



Non-destructive assessment of vitamin C in foods: a review of the main findings and limitations of vibrational spectroscopic techniques

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Abstract

The constant increase in the demand for safe and high-quality food has generated the need to develop efficient methods to evaluate food composition, vitamin C being one of the main quality indicators. However, its heterogeneity and susceptibility to degradation makes the analysis of vitamin C difficult by conventional techniques, but as a result of technological advances, vibrational spectroscopy techniques have been developed that are more efficient, economical, fast, and non-destructive. This review focuses on main findings on the evaluation of vitamin C in foods by using vibrational spectroscopic techniques. First, the fundamentals of ultraviolet–visible, infrared and Raman spectroscopy are detailed. Also, chemometric methods, whose use is essential for a correct processing and evaluation of the spectral information, are described. The use and importance of vibrational spectroscopy in the evaluation of vitamin C through qualitative characterization and quantitative analysis is reported. Finally, some limitations of the techniques and potential solutions are described, as well as future trends related to the utilization of vibrational spectroscopic techniques.

Keywords Vitamin C · Ascorbic acid · Spectroscopy · Electromagnetic spectra · Food quality

Introduction

Over the years, the demand for high-quality food has increased substantially [1]. Consumers require products with minimal risk for disposal to negative health effects. There is a global need to improve food safety and quality [2] since in many countries economic profit is emphasized ahead of nutritious products that meet strict quality and safety standards [3].

The food industry is of utmost significance as it is one of the most important economic axes in the world [2]. To meet the challenges, scientists and specialists of the food

sector are designing, developing, and improving technologies to enable trustworthy, fast, and economically feasible analysis of the quality of food. Most important traditional detection techniques used in food analysis have included high performance liquid chromatography (HPLC), mass spectroscopy (MS), lateral flow strip (LFS), Southern Blot (SB) and enzyme-linked immunosorbent assay (ELISA) [4, 5]. Although these techniques often give accurate results, they are complex, costly, require chemical reagents, are time-consuming, and, above all, destructive (i.e., they alter the physical, chemical and/or nutritional characteristics of the food), which makes accurate measurement of labile food components like vitamin C difficult. Due to continuous technological advancement especially in the area of computational and data processing, other techniques have been developed that do not require prior sample preparation and are more efficient and non-destructive [6, 7]. These include computer vision (CV) and vibrational spectroscopies, encompassing infrared (IR), near (NIR), mid (MIR) and far infrared (FIR) spectroscopy, Raman spectroscopy, ultraviolet–visible (UV–Vis) spectroscopy, and hyperspectral imaging (HSI) [8, 9]. When vibrational spectroscopy techniques are combined with chemometric methods, they become more

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useful [9]. This combination can be successfully utilized for the simultaneous qualitative and quantitative evaluation of different characteristics [3] and/or compounds in fruits, vegetables, cereals, and legumes [7] to measure and monitor their quality [10].

Monitoring the level of vitamin C is fundamental as it is an indicator of the quality of a food product. It is essential to control the concentration of vitamin C during food processing, storage and transport, especially in stages that include high temperatures [11, 12]. However, due to the heterogeneity of vitamin C in complex food matrices and its susceptibility to rapid degradation, use of non-destructive techniques is essential for its detection and accurate quantification [13]. This review focuses on compiling and analyzing the main findings related to evaluation of vitamin C in foods by vibrational spectroscopic (UV–Vis, IR, and Raman) techniques including their limitations and future trends.

Fundamentals of vibrational spectroscopy

IR spectroscopy was discovered between the 1940s and 1950s with the aim of identifying the structure of organic compounds. At present, there is more knowledge about the technique, which, with respect to the electromagnetic spectrum, includes the wavelength range from 780 to 100,000 nm. IR spectroscopy is divided into subregions called the NIR spectral regions with a wavelength range of 714–2500 nm, 2500–25,000 nm in the MIR spectral region and 25,000–100,000 nm in the FIR spectral region [6]. These ranges are not definitively set and their values are based on what has been suggested by various scientific studies [14]. IR spectroscopy examines the relationship between light transmitted into samples and absorbed radiation, yielding data on the molecular structure of foods [15], specifically on the C–O, C–N, C–C, C–H, O–H, N–H, and N–O chemical bonds [10].

UV–Vis spectroscopy covers a spectral range of 200–780 nm, specifically, 200–380 nm in the UV range and 380–780 nm in the Vis range [16]. The basis of UV–Vis spectroscopy begins with the projection of light onto the sample, which is absorbed by the excitation of the electrons that form part of the chemical bonds in the molecules, decreasing the amount of transmitted light [9]. The principle of UV–Vis spectroscopy is based on the Lambert–Beer law, which indicates that the absorption spectrum (sequence of frequencies according to the absorbed light) depends on the concentration of the substance to be evaluated, i.e., the absorbed light is proportional to the sample thickness [6, 17].

Raman spectroscopy can utilize wavelengths from approximately 2500–100,000 nm [8]. When the sample is illuminated with monochromatic light, a low proportion of

the radiation interacts with the sample molecules, generating a scattered light, which has a different frequency compared to incident light. As the product of this inelastic collision, Raman spectrum is produced [18], which reflects the characteristics of the sample and generates a "fingerprint" [4]. This is useful for obtaining information about the chemical bonds and/or the energy of the vibrational bands of the molecules of the organic matrix; therefore, it can be successfully employed for qualitative and quantitative evaluation of various compounds [8]. The physical mechanism of the technique was proposed by Smekal [19], but was later named Raman Effect by Raman and Krishnan [20]. A few decades later, Fleischmann et al. [21] used Raman spectroscopy to study adsorption on rough silver electrodes, achieving improved signals for the Raman spectra. Subsequently, Jeanmaire et al. [22] published similar research, but they used rough gold, silver, and copper surfaces and obtained better results in terms of sensitivity, speed of analysis, and interference. This improved technique was named surface enhanced Raman spectroscopy (SERS) [4]. This spectroscopy is simply based on the amplification of Raman signals from molecules located in an electric field (interacting with a magnetic or chemical field), which is generated due to the excitation of electrons of nanostructures of metals such as silver and gold [23, 24].

Chemometrics: spectrum data processing

There are some undesirable factors that interfere the analysis of data, such as the effects of scattering, instrumental noise and sensitivity, and environmental conditions [2, 8]. It is important to preprocess the information with the use of chemometrics using mathematical techniques and multivariate statistics [25]. For this purpose, a number of smoothing methods can be employed such as first and second order derivative methods, orthogonal signal correction (OSC), Gaussian filter (GF), standard normal variant (SNV), Savitzky–Golay filter (SG), wavelet transform (WT), multiplicative signal correction (MSC), and net analyte signal (NAS) [10, 26]. Especially Fourier transform (FT) has been proven useful since it increases the sensitivity of various vibrational spectroscopy techniques, resulting in improved data acquisition [27].

Due to the complex food matrices, the spectral information obtained is very large and much of it is not of interest to the researcher. Therefore, other discrimination and modeling algorithms must also be applied to reduce the amount and complexity of the information. Some discriminant methods are hierarchical cluster analysis (HCA), particle swarm optimization (PSO), genetic algorithm (GA), partial least squares regression (PLSR), successive projections algorithm (SPA), artificial neural networks

(ANN), support vector machine (SVM), random frog algorithm (RFA), linear, quadratic and partial least discriminant analysis (LDA, QDA, and PLSDA, respectively), soft independent modeling of class analogies (SIMCA), cluster analysis (CA), regularized discriminant analysis (RDA), principal component regression (PCR), and principal component analysis (PCA) [1, 16, 28]. PCA is widely used to classify and make predictions from a database without affecting its patterns and/or trends. As an example, Zilhada et al. [29] were unable to determine by direct FT-NIR data analysis whether vitamin C gummies from the Ciputat market in Indonesia were made from bovine or porcine gelatin; however, by applying PCA to the technique, it was possible to conclude that the commercial gummies contained gelatin derived from cows.

Finally, the robustness of the models must be analyzed using techniques such as the correlation coefficient (r), coefficient of determination (R^2), root-mean-square error of validation (RMSEV), of calibration (RMSEC), and of prediction (RMSEP) [17]. In addition, the residual prediction deviation (RPD) is used commonly; the value of the factor must be greater than 2.5 [10].

Hemrattrakun et al. [30] employed Vis–NIR spectroscopy to evaluate vitamin C content, total soluble solids (TSS), and firmness of persimmon. They applied OSC and PLS as the preprocessing and discrimination technique, respectively, in addition to using RMSEC, RMSEP and RPD as accuracy models. The authors emphasized the importance of chemometrics in obtaining results of good quality in the quantification of vitamin C. In another investigation, Soltanizazemi et al. [31] analyzed the °Brix, titratable acidity, TSS, total anthocyanins, and acid ascorbic of mulberry juice. UV–IR spectroscopy was used, in addition to MSC and SNV as preprocessing methods, and PLS and GA-PLS as multivariate calibration methods. According to the r value (0.96–0.98) obtained when using GA-PLS, it was determined that it was better for the analysis compared to the use of PLS (r : 0.88–0.95).

In another study, UV–Vis spectroscopy was used to analyze herperidin, rutin, and vitamin C in solution. In this case, although no preprocessing methods were employed, calibration methods (PLS, ANN, and multivariate curve resolution-alternating least squares) enabled successful quantification of each compound [32].

As mentioned, FT and PCA are widely used for data pretreatment and discrimination, respectively. Gedikoğlu et al. [33] employed FT and PCA with IR spectroscopy to evaluate polyphenol and flavonoid content and antioxidant activity in citrus fiber. In the study, citrus fiber was added to ground beef meatballs and its quality was evaluated during refrigeration for 7 days. The results demonstrated an overall R^2 value of 0.96 and encouraged usage of FT

and PCA -based spectroscopy in predicting lipid oxidation in meat products.

Spectroscopy in the analysis of vitamin C in food

Due to the increasing demand for quality of food products and the constant concern in public health [23], vibrational spectroscopy is mostly used in the on-line evaluation of various compounds. This is to ensure the safety and high quality of a foodstuffs [3, 10, 26, 34] in sensory, physical, chemical, microbiological, and physiological terms [7]. Many of the compounds maintain food quality are antioxidants [3], and vitamin C is one of the most relevant antioxidant quality indicators. The nutrient is the main water-soluble antioxidant, comprising approximately in average 65% of biological antioxidant activity of many fruits and vegetables [11]. In addition, vitamin C is indispensable for life because it influences various physiological processes due to its antimicrobial, anti-inflammatory, and immunomodulatory properties [5]. Vitamin C deficit generates scurvy [13]. Vitamin C consists of L-ascorbic acid (LAA) and L-dehydroascorbic acid (LDAA), which are its reduced and oxidized form, respectively; therefore, for its quantification it is necessary to determine the sum of both [35]. LAA is easily oxidized to LDAA in the presence of oxygen and metals under conditions of high temperature and pH [5].

There are multiple conventional techniques for vitamin C assessment, including titrimetry, voltammetry, fluorometry, electrochemistry, potentiometry, chemiluminescence, capillary electrophoresis, and chromatography [12, 36–38], but these methods have drawbacks especially because of instability, lack of accuracy, and the use of chemical reagents. Vitamin C can be determined more efficiently and non-destructively by spectroscopy, which has first utilized for vitamin C measurement in 1937 by Williams and Rogers [39]. Da Silva et al. [40] compared two methods for the quantification of vitamin C in industrialized fruit juices, concluding that by UV–Vis spectroscopy error values were less than 5% and by titrimetry over 15%. In the evaluation of vitamin C in several fruits by titrimetry and UV–Vis spectroscopy, Elgailani et al. [41] concluded that there was no significant difference between the techniques, but they recommend spectroscopy due to the ease and speed of the technique. Likewise, no significant difference was established in the quantification of vitamin C in orange juice by voltammetric method and UV–Vis spectroscopy [42]. In addition, UV–Vis and FT-IR spectroscopy were compared with fluorometry in the computational assessment of vitamin B9, vitamin C and vitamin K3 and their interactions with β -lactoglobulin [43]. Without significant difference, all spectroscopic techniques suggested that the interaction between nutrients and β -lactoglobulin caused conformational changes in the protein.

To date, by employing UV–Vis spectroscopy, vitamin C has been quantified in many types of food products such as orange, lemon, mandarin, grapefruit, kiwi, red bell pepper, green bell pepper, cauliflower, parsley, Brussels sprouts, kale, cabbage, orange and peach juices, apple, peach, as well as in banana/pear, apple/carrot and currant/cherry/apple cocktails [44]. Vitamin C content was also evaluated in tangerine, grape, orange, lemon, apples [41], in apple and carrot purees, and in apple puree whey [35]. Using UV–Vis spectroscopy with HPLC, vitamin C was evaluated in fortified cereal, dry cereal, freeze-dried Brussels sprouts, whole milk powder, low-calorie cranberry juice cocktail, adult and children's nutritional formula powder, freeze-dried green beans, fresh pasteurized orange juice, slurried spinach, chips, pineapple, broccoli, potatoes, cassava chips, plantain chips, dried oregano, parsley [45], raw and boiled green leafy vegetables [46], oranges, grapefruit, pink grapefruit, apples, and pineapples [47]. Using UV spectroscopy with HPLC, vitamin C was also evaluated in fruit cream powder, multivitamin syrup, infant milk powder, multivegetable juice, grapefruit and orange juices, banana, kiwi, broccoli,

tomato, cauliflower, cucumber, and parsley leaves [48]. The vitamin C content of jujube [49], tomatoes [50], and mango [51, 52] was measured by NIR spectroscopy. FT-NIR spectroscopy was also used to evaluate the vitamin C content of pomegranate [53]. Cimpoiu et al. [54] employed Raman spectroscopy to identify and separate vitamin C in a solution.

Vibrational spectroscopy can be also employed to evaluate possible adulteration. Mohammadian et al. [55] detected the authenticity of lime juices by assessing their vitamin C content by employing FT-IR spectroscopy. To evaluate the quality of Kakadu plum, its vitamin C content is usually taken as an indicator. Recently, an investigation analyzed the efficiency of attenuated total reflectance (ATR)-MIR spectroscopy to discriminate Kakadu plum powder with synthetic ascorbic acid. Using the second derivative and PLS as a chemometric analysis, Cozzolino et al. [56] were able to identify the adulteration of the product with an R^2 value of 0.85.

UV–Vis (Table 1) and IR (Table 2) spectroscopies are the vibrational spectroscopic methods that are the most widely

Table 1 Quantification of vitamin C by UV–Vis spectroscopy

| Food | Equipment | Results | Reference | | |
|--|---|---|-----------|------------------|------|
| Gelatin with 30, 40 and 50% moringa leaf flour | Not specified | 1.83, 6.74 years 10.85 mg/L | [59] | | |
| Apple | UV–visible spectrophotometer model PD303UV (APEL CO., LTD, Japan) | 15 (mg/L) | [41] | | |
| Tangerine | | 15 | | | |
| Orange | | 13 | | | |
| Lemon | | 12 | | | |
| Grapes | | 9 | | | |
| Black currant | UV–Vis spectrophotometer of double beam model Shimadzu 1800 (Shimadzu, Japan) | 446.83 (mg/100 g) | [60] | | |
| Guava | | 181.79 | | | |
| Lemon | | 56.40 | | | |
| Melon | | 44.73 | | | |
| Karanda | | 44.68 | | | |
| Mulberry | | 41.8 | | | |
| Mango | | 36.41 | | | |
| Wax apple | | 18.89 | | | |
| Watermelon | | 9.79 | | | |
| Gooseberry | | 8.29 | | | |
| Pomegranate | | 8.22 | | | |
| Grapes | | 5.58 | | | |
| Lemon juice | | Spectrophotometer model UV-1601 (Shimadzu, Japan) | | 91.21 (mg/100 g) | [61] |
| Orange | | | | 76.62 | |
| Apple | | | | 35.83 | |
| Lemon | 29.10 | | | | |
| Orange juice | 21.75 | | | | |
| Grapes | 21.70 | | | | |
| Grape juice | 19.59 | | | | |
| Apple juice | 12.20 | | | | |

Table 2 Quantification of vitamin C by IR spectroscopy

| Food | Equipment | Method | Results | References |
|--|--|--------|--|------------|
| Fresh tomatoes | Portable/handheld NIR spectrometer model Neospectra (Si-ware Systems, Egypt) | NIR | RMSEV: 3.78 (mg/100 g) RMSEP: 4.09 | [62] |
| Valencia Orange | Spectrometer model Spectrum 100 N (Perkin-Elmer Corp., USA) | MIR | RMSEV: 103.4 (mg/L) RMSEC: 89.7 RMSEP: 75.1 | [63] |
| | | NIR | RMSEV: 107.2 RMSEC: 89.3 RMSEP: 94.9 | |
| Newton tomatoes | Spectrometer NIR model EPP 2000 (Stellarnet, Inc. USA) | NIR | RMSEV: 1.087 (mg/100 g) RPD: 1.701 | [50] |
| Kakadu plum powder | Spectrophotometer model Bruker Alpha (Bruker Optics, Germany) | MIR | R^2 : 0.93 RMSEV: 18.1 g/1 kg dw RPD: 4.1 | [56] |
| | | NIR | R^2 : 0.91 SEV: 18.4 mg/1 kg dw RPD: 4 | |
| Cultivars of <i>Fragaria x ananassa</i> Duch | GX FTIR spectrophotometer (PerkinElmer®, USA) | MIR | RMSEC: 21.14 (mg/100 g) RMSEP: 22.11 | [64] |
| Acerola | Frontier FT-IR/NIR Spectrum 100 N spectrometer (PerkinElmer®, USA) | NIR | RMSEP: 166.27 mg/100 g R^2 : 0.99 | [65] |
| Apple | Scanning monochromator model 6500 (FOSS NIRSystems Inc., USA) | NIR | RMSEC: 3.4 (mg/100 g) RMSEP: 4.9 RPD: 2 | [66] |
| Cashew apple | FT-NIR spectrometer model Spectrum 100 N (PerkinElmer®, USA) | NIR | R^2 : 0.84 RMSEC: 4.61 (mg/100 g) RMSEP: 4.8 | [67] |
| Guava nectar | | NIR | R^2 : 0.86 RMSEC: 6.41 RMSEP: 7.44 | |

dw dry weight

employed for vitamin C analysis because they are generally regarded as the best techniques for the purpose [57]. Yang and Irudayaraj [57] compared different spectroscopic techniques for the evaluation of vitamin C in liquid and powder mixtures; the R^2 values for FT-IR attenuated total reflectance, FT-NIR, NIR, FT-IR photoacoustic, and FT-Raman spectroscopy were 0.999, 0.992, 0.988, 0.966, and 0.950, respectively. In another study, the results of vitamin C quantification in Kakadu plum powder were compared. It was observed that MIR spectroscopy (R^2 : 0.93, RPD: 4.1) was better than NIR spectroscopy (R^2 : 0.91, RPD: 4), but coupling it with FT (FT-NIR) also yielded efficient models [58].

Current challenges and opportunities

Despite the many benefits of using vibrational spectroscopy, it also has its limitations. First and foremost, traditional vibrational spectroscopy equipment has a relatively high cost. However, thanks to technological advances, handheld/portable spectrometers are available. These have all the components of benchtop spectrometers, but at a smaller size and lower cost [14]. In addition, they are fast, lightweight, compact and rugged with ease of use on site [68–72]. Thus, miniaturized spectrometers enable rapid, real-time monitoring of food quality and safety at any point in the food supply chain [73, 74]. Portable NIR spectrometer was used to assess the quality of mango cv. Tommy Atkins [75], oranges [76], tomato paste [77], oregano [78], green tea [79], and ground meat [80]. With portable FTIR spectrometer, the quality of butter [81], milk powder [82], and pistachio was evaluated [83]. Portable Raman spectrometers were used to evaluate

the quality of vegetable juice (NIR-excited Raman) [84], tomato [85], and Parmesan cheese [86]. A portable Vis spectrometer was used to evaluate the quality of apples [87], and a portable SERS spectrometer was used to evaluate the quality of cabbage and apples [88].

Santos et al. [89] used a handheld NIR spectrometer to predict the vitamin C content of clementine, lemon, tangerine, orange, and lime; R^2 values were determined to be between 0.766 and 0.864. Aykas et al. [77] employed a portable ATR-FTIR spectrometer to predict the vitamin C content of tomato paste. Compared with reference values, there was a high coefficient of cross-validation (0.85 and 0.99). Similarly, Borba et al. [62] compared a portable NIR spectrometer with conventional techniques in measuring vitamin C content of tomatoes; the validation coefficient obtained was 0.81. Akpolat et al. [90] obtained a validation coefficient of 0.79–0.91 in predicting the vitamin C content of fresh tomatoes. Beghi et al. [91] used a portable vis–NIR spectrometer to monitor the vitamin C content of Golden Delicious and Stark Red Delicious apples. In this case, the validation had a low R^2 value of 0.50. Similarly, the correlation coefficient between the evaluation with a portable NIR spectrometer and the reference values for vitamin C content in Kakadu plums and plum puree was 0.55 and 0.86, respectively [92]. Even smartphone-based spectrometers have been developed as demonstrated in the studies of Kong et al. [93] and Aguirre et al. [94], whose equipment was successfully employed to assess the vitamin C content in a lemon beverage and orange juice, respectively.

The development of this miniaturized equipment is a great achievement in the field of spectroscopy, but there are some limitations that influence the results obtained. The size of the portable equipment limits the evaluation of high volume samples. When performing the evaluation in the field (in situ), there is a high risk of contamination and interference from environmental factors [74]. They also have somewhat higher detection limit and lower sensitivity compared with conventional equipment. In a study predicting the quality of mushrooms of the genus *Tuber*, the accuracy of the benchtop NIR spectrometer was from 93.33–100%, and the values of three portable NIR spectrometers were 83.33–100%. Similar results were shown when evaluating bioactive compounds from green tea [79].

Another disadvantage is that the construction of calibration models for each portable equipment requires considerable cost and time [95]. One option is for models to be built on benchtop spectrometers (master or primary unit) and transferred to portable spectrometers (slave or secondary unit) [96] to avoid the whole calibration process. It has been reported that large spectral databases of various samples have been transferred from benchtop to portable spectrometers [74]. The transfer can also be made between equipment of different makes/models [97, 98]. There are several

chemometric or standardization techniques to achieve this and maintain model accuracy [99]. For example, Igne et al. [100] evaluated the quality of soybean with four benchtop NIR spectrometers of two different brands by employing eight calibration transfer techniques based on the removal of orthogonal signal. Zeng et al. [96] evaluated pigments in tea leaves with a laboratory Raman spectrometer and the calibration models were transferred to a portable Raman spectrometer with the direct standardization (DS) technique. For the evaluation of fresh cow milk, Melenteva et al. [101] transferred calibration models from a diode-array spectrometer to a shortwave visible–NIR spectrometer with model transfer by slope and bias correction (SBC). To transfer the calibration model between three NIR spectrometers of different brands to predict apple TSS, Hayes et al. [95] employed orthogonal projection (TOP), piecewise direct standardization (PDS), difference spectrum adjustment (DAS), and model updating (MU). Salguero-Chaparro et al. [102] used PDS, TOP, and SBC to transfer calibration models on olive quality assessment from a benchtop NIR monochromator to a portable NIR spectrometer. The disadvantage of the transfer is that, after a certain time, the model obtained loses accuracy. To avoid this, the models should be recalibrated gradually [102].

UV spectroscopy has degradative effects on bioactive compounds such as vitamin C. The use of IR spectroscopy is not recommended for foods with water content higher than 80% [103] since water is a strong absorber whose hydrogen bonds interfere significantly in the IR region [104]. This is a serious limitation for many foods of plant origin that are significant sources of vitamin C, but also have a high proportion of water in their composition. This problem can be solved with a suitable preparation of the sample, but this demands time and is costly. Raman spectroscopy is a potential option in these cases because the weak Raman scattering has less interference with water, and it can be used in solid, semi-solid, and liquid samples quickly and economically; in addition, by omitting the sample preparation, the analysis would be non-destructive [8]. This has been demonstrated in several studies such as in the evaluation of milk; El-Abassy et al. [105] were able to successfully (R^2 : 0.92–0.99) determine milk fat content using Raman spectroscopy.

Despite the potential of Raman scattering, it is weak, resulting in low analytical sensitivity [106] compared to other spectroscopy techniques such as NIR and MIR spectroscopy. To counteract this, enhancement of Raman spectroscopy can be utilized in form of SERS. Another disadvantage of the Raman spectrum is that it can only collect a small amount of information from the sample and, therefore, the results obtained are not complete [106]; the same is also true for IR spectroscopy [107]. The low sensitivity of Raman spectra was demonstrated by He et al. [108], who were unable to discriminate the Raman spectra of three prohibited

food additives dissolved in ethanol. On the other hand, by employing gold-plated silicon as SERS substrate, the weak signal was improved, enabling successful distinguishment of the samples.

Considering the above, before performing any analysis in food, it is necessary to define which vibrational spectroscopy technique is going to be used, taking into account its advantages and disadvantages in relation to the nature and composition of the sample. For example, many compounds cannot be detected based on IR spectrum; specifically, minerals are not active in the NIR region, but they are active in the Raman region [107]. It should be noted that, even if the most optimal vibrational spectroscopy technique is chosen, it is challenging to analyze multiple compounds simultaneously [24]. This can, however, be solved with correct data processing of the spectrum using chemometrics. Yang and Irudayaraj [57] concluded that infrared spectroscopy (NIR and IR-photoacoustic) is better than Raman spectroscopy for the prediction of vitamin C content in some foods and pharmaceuticals. The authors also used FT-Raman spectroscopy and highlighted the importance of such a chemometric method for improving the sensitivity of the technique and reducing data acquisition time. In the same study, it was established that the O–H groups have a weak absorbance in the Raman spectrum, but a strong absorbance in the infrared region, with the opposite occurring with the non-polar C–C groups.

Finally, to enhance the robustness of the models generated with respect to vitamin C assessment, it is necessary to have a comprehensive database. This can be achieved by analyzing different foods or, if the focus is on a specific food, samples of different species and origins should be used [7, 28]. Relatively more robust models were obtained when evaluating vitamin C in three bell pepper cultivars at different growth stages by using Vis–NIR spectroscopy (average R^2 : 0.74 and RPD: 2.2) compared to shortwave NIR spectroscopy (average R^2 : 0.72 and RPD: 2.13) [109]. In addition, excellent results were obtained in the evaluation of vitamin C in two green-fleshed kiwifruit cultivars employing FT–NIR spectroscopy [110]; in eleven yellow-fleshed peach cultivars, in three white-fleshed peach cultivars, in four yellow-fleshed nectarine cultivars and in one white-fleshed nectarine cultivar using UV spectroscopy [111]; in four plum cultivars, using NIR, MIR and Raman spectroscopy [112]; and in apricot pastes of eight cultivars using FT-IR spectroscopy with attenuated total reflectance [113].

Vibrational spectroscopy techniques and chemometric methods will continue to evolve in parallel with other technological advances to address the above limitations. On the other hand, researchers should be informed and trained on the importance of using these techniques not only in the evaluation of vitamin C, but also in the evaluation of other compounds in different food matrices. If the use of spectroscopy expands further, this will increase the volume of the production

of equipment and, consequently, lead to a significant cost reduction.

Conclusions

Vibrational spectroscopy and its recent advancements are attracting the attention of researchers around the world due to its possibilities in food quality assessment, the benefits including rapid, accurate and inexpensive non-destructive analysis. Specifically, the usage of UV–Vis, IR and Raman spectroscopies has increased in the quantification of vitamin C as a quality indicator of various food products; the techniques are used together with chemometric preprocessing, discrimination, and modeling tools to, in addition to improving the efficiency of obtaining spectral data, help researchers in the subsequent data analysis and interpretation of the results. To avoid limitations of vibrational spectroscopy techniques, it is necessary to define the appropriate technique according to its advantages and disadvantages with respect to its compatibility with the nature of the food sample.

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