

Spectroscopic, Chromatographic, and Chemometric Techniques Applied in Food Products Characterization

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1. Introduction

Spectroscopy is a technique indispensable for evaluating the quality of foods. It includes ultraviolet–visible (UV-Vis), fluorescence (FL), infrared (IR), mid-infrared (MIR), near-infrared (NIR), Raman, and nuclear magnetic resonance (NMR) methods that can be used to determine food composition and to detect food adulteration [1]. On the other hand, chromatography is a powerful analytical tool for separating individual compounds in foods. Several chromatography methods have been developed to that end. Some include column chromatography, thin-layer chromatography (TLC), paper chromatography (PC), gas chromatography (GC), ion exchange chromatography (IEC), gel permeation chromatography (GPC), high-pressure liquid chromatography (HPLC), and affinity chromatography (AC) [2]. Chemometric techniques in analytics use mathematical and statistical methods to obtain relevant information on food matrices [3]. Coupled with spectroscopic or chromatographic characterization, it serves as an essential and incredibly flexible tool for food analysis at all levels [4].

The Special Issue (SI) entitled “Spectroscopic, Chromatographic, and Chemometric Techniques Applied in Food Products Characterization” was proposed to collect full-length original research articles, short communications, and review articles regarding:

- techniques for the extraction, separation, estimation, and isolation of natural products;
- analytical method development and validation for food analysis;
- development and validation of rapid methods using calibration models based on near-infrared (NIR) and/or middle infrared (MIR) spectra and chemometrics;
- physicochemical characterization of foods by spectroscopic and/or chromatographic and/or chemometrics techniques;
- detection of food fraud and adulteration;
- determination of food authenticity and origin;
- assessment of chemical contaminants in food;
- evaluation of natural and synthetic additives;
- and chemometrics tools for comparing and classifying agro-food products based on their physicochemical properties, biological activities, and the sensory and texture parameters.

There is rising interest among consumers, scholars, and professionals from the research and industry sectors regarding recent advances in food analysis. In this sense, this Special Issue aimed to provide interested parties with the latest findings on the abovementioned topics.

2. Summary of the Special Issue

The study by Pinto et al. [5] aimed to provide new information on supercritical carbon dioxide extraction and composition of rice bran oil derived from eight rice types grown exclusively in the Sado River, Portugal (three short-grain Japonica and five long-grain



Citation: Semeniuc, C.A.; Mureşan, V. Spectroscopic, Chromatographic, and Chemometric Techniques Applied in Food Products Characterization.

Separations **2023**, *10*, 55.

<https://doi.org/10.3390/separations10010055>

Received: 21 December 2022

Accepted: 3 January 2023

Published: 14 January 2023



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Indica). As a result, it has been shown that SC-CO₂ is an effective method to extract oil from rice bran, assisting in valorizing this byproduct and facilitating the transition to a circular economy.

The primary objective of the work by Pasvanka et al. [6] was to develop a simple, robust, and respectively rapid analytical method for the authentication (characterization and discrimination) of a number of Greek wines based on their elemental profile with minimal sample pretreatment and low risk of analyte loss or contamination. For this reason, wine samples produced in six distinct locations in Greece from nine different types were subjected to the direct determination of forty-four metals using ICP-MS equipment.

The objective of the study by Saluti et al. [7] was to create a confirmatory multiclass method for more than seventy of the most used and regulated antibiotics in eggs (aside from aminoglycosides and colistin) and to apply it to two hundred commercial egg samples from Italy produced using conventional and organic approaches and gathered between 2018 and 2021.

The study by Manousi et al. [8] aimed to determine whether there are any notable differences in the elemental profiles of oils obtained from walnuts of the same botanical variety, cultivated organically and conventionally in Greece, by their analysis using ICP-AES. A total of twenty walnut oil samples were evaluated for elemental composition, and calcium and magnesium were the most abundant elements found in the tested oils, followed by iron and zinc.

The study by Dini et al. [9] assessed the efficacy of FT-infrared reflectance (FT-IR) for measuring total acid, alcohol, and SO₂ in wines. One hundred and fifty-six DOC Italian wines were analyzed using IR technology, and results were compared to those obtained using official analysis methods. Findings demonstrated that spectrophotometric methods include inaccuracies due to the interferences of impurities in the sample, which can be corrected by blank determination.

The goal of the study of Longodor et al. [10] was to determine the potential toxicity of the food additive monosodium glutamate (E-621, MSG) and the health benefits of spirulina (*Spirulina platensis*) as a dietary supplement. The biochemical parameters of blood and the organ damage of *Swiss mice* who received an additional daily dose of MSG for four weeks were studied. In addition, the spectra of MSG and spirulina powders were also measured in the treated mice with FTIR spectroscopy being used to identify these groups' marker bands.

The study of Greco et al. [11] aimed to determine whether the capsules' performance was able to affect the intensity of coffee aroma, particularly if the volatile intensity of each compound was increased due to the capsule's compression during extraction. Gas chromatography and mass spectrometry (GC-MS) analysis were used to investigate the volatilome, examining the abundance of various components in coffee extracted with and without capsule protection.

The study objective of Papastavropoulou et al. [12] was to assess the key quality characteristics of olive oil, with a particular emphasis on biophenolic content and its health benefits. In this sense, an HPLC analytical method was used to determine the biophenolic content in oil samples collected from various traditional oil-producing regions of Greece.

In another study, Papastavropoulou et al. [13] investigated a number of plants of Greek origin for their polyphenol content, antioxidant capacity, and antimicrobial activity. Plant polyphenols were identified and characterized using GC-MS and HPLC-DAD analyses. Plant extracts under study showed antioxidant and antibacterial properties. The most prevalent polyphenols were ferulic acid, quercetin, and catechin.

The paper of De Grazia et al. [14] aimed to draw attention to the possibility of registering analytical data in searchable MS databases, making them rapidly and reliably available, and to enhance researchers' ability to identify unknown compounds. In contrast to traditional methods, a three-dimensional prep-MDGC system was used in this investigation to efficiently and quickly capture mg quantities of a target chemical from the volatile myrtle fraction.

Hacini et al. [15] sought to characterize ten durum wheat genotypes protein profiles using chromatographic methods (reversed-phased RP and size exclusion SE high-performance liquid chromatography HPLC), as well as to investigate the diversity in these cultivars' protein profiles based on the agro-ecological zones where they were grown in Algeria. The findings demonstrate that, in the studied year, the agro-climatic conditions in Constantine (subhumid and semiarid) were more favorable for protein accumulation than those in Setif (semiarid) and Algiers (subhumid). These findings suggest that the quantity, as well as the quality, to a lesser extent, of these proteins are influenced by these conditions.

Author Contributions: Writing—original draft preparation, C.A.S.; writing—review and editing, V.M. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, project number PN-III-P2-2.1-PED-2019-5346, within PNCDI III.

Acknowledgments: We thank all the authors who made this Special Issue possible and the *Separations* editorial team for their trust and support.

Conflicts of Interest: The authors declare no conflict of interest.

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