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Applications of spectroscopic-based techniques for quality and safety evaluation of tomatoes: A mini-review

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Abstract: *This review article summarizes the application of spectroscopic-based techniques as non-destructive techniques for the quality and safety evaluation of tomatoes. Spectroscopic techniques such as near-infrared (NIR), visible/near-infrared (Vis/NIR), and Raman spectroscopy have been widely used for the evaluation of various quality attributes of tomatoes, including soluble solids content, pH, firmness, color, and lycopene content. Moreover, the use of spectroscopic techniques has also shown promising results in the detection and quantification of contaminants such as pesticides and pathogens in tomatoes. This technique has been widely used for internal quality evaluation of tomatoes and future studies should focus further on investigating the feasibility of this approach in the evaluation of external qualities. The advantages of spectroscopic techniques include their non-destructive nature, rapid analysis time, and potential for on-site analysis. However, the limitations of these techniques include the need for calibration models, sample preparation, and sensitivity to environmental factors such as temperature and humidity. Overall, spectroscopic-based techniques have great potential in the quality and safety evaluation of tomatoes, and further research is needed to explore their full capabilities and optimize their use in the tomato industry.*

Keywords: tomato, spectroscopic-based, quality evaluation, Vis/NIR spectroscopy, Raman spectroscopy

1. INTRODUCTION

Quality and safety evaluation of horticultural products has shown a great deal of interest in academia and industry because food producers must adhere to more restrictive standards from regulatory agencies and satisfy consumer demands for fresh produce and processed foods of higher quality and safety [1]. Tomato, as shown in Figure 1 is an example of a horticultural product and is popular, versatile, and is considered the world's largest vegetable crop [2]. Tomatoes have diverse applications in both fresh and processed forms. Ketchup, sauces, pastes, and juice are examples of processed goods [3]. Tomatoes are the most well-known source of lycopene, the major component responsible for the bright red color of ripe tomatoes and tomato products [4]. Tomatoes are a rich source of minerals, vitamins, and carotenoids, including phosphorus, potassium, lycopene, and vitamin C, and they can complement a wide range of processed food products [5]. Tomatoes and their derivatives offer not only nutritional value but also significant anti-inflammatory, antioxidant, and anticancer properties [6]. From an economic standpoint, tomatoes are the most crucial crop for many farmers and are among the most cultivated crops globally. According to FAOSTAT, tomato production worldwide was approximately 186.821 million metric tons in 2020, cultivated on 5,051,983 hectares, with a yield of 37.1 metric tons/hectare (mT/ha). In the Asia-Pacific region, the Philippines emerged as the top tomato producer, with a total production volume amounting to about 225.5 thousand metric tons in 2022 [7]. However, tomatoes are perishable in nature, and they are susceptible to losses during postharvest storage and handling, affecting their

both economic and nutritional benefits. This is because the fruit releases ethylene, a plant growth regulator which plays a vital role in fruit ripening or deterioration [8]. The perishable nature of this commodity is one of the reasons why the number of postharvest losses or the decline in both quality and quantity during postharvest stages is relatively high [9]. Owing to these reasons, quality, and safety evaluations for tomatoes particularly during the phase of production, postharvest processes are of high significance.

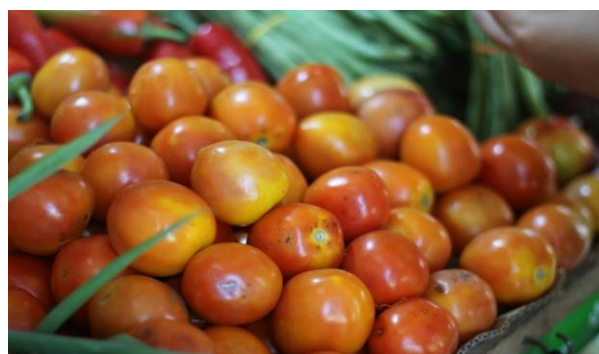


Figure 1. Tomatoes (*Solanum lycopersicum*)

However, the traditional method for quality evaluation of tomatoes relied on destructive techniques such as chemical and sensory analyses. However, these methods are time-consuming, costly, and may damage the product after the test is carried out [10]. Therefore, non-destructive techniques based on spectroscopy have been developed as an alternative approach for evaluating tomato quality. The principle of spectroscopy involves the interaction of matter and the electromagnetic spectrum according to a specific wavelength [11]. This

technique can determine the various quality indicators of tomatoes such as sugar content, acidity, and firmness, which are indicators of tomato quality.

In recent years, spectroscopic-based techniques have been successfully used for rapid and non-destructive monitoring of the different quality indicators of tomatoes during storage, hence predicting quality changes. The most promising spectroscopic-based techniques involve Visible/Near Infrared (Vis/NIR), Near Infrared (NIR), Fourier Infrared (FTIR), and Raman spectroscopy, which has been successfully employed as a rapid and non-destructive tool for quality and safety evaluation of tomatoes from pre- to postharvest processes. However, there has been no research study that summarizes the recent advances and applications of spectroscopic-based techniques for the quality and safety evaluation of tomatoes. As a response, this mini-review article aims to collect and summarize the different published works about the applications of spectroscopic-based techniques for tomatoes' quality and safety evaluation. Challenges, advantages, and future trends will be discussed also.

2. QUALITY EVALUATION

The quality and safety evaluation of tomatoes involves accessing both internal and external qualities. External quality is crucial and significant since it displays a clear perception based on the exterior surface of most agricultural products [12]. For instance, the external quality of tomatoes is characterized by size, shape, color, and external defects such as bruises. The size of a tomato is the most important aspect of its outside appearance because the commercial value of the fruits is graded in different size categories throughout the postharvest handling process. Thus, it has become one of the important focuses for tomato growers, fruit retailers, and cultivar genetic researchers. The measurement of tomato quality based on its size is more challenging because of its irregularities in size and shape. Furthermore, the conventional method called "visual grading" for size measurement is a manual operation that is tedious, labor-intensive, and subjective [13]. To overcome these drawbacks, Yang et al. [14] established the application of spectroscopic-based technology for rapid measurement of tomato size and the approach was able to determine the fruit quality based on size.

For the postharvest handling of tomatoes, size determination is essential in the food industry to meet the requirements for the grading and sorting process of the fruit. As reported by Gastélum-Barrios et al. [3], size determination for tomatoes is a factor of weight, diameter, and form. The process of fruit grading and sorting is used to increase the homogeneity, economic worth of the commodity, and consumers' acceptability [15]. This process can also be performed using the color property of the fruit, an attribute that is directly linked to the external property of the fruit. The most important visible attribute of tomato used to determine ripeness and postharvest life is color, which also plays a significant role in the consumer's buying choice. A manual inspection for fruit ripeness is performed by comparing the tomato color to the classification chart [3]. However, the conventional

method for maturity classification is laborious, and non-accurate as judgment is subjective.

External defects are another important factor to consider during the external quality inspection of tomatoes. Common external defects of tomatoes include cracks, bruises, scars, and discoloration. These defects can be caused by various factors such as physical damage during harvesting, handling, and transportation, as well as environmental stressors such as temperature and humidity. External defects can also serve as entry points for pathogens and increase the risk of spoilage and contamination. It was emphasized by Mohd Ali et al. [15] the early detection of surface defects could forestall further deterioration throughout the entire product. Therefore, it is notable to give importance to external defects, particularly for tomatoes where they may have an impact on market pricing.

The internal quality of tomatoes refers to their flavor, texture, and nutritional value. It includes characteristics such as aroma, sweetness, firmness, and hue. When evaluating internal quality, factors such as sugar concentration, acidity, and aroma are taken into account. Tomatoes that are ripe and of high quality typically have a balance of flavor and acidity, a vibrant color, and a delightful aroma. The internal quality of tomatoes plays a vital role in consumer satisfaction and is a crucial factor for food processors, caterers, and consumers.

3. PRINCIPLES OF SPECTROSCOPY

Spectroscopy is a science that covers the study and measurement of spectra generated when a specific material interacts with or produces electromagnetic radiation [16]. This technology depends on the changes in the photophysical properties of the material and has gained relevant attention due to its wide range of applications [17]. According to Wang [18], a typical spectrometer has seven important parts, as illustrated in Figure 1. These components work together to analyze a sample by measuring the intensity of the radiation reflected and transmitted by the sample, which is then processed by a computer to produce a spectrum.

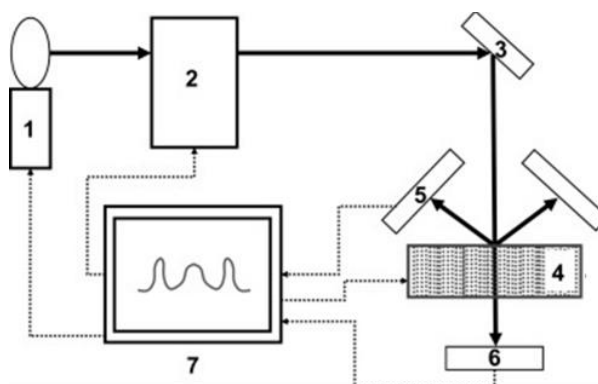


Figure 1. A schematic illustration of a Near Infrared spectrometer. Where 1. Light source, 2. Beam splitter, 3. Reflector, 4. Sample, 5. Diffuse reflection detector, 6. Transmission detector, and 7. Computer. Source: [18]

This method is usually classified based on the wavelength area employed, the nature of the interaction involved, or the sort of products investigated. In the interest of quality and safety evaluation of tomatoes, the most employed spectroscopic-based techniques involved Vis/NIR, spectroscopy that covers the electromagnetic spectrum from 380-2500 nm [19]. Spectra in the Vis/NIR region are often utilized for analysis since practically all-important structures and functional groups of organic substances may be recognized in the spectrum with a very stable spectrogram [20]. Through the examination of spectra within the visible/near-infrared range, it is possible to discern significant structures and functional groups present in tomatoes. This process yields crucial insights into the quality attributes and safety parameters of said tomatoes. The utilization of this technique provides a consistent spectrographic representation, enabling dependable and effective evaluation of tomatoes while avoiding the necessity for destroying sampling or extensive sample conditioning.

Another promising spectroscopic-based technique is Raman spectroscopy, a technique that gives detailed information about samples by analyzing the molecules' basic vibrational modes, resulting in precise chemical identification [21]. The utilization of Raman spectroscopy for the purpose of quality assessment of tomatoes entails the exposure of the sample to a laser beam followed by the examination of the dispersed light. The tomato sample's chemical composition and structure can be inferred from the energy shifts in the scattered light, which are caused by its molecular vibrations.

Raman spectroscopy is a non-destructive technique that enables the rapid assessment of tomato quality by analyzing the unique molecular fingerprint of the sample through its scattered light.

Likewise, Fourier Transform Near Infrared spectroscopy (FT-NIR), a spectroscopic technique used for quality assessment of tomatoes, works by measuring the absorption and reflection of near-infrared light by tomato samples.

4. APPLICATIONS OF SPECTROSCOPIC-BASED TECHNIQUES IN TOMATOES

The applications of spectroscopic-based techniques in the field of quality and safety evaluation of tomatoes have shown great results in previous years. The spectroscopic-based techniques highlighted in this paper are Visible/Near Infrared (Vis/NIR), Near Infrared (NIR), Fourier Infrared (FTIR), and Raman spectroscopy. Different studies underlining the application of this approach in the quality evaluation of tomatoes were summarized as encapsulated in Table 1. It is observed that the results from diverse studies demonstrate a good finding with a higher coefficient of correlation. Among the two categories of quality parameters, this approach has been widely used to characterize and detect the internal qualities of tomatoes. This means that the feasibility of spectroscopic-based techniques in terms of the evaluation of the external qualities of tomatoes should be further investigated.

Table 1. Summary of recently published studies for the quality and safety evaluation of tomatoes using spectroscopic-based techniques.

Approach	Quality Parameters	Data Analysis	Accuracy/Results	References
Vis-NIR	Color, titrable acidity, dry matter	PCA, PLS	RMSEP = 2.89, $R_p^2 = 0.94$, SDR = 4.11 (color) RMSEP = 0.46 %; $R_p^2 = 0.59$ % SDR = 1.92 (dry matter) RMSEP = 0.07 %; SDR = 1.15 (TA)	[22]
Vis/NIR	Classification	PCA, SIMCA, DPLS	100% accuracy	[23]
Vis/NIR	Lycopene content and color properties based on L^* , a^* , a^*/b^*	ANOVA	$R^2 = 0.94, 0.90, 0.87$, and 0.91 (L^* , a^* , a^*/b^* , & (TCI) $r_{cv}^2 = 0.92-0.96$ RMSE _{cv} = 12.3-17.1 (Lycopene content)	[24]
Vis/NIR	SSC	PLSR	$R_p = 0.85$ to 0.87 RMSEP = 0.20 to 0.35	[25]
Vis-NIR	Sensory quality	PLSR, SWSR	$r = 0.92$	[26]
Vis-NIR	total soluble solids (TSS), acidity (pH), titratable acidity (TA), and lycopene content	PLS	$R^2 = 0.77$ (TA) $R^2 = 0.79$ (lycopene) $R^2 = 0.85$ (TSS) $R^2 = 0.82$ (pH)	[27]
Vis-NIR	SSC, TA, lycopene	PLSR	$R^2 = 0.91$ (SSC) $R^2 = 0.73$ (lycopene)	[28]
Vis/NIR	soluble solids content (SSC), titratable acidity (TA), taste (SSC/TA) and firmness	PCA, PLS	$R^2 > 0.85$ (For all quality parameters except for firmness)	[29]
Vis-NIR	detection of Tomato chlorosis virus	NCA	88.3% to 100% overall accuracy	[30]
Vis/NIR	detection of tomato pesticide residues	PLSR, ANN	RC = 0.988, RP = 0.982, RMSEC = 0.141, RMSEP = 0.166	[31]

NIR	lycopene, b-carotene, total phenolic content (TPC), total flavonoids content (TFC), and firmness	ANOVA, LSD, PCA	$R^2 = 0.834$ (TPC) $R^2 = 0.864$ (lycopene) $R^2 = 0.790$ (TFC) $R^2 = 0.708$ (b-carotene) $R^2 = 0.679$ (firmness)	[32]
NIR	Taste-related compounds	PLS	RMSEP<6.1%, 13.3%,14.1% 12.7%, 13.8%, 21.9% (for SSC, fructose, glucose, citric acid, malic acid, glutamic acid, respectively)	[33]
NIR	SSC	PLS	RMSE=0.32% (cross-calibration, prediction)	[34]
NIR	textural properties, alcohol insoluble solids, soluble solids content of the tomatoes	PCA, SIMCA, PLS	96.85% accuracy (PCA) 100.00% accuracy (SIMCA)	[35]
NIR	Chemical and sensory properties	PLS	$R^2 = 0.97$ (fructose, glucose, soluble solids content, and dry matter) $R^2 = 0.702$ to 0.917 (taste-related attributed) $R^2 = 0.009$ to 0.849 (texture-related attributes)	[36]
NIR	Total sugar	PLS	$R = 0.930$ RMSECV=0.466% PMSEC=0.469%	[37]
NIR	SSC, lycopene	PLS	$R_p = 0.8988$ (SSC) $R_p = 0.8023$ (lycopene)	[38]
NIR	sugars, acids, soluble solids, titratable acidity, and pH	PLSR	$R_{val} > 0.80$; <10% SEP	[39]
NIR	firmness, SSC, pH	PLS, SVM, ELM, MSC, SNV	$R_p^2 = 0.9666$ (firmness) $R_p^2 = 0.9179$ (SSC) $R_p^2 = 0.8519$ (pH)	[40]
NIR	SSC, pH	MSC, PLS	$RC = 0.92$, RMSEC=0.0703°Brix, RMSEP=0.150°Brix, RMSECV=0.138°Brix (SSC) $RC = 0.90$, RMSEC=0.0333, RMSEP=0.0316, RMSECV=0.0489 (pH)	[41]
NIR	SSC, fructose, glucose, titratable acidity (TA), ascorbic, citric acid contents	PLSR	$R_p = 0.87$ (SSC) $R_p = 0.83$ (glucose) $R_p = 0.87$ (fructose) $R_p = 0.81$ (ascorbic acid) $R_p = 0.86$ (citric acid)	[42]
Raman	disease detection	PCA	>75% accuracy (14 days after inoculation) >85% accuracy (8 days after inoculation)	[43]
Raman	maturity index	PLS	93.8 classification accuracy	[44]
Raman	carotenoids quantification	SIMCA, ANN, PLSR	93% classification accuracy (SIMCA) 100% classification accuracy (ANN)	[45]
Raman	carotenoids composition	PLSR	$R^2 = 0.94$	[46]
Raman	pesticide residue determination	PCA	Accuracy was not specified	[47]
Raman	carotenoids characterization	PCA-PLSR	RMSE=11.7%	[48]
Raman	Tomato freshness	PLSR	85.6% accuracy	[49]
Raman	Infection detection	PLS	80% accuracy	[50]
Raman	Pesticide residue detection	LSSVM	R_p^2 up to 0.960	[51]
Raman	Pesticide residue detection	PLS, PCA	99.86% accuracy	[52]
Raman	Pesticide residue detection	PLSR	93.2% to 99.3% accuracy	[53]
FT-NIR	Textural property	PLSR	$R^2 = 0.7$ to 0.97, RPD=1.8 to 6.1	[54]
FT-NIR	Surface and overall elasticity	Not identified	$R^2 = 0.75$ to 0.88	[55]

FT-MIR	Taste-related compounds	PLS	$R^2 > 0.84$ (SSC, fructose, glucose, and citric acid)	[56]
ATR-FTIR	Ripening stages	SVM	99%-100% accuracy	[13]

SIMCA, soft independent modeling of class analogy; **PCA**, Principal component analysis; **DPLS**, discriminant partial least squares; **R²**, coefficient of determination; **NCA**, Neighborhood component analysis; **MSC**, Multiplicative signal correction; **MSC**, multiplicative scattering correction; **ELM**, extreme learning machine; **SVM**, support vector machine; **SNV**, standard normal variate; **SWSR**, stepwise selectivity ratio; **PCR**, Principal Component Regression; **ATR-FTIR**, Attenuated total reflection Fourier-transform infrared; **LSSVM**, least squares support vector machine; **ELM**, Extreme learning machine;

5. BENEFITS AND DRAWBACKS

The applications of spectroscopic-based techniques for the quality and safety evaluation of tomatoes offer both benefits and drawbacks. On the one hand, these techniques provide a non-destructive and rapid approach to determining the chemical and physical characteristics of tomatoes, enabling a more efficient and reliable evaluation of their quality and safety. The use of spectroscopy eliminates the need for time-consuming and costly laboratory analyses, which can save time and reduce costs for tomato producers and processors. Moreover, the information obtained through spectroscopy can aid in the optimization of processing and storage conditions to maintain the quality and safety of tomatoes. However, there are also some limitations associated with the use of spectroscopic-based techniques, such as the need for extensive and representative calibration datasets and the potential for interference from external factors such as environmental conditions. Additionally, the cost of equipment and the need for specialized knowledge to operate and interpret the results can pose a barrier to widespread adoption. In brief, while spectroscopic-based techniques offer great potential for the quality and safety evaluation of tomatoes, it is important to carefully consider their benefits and limitations to optimize their use in practice.

6. FUTURE PERSPECTIVES

In recent years, there has been increasing interest in the use of spectroscopic-based techniques for the evaluation of the quality and safety of agricultural products, including tomatoes. Spectroscopy offers a non-destructive and rapid approach to determining the chemical and physical characteristics of tomatoes, allowing for a more efficient and reliable evaluation of their quality and safety. Spectroscopic-based techniques, such as near-infrared spectroscopy (NIRS), Raman spectroscopy, and fluorescence spectroscopy, have been successfully used for the assessment of various parameters related to tomato quality and safety, such as nutritional content, ripeness, and the presence of contaminants such as pesticides and pathogens. Despite the promising results, there are still challenges to be addressed, such as the need for more accurate and robust calibration models and the standardization of analytical protocols. Nevertheless, the future perspectives for the application of spectroscopic-based techniques in the tomato industry are bright, with the potential for the development of portable and user-friendly devices for on-site and real-time evaluation of tomato quality and safety. These advancements will not only benefit the

tomato industry but also have broader implications for food safety and security.

7. CONCLUSIONS

In conclusion, the applications of spectroscopic-based techniques have shown great potential for the quality and safety evaluation of various agricultural products, including tomatoes. Among the different spectroscopic-based techniques, NIR, FTIR, Raman, and Vis-NIR have emerged as the most prevalent ones according to the published studies. Recent studies underlined the applications of spectroscopic-based techniques for rapid and non-destructive evaluation of internal qualities of tomatoes. This means that future studies should focus further on evaluation of external qualities such as textural properties, color properties, classification and detection.

Although, these techniques provide a non-destructive and rapid approach to determining the chemical and physical characteristics of tomatoes, enabling a more efficient and reliable evaluation of their quality and safety. However, the successful implementation of spectroscopic-based techniques for tomato evaluation requires careful consideration of the benefits and drawbacks of each technique, as well as proper calibration and validation of the models. Future research should focus on improving the accuracy and robustness of calibration models, standardizing analytical protocols, and developing portable and user-friendly devices for on-site and real-time evaluation of tomato quality and safety. Overall, the applications of spectroscopic-based techniques have the potential to revolutionize the tomato industry, as well as the food safety and security landscape more broadly.

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