of flight system (LC-DAD-QTOF) as a screening method for detecting allergenic agents in *Zuccagnia punctata* and in two north-western Argentinean propolis (NAPs) collected in the provinces of Catamarca and Tucumán. The LC-DAD-QTOF analysis highlighted that, among the diverse sensitizing agents investigated, *Z. punctata* contained only one (geranyl caffeate), while geranyl, pentenyl, and benzyl caffeates were found in NPAs.

The second paper of the special issue, aimed at the evaluation of the sanitary compliance of food, is the one by Tsagkaris et al. [2], who developed an acetylcholinesterase (AChE) assay for carbamates (CMs) and organophosphates (OPs). The analytical performance of the novel assay was confirmed by an accredited liquid chromatography-tandem mass spectrometry (LC-MS/MS) method, demonstrating that the developed device reaches low limits of detection (at ppb level) and good repeatability, and indicating that it represents a fast and easy-to-use alternative to LC-MS/MS for CMs and OPs detection.



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Eventually, the last paper, on this regard, is the one published by Nguyen and collaborators [3], where fluorescence resonance energy transfer method (FRET) is used to quantify aflatoxin B1 in maize. The comparison of the outcome of the proposed approach with HPLC analysis indicated the suitability of the FRET-based approach for the quantification of this aflatoxin in real samples.

3. Quantification of Constituents in Food

The quantification of specific food constituents may be of interest, as these can provide information on the quality/organoleptic properties of a product. Often, food matrices represent a complex system, where the quantification of substances is difficult, in particular, due to the presence of interferents other than the compound of interest. Nevertheless, this problem can be overcome thanks to the combination of spectroscopy and chemometrics. In the special issue, two papers where constituents in matrix are quantified coupling analytical techniques and chemometrics were proposed. One of these is the paper by Quijano-Ortega et al. [4], where FTIR with attenuated total reflectance coupled with partial least squares (PLS) [5] regression was used to assess total carotenoid content (TCC) in *Cucurbita* spp. samples. The proposed strategy achieved excellent results, providing an R^2_{pred} of 0.93 and an RPD of 3.78.

The second paper where chemometric regression methods are used for the quantification of a constituent in food is the one by Roger and collaborators [6]. In this work, a NMR-based method for predicting fat content in butter, margarine, and milk-derived samples is proposed. In order to achieve this goal, the authors applied two different multi-block classification methods, sequential and orthogonalized partial least squares (SO-PLS) [7] and sequential and orthogonalized covariance selection (SO-CovSel) [8] to handle the nuclear magnetic resonance longitudinal (T1) relaxation measurements of the liquid and the solid sample phase. Both approaches provided excellent results (RMSEP \approx 1.00%), more accurate than those obtained by the individual PLS handling of the individual data blocks (liquid phase: RMSEP \approx 1.33; solid phase: RMSEP \approx 5.27%).

4. Authentication, Tracing and Fraud Detection

Traceability, i.e., defining the geographical origin of a food, is important for different reasons; for instance, as properly described by Power and Cozzolino in their review [9], in situations where high quality species are replaced by less valuable ones. This practice frequently occurs for seafood, whose origin identification is a complex issue. In their review paper, the authors provide a complete overview of recent applications of vibrational spectroscopy coupled with chemometrics for solving this kind of issues.

Additionally, traceability is a key concept also for agro-food; in particular, for those foodstuffs presenting peculiar organoleptic characteristics ascribable to the growing area or the know-how of local farmers. As a consequence, the verification of the origin of high-valued food products is of crucial interest. Tracing, authentication and characterization of agro-foods are complex problems, commonly accomplished by classification methods. The main chemometric tools adopted to solve these kind of issues have been briefly described by Biancolillo and co-authors in a review included into the special issue [10]. The same approaches are also used for the detection of frauds in foodstuff, such as sophistications or adulterations.

The remaining research articles of the special issue belong to this field, and they are based on the combination of chemometric classifiers and spectroscopic techniques.

An example of this is the paper published by Di Donato and collaborators [11], where three potato (*Solanum tuberosum* L.) grown in the area of Majella National Park (Abruzzo, Italy) and five commercial varieties cultivated in the same area were characterized by means of morphological descriptors and microsatellite (SSR) DNA markers. Eventually, samples were also analyzed by infrared spectroscopy and partial least squares discriminant analysis (PLS-DA) [12] was used to classify them according to their origin. The developed

methodology achieved high accuracy, leading to 97% and 80% correct classification, for training and test samples, respectively.

Similarly, the paper published by Amendola and co-authors [13] is focused on predicting the geographical origin of a typical agro-food, the “walnuts of Sorrento”, grown in Southern Italy. In order to hit this goal, walnuts were analyzed by near infrared spectroscopy and then classified by different approaches. Data was collected either on the shell, or on the kernel of the fruits. The two sets of spectra were separately analyzed by PLS-DA, and by multi-block strategies. The most accurate results were obtained when data was handled by SO-PLS-LDA; in this case, the classification model led to a total error rate of ~1% in external prediction.

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