

The Importance of UV-Vis Spectroscopy: Application in Food Products Characterization



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Abstract

There is a great concern about the quality of food products in the current market, since adulterations of them can lead to financial loss and damages to consumer health. In this context, the techniques for food characterization have been useful tools, specially the spectroscopic techniques, since they do not destroy the sample under analysis nor do they produce toxic residues. One of these techniques is the absorption spectroscopy in the Ultraviolet and Visible region, which is used for qualitative and quantitative characterization of sample compounds. This study is a bibliographical review that seeks to demonstrate the effectiveness and relevance of using this technique in food products characterization. Therefore, a bibliographic survey of publications in national and international journals in the last eight years was carried out.

Introduction

All the analytical techniques used to collect physicochemical data obtained by absorbing, transmitting or reflecting the incident radiant energy in a sample are called spectrophotometry [1]. Among these analytical techniques, there is the light absorption spectroscopy in the Ultraviolet and Visible region (UV-Vis) (200-800nm) as one of the most used technique for the characterization and determination of several organic and inorganic substances [2]. The UV-Vis analytical method has become very important and widespread in different scientific areas around the world due to its availability, simplicity, flexibility and wide applicability in several areas, including biochemistry and analytical chemistry. Currently, it is necessary to reduce sample and reagents quantity to develop an analytical measurement, especially for scarce samples or toxic solvents; therefore, a UV-Vis microvolume spectrometric instrumentation has been developed [3].

Currently, spectroscopy techniques and chemometric methods are largely used in the food industry analyses to improve quality control of foods and beverages, such as: detection of falsification or adulteration, identification of origin [4], differentiation of caffeinated and decaffeinated coffee, origin and variety of wine or the origin of olive oils [5], and others. This study presents a bibliographic review in order to evaluate the effectiveness and the relevance of using the analytical technique of molecular

spectrophotometry in the Ultraviolet and Visible region in the food industry.

Methodology

The literature survey was carried out through searches in ScienceDirect journal portal (www.sciencedirect.com), which provided nine international paper, by using the following search terms: "Use of UV-Vis spectroscopy in food" and "Application of UV-Vis spectroscopy in food analysis". These search terms were also used in the CAPES journal portal (www.periodicos.capes.gov.br) and one national paper was also selected. The collected papers were published in the last eight years in order to maintain the updated data. The parameters analyzed in the paper are presented in Table 1: The study objectives, the methodology applying UV-Vis analysis, and the main results. It could be noted various objectives of using UV-Vis spectroscopy in food industry, highlighting the analyses to identify possible frauds in general foods and beverages.

Result and Discussion

Table 1 presents ten papers selected in the bibliographic survey, describing the objectives of the authors, the methodology used to reach these objectives and the main results obtained in the studies. Problems involving food adulteration can be identified in two ways: using quantitative analysis, when the adulterant is known,

otherwise, the qualitative analysis is able to provide satisfactory results. The qualitative methods such as UV-Vis, for example, have been highly applied in quality control of food and beverages, and they have increasingly attracted interest due to their screening potential, which allows the identification of possible frauds that may occur in food products [6].

Table 1: Articles selected by means of a bibliographical survey carried out in this study (2010-2017).

Literature	Stuty Objective	Methodology	Main Result
[12]	To propose a method to verify the characteristics of tea infusions prepared with boiling water only, using UV-Vis spectroscopy and resolution of variables through the algorithm of successive projections associated to linear descriptive analysis.	20 types of Brazilian black tea, 20 types of Argentinean black tea, 20 types of Brazilian green tea and 20 types of Argentinean green tea were used. Samples were prepared using 1 g in 100 mL of distilled water at 90 °C. Quartz cuvettes were used to obtain the spectra in the UV-Vis.	Two absorption bands were easily seen from 190 to 250nm, and from 250 to 300nm, and another wide absorption range appears around 300-400nm. These absorption bands are characteristic of phenolic compounds present in tea infusions.
[12]	To investigate the application of synchronous fluorescence spectroscopy and UV-Vis spectroscopy to quantify coffea canephora var, addition of robusta to coffea arabica, as well as the complementarity of data obtained with both techniques.	Coffee extracts were prepared at 6 % (w/v) with distilled water at 95°C, they were filtered and diluted in the ratio 1:120 (v/v). In total, 147 spectra were measured. All analyses were performed in triplicate for each sample of genuine coffee or in duplicate for the blends of coffee samples.	The spectra analyzed could evidence the potential of UV-Vis spectroscopy to discriminate coffea arabica, coffea robusta and their blends samples. The study showed that the aqueous extracts of Coffea arabica and Coffea canephora var. presented significant differences in their UV-Vis spectra.
[13]	To use UV-Vis and HPLC-DAD to investigate pigments in samples of extra virgin olive oils (EVOOs) produced from olives harvested in different countries.	The oil samples were analyzed in quartz cuvettes without any treatment, and the spectra were obtained in 390-720nm spectral range, with spectral and band resolution set at 1nm.	The study showed that the optimized HPLC-DAD method was not able to quantify feofitin B pigment with sufficient accuracy. In contrast, the feofitin B can be accurately determined by UV-vis spectroscopic approach.
[4]	To discriminate whiskey brands and identify the occurrence of falsification, using the UV-Vis spectroscopy method combined with the partial least squares for discriminant analysis (PLS-DA).	Authentic samples consisted of m different brands bottles and seventy-three false samples. Absorbance data were acquired at 1nm of resolution and from 190 to 1100 nm. They were exported to worksheet using the UV-Visible Chemstation software.	A significant difference in the spectra was identified around 205nm; there was a clear separation between 12-year-old brands spectra (Black Label, Old Parr e Chivas Regal) and 8-year-old brands spectra (Red Label, Ballantine's Finest, White Horse e Natu Nobilis), and older brands presented higher absorbance values.
[8]	To present a comparative study of chemometric methods used to quantify extra virgin olive oil (EVOO) adulterated with edible soy oil, applying fluorescence and UV-Vis spectroscopy.	39 adulterated EVOO samples were prepared by adding different concentrations of edible soy oil. The spectrum was recorded in the range from 190 to 1100nm with 1 nm resolution. The transmittance signal calibration was performed using isoocane as the blank.	Preliminary results are indicative that the screening approach is promising and can support official analytical methods to identify the adulteration of EVOOs with lower quality vegetable oils.
[9]	To identify adulteration in ground roasted coffee (due to the presence of peels and sticks) using UV-Vis and the algorithm of successive projections for variable selection associated with linear discriminant analysis (SPA-LDA).	The ground roasted coffee extracts were prepared in hot water. Principal Components Analysis (PCA) was applied in UV-Vis spectra of all samples in order to evaluate the capacity of UV-Vis spectra to discriminate aqueous extracts of adulterated and non-adulterated coffee.	This approach has intrinsic advantages because it provides a simple and quick analysis of ground roasted coffee extracts prepared in hot water only, which represent the final product as taken by consumers.
[14]	To determine the pre-concentration of mercury in water and fish samples using UV-Vis spectrophotometry.	The stock solution (0.1 mol L ⁻¹) of 1-(2-pyridylazo)-2-naphtol (PAN) was prepared by dissolving 0,622 g of it in 25mL of methanol. The working solution (0,002 mol L ⁻¹) was prepared by diluting the stock solution in methanol. UV-Vis spectrophotometric measurements monitored the absorbance of the mercury/PAN complex (λ máx = 554nm). The maximum absorbance for PAN (methanol as the blank) was measured at 460nm.	The proposed sample preparation procedure, associated with the the UV-Vis spectrophotometric determination of mercury/PAN complex microvolume, provided a simple, fast and accurate determination of total mercury in water and fish samples.

[15]	To compare the oxidative stability of various edible oils using UV-Vis spectroscopy and Multivariate Curve Resolution Alternating Least Squares (MCR-ALS) as a viable tool to monitor edible oils in the visible ultraviolet.	Samples of oil from soy, corn, sunflower, canola and olive were analyzed. UV-Vis spectra were acquired in the range from 300 to 540nm (2 nm steps) using 1 mm quartz cuvette.	UV-Vis spectra from heated samples showed a different value for peak maximum intensity. This effect is typical in cases of temperature variation, but it does not affect MCR-ALS curve resolution. MCR-ALS method was able to provide information related to the appearance of tocopherol degradation and oxidation product due to the heating process, even when evaluated by UV-Vis spectroscopy.
[7]	To detect adulteration of commercial pomegranate molasses with date molasses. Some different parameters that could indicate adulteration were determined, such as: total acidity, polyphenol yield, anthocyanin concentration, color intensity and antiradical activity. UV-Vis spectroscopy was used as the screening method to detect adulteration, and then ATF-FTIR and HPLC.	Sampling consisted of 2 authentic natural pomegranate molasses (NPM1 and NPM2), 3 commercial pomegranate molasses (CPM1, CPM2 and CPM3) and 1 natural date syrup (DS). The samples were diluted 1:50 (p/v). The absorption spectra were obtained in the range from 190 to 1100 nm in the visible ultraviolet region, using quartz cuvettes.	The natural pomegranate molasses samples presented higher values of peak amplitudes with similar maximum optical density values varying from 1.01 to 1.12 for NPM1 and NPM2. In contrast, the commercial pomegranate molasses and date syrup showed lower values of peak amplitude, from 0.41, 0.35, 0.42 and 0.34 for CMP1, CMP2, CMP3 and DS. This phenomena may be attributed to a different concentration and / or diversity of the absorbent molecules of phenolic compounds.
[18]	Simultaneous determination of Tartrazine and Twilight Yellow via UV-Vis spectrophotometry and comparison of the results obtained through the Partial Least Squares Regression (PLSR) methodology and two conventional mathematical methodologies (first derivative of spectral data and principle of spectrophotometric additivity) .	An extraction using wool was performed in this study. Sample aliquots were transferred to a beaker with about 50 mL of distilled water, five drops of concentrated HCl and wool pieces. It was stirred until the obtainment of a colorless solution. Then, the colored wool was washed with distilled water and transferred to another beaker with 20 mL of buffer solution NH ₄ OH/NH ₄ Cl pH 10. Finally, the UV-Vis spectrophotometer was used to analyze absorbance.	The dye analyses using UV-Vis spectrophotometry associated with mathematical methodologies allowed an adequate determination of multi components in food matrices.

Source: Author, 2018.

According to Darra, et al. [7] food fraud is a serious ethical and economic problem that affects food industries around the world. In their study, the determination of frauds occurrence in pomegranate molasses syrup was performed using polyphenol characteristics such as its diversity, quantity and bioactivity. The UV-Vis spectroscopy was used as a screening method to determine the adulteration level of pomegranate molasses with date syrup, the HPLC was used to perform an identification of sample adulterants, and ATR-FTIR provided an additional evidence for the perceived differences in the analyzed samples.

In the study accomplished by Martins, et al. [4] the UV-Vis technique was used in order to identify counterfeit Whiskey, which is an high value alcoholic beverage and widely commercialized. It has been constantly adulterated with the substitution with another whiskey of lower quality using the original commercial bottle. The UV-Vis spectroscopy technique was combined with partial least squares for discriminant analysis (PLS-DA), which showed great efficiency in the discrimination of different brands and identify adulteration such as dilution and mixing.

The UV-Vis technique has a very wide application also in vegetable oils, this can be validated by four papers showed in Table 1. One of these studies was developed by Milanez, et al. [8] who

verified the adulteration of extra virgin olive oil with soy oil. The results showed the screening approach as very promising, and could support other official analytical methods currently used to identify adulterations in oils. One of the most important concern related to food adulteration is the possible risk for consumer health or an economic benefit. Olive oil has high nutritional value and pleasant sensory characteristics and also a higher commercial value than common oils, therefore, olive oil is constantly adulterated with the addition of vegetable oils with lower quality [9].

Coffee is one of the most consumed beverages in the world, due to its intrinsic characteristics, stimulant property and some benefits to health. The variety of coffee types is relatively large, due to this, the normative instruction n. 16 of Ministry of Agriculture, Livestock and Food Supply (MAPA) has established a maximum limit of 1 g/100 g for some impurities (stones, peels, stick) in roasted coffee, in order to avoid illegal practices of adulteration [10-18]. In this context, Souto, et al. [19] used UV-Vis spectroscopy associated with linear descriptive analysis to identify irregularities in coffee extracts. According to authors, the technique presented advantages over other methods normally used for this kind of analysis because it provided a simple and quick analysis of coffee extracts, besides it may offer safety to consumers and regulatory agencies, avoiding fraudulent labeling of these products. The bibliographic survey

carried out in this study showed a great concern of food industries to use analytical methods that present easy access, low cost, simplicity and reliable experimental parameters. Among these analytical techniques, the UV-Vis spectroscopy congregates numerous and important methodologies applied in the improvement of food products quality control.

Conclusion

The spectroscopy in the visible ultraviolet region is a very useful technique for qualitative and/or quantitative studies related to characterization of organic and inorganic compounds in food matrices. In this context, the scientific community has used this technique in several research areas of food science and technology sector; its application in quality laboratories of food industries has been very important, because it satisfies both the economic scope and the public health issues, since it allows the quality verification of various products widely commercialized and consumed around the world.

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