Critical Reviews in Biotechnology

ISSN: 0738-8551 (Print) 1549-7801 (Online) Journal homepage: www.tandfonline.com/journals/ibty20

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To cite this article: Ravi Pandiselvam, Alev Yüksel Aydar, Zeynep Aksoylu Özbek, Didem Sözeri Atik, Özge Süfer, Bilge Taşkin, Emine Olum, Seema Ramniwas, Sarvesh Rustagi & Daniel Cozzolino (2025) Farm to fork applications: how vibrational spectroscopy can be used along the whole value chain?, Critical Reviews in Biotechnology, 45:4, 938-981, DOI: 10.1080/07388551.2024.2409124

To link to this article: https://doi.org/10.1080/07388551.2024.2409124

Published online: 04 Nov 2024.

CRITICAL REVIEWS IN BIOTECHNOLOGY
2025, VOL. 45, NO. 4, 938–981
https://doi.org/10.1080/07388551.2024.2409124

REVIEW ARTICLE

Farm to fork applications: how vibrational spectroscopy can be used along the whole value chain?

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ABSTRACT
Vibrational spectroscopy is a nondestructive analysis technique that depends on the periodic variations in dipole moments and polarizabilities resulting from the molecular vibrations of molecules/atoms. These methods have important advantages over conventional analytical techniques, including (a) their simplicity in terms of implementation and operation, (b) their adaptability to on-line and on-farm applications, (c) making measurement in a few minutes, and (d) the absence of dangerous solvents throughout sample preparation or measurement. Food safety is a concept that requires the assurance that food is free from any physical, chemical, or biological hazards at all stages, from farm to fork. Continuous monitoring should be provided in order to guarantee the safety of the food. Regarding their advantages, vibrational spectroscopic methods, such as Fourier-transform infrared (FTIR), near-infrared (NIR), and Raman spectroscopy, are considered reliable and rapid techniques to track food safety- and food authenticity-related issues throughout the food chain. Furthermore, coupling spectral data with chemometric approaches also enables the discrimination of samples with different kinds of food safety-related hazards. This review deals with the recent application of vibrational spectroscopic techniques to monitor various hazards related to various foods, including crops, fruits, vegetables, milk, dairy products, meat, seafood, and poultry, throughout harvesting, transportation, processing, distribution, and storage.

ARTICLE HISTORY
Received 4 July 2023
Revised 28 June 2024
Accepted 8 August 2024

KEYWORDS
Food safety; Fourier transform infrared spectroscopy; Infrared spectroscopy; Nondestructive methods; Raman spectroscopy; Value chain; Vibrational Spectroscopy

Introduction

The current worth of the global food system is around $8 trillion, which represents around 10% of the worldwide economy. As a result, the quality of food and food products affects not only end customers but also millions of employees and entrepreneurs in the global food business. To achieve the best possible food quality across all involved processes, it is necessary to constantly trace and monitor numerous critical environmental factors that may have a substantial impact on the product's quality [1]. The growth and globalization of the market necessitate that every organization seeks assurance in its supply chain to ensure that the manufactured products meet specifications. Production quality is considered a socio-economic category and is perceived as a collection of properties and characteristics that aim to satisfy the ever-increasing consumption needs and demands of customers. The foundation of global food safety policies is health insurance coverage for all consumer groups. The assurance of food safety, which is the most important aspect of quality, must be regarded as an integral part of all management activities [2].

Numerous factors, including preserving public health, promoting consumer confidence, and facilitating international trade, make ensuring the quality and

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safety of food of the utmost significance. The primary reason for prioritizing food quality and safety is to safeguard public health. Foodborne illnesses pose a significant global burden, resulting in substantial morbidity and mortality. Every year, contaminated foods cause 600 million cases of foodborne disease and 420,000 deaths worldwide. Children under the age of five account for 30% of all foodborne deaths. The World Health Organization estimates that, 33 million years of good life are lost owing to eating unsafe food each year, and this figure is certainly an underestimation. The incidence of food-borne infections is highest in developing countries, but it is still very common in wealthy countries as well [3]. Over 128,000 people are hospitalized in the U.S. alone, and 3000 people die from the foodborne illness [4,5]. The typical restaurant inspection process has little influence due to the predictability and infrequent nature of inspections as well as the dynamic nature of the cooking environment, even if food safety violations are preventable with adequate procedures. Despite this fact, the inspection procedure has mainly not changed over the years. Food safety has even been named as one of seven "winnable battles" by the Centers for Disease Control and Prevention, but progress has been slow so far [5].

Ensuring food quality and safety is vital for maintaining consumer confidence and trust in the food industry. Consumers expect that the food they purchase and consume is safe, nutritious, and accurately labeled. It is absolutely necessary, in order to lower the number of illnesses caused by foodborne pathogens, to understand the behaviors of consumers and how they handle high-risk foods in their own homes. According to Smigic et al. [3] social network-distributed awareness-raising initiatives may significantly enhance people's daily routines, hence lowering risk. Additionally, it is crucial to improve customer awareness of food labeling. Second, in addition to raising consumer awareness generally, it is also necessary to facilitate and enhance consumer-facing messages from food producers [3,6]. Any breach of this trust can have significant consequences, including loss of reputation, decreased consumer loyalty, and negative economic impacts. Liu er al. [7] revealed that, consumers' perceptions of food safety significantly influence their purchasing decisions. By upholding high standards of quality and safety, food businesses can establish trust with consumers and enhance their reputation.

The economic impact of compromised food quality and safety cannot be understated. Foodborne illnesses result in substantial healthcare costs, productivity losses, and reduced consumer confidence. Risk assessment should be used to identify risk factors in order to lower the socioeconomic costs associated with foodborne disease. According to conservative estimates, the average case of a foodborne disease costs $1068 and has a $51.0 billion yearly economic burden in the U.S. [4]. Moreover, when countries fail to meet food safety standards, it can lead to trade disruptions, import bans, and reduced market access. By ensuring high food safety standards, countries can enhance their competitiveness in the global market and protect public health simultaneously. Globally, food quality and safety standards are enforced by legal and regulatory frameworks that are among the most stringent in the world. To make sure that certain quality and safety standards are met, these rules set forth principles for the food industry to follow. The failure to comply with these regulations may result in fines, product recalls, or even the closure of the business. In addition, the Codex Alimentarius Commission's international standards help to streamline international trade by standardizing food safety rules worldwide [8]. In the past quarter of the century, the concept of sustainability, as well as the concept of sustainable development, has emerged as an essential component in the management of food production and consumption. It is of the utmost importance that food and agricultural systems be sustainable. The production of food, feed, and fiber in an environmentally responsible manner in order to attain food security is the primary focus of sustainable agriculture, which has been embraced as the ultimate policy aim by a significant number of states all over the world [9].

Moreover, sustainability has emerged as a crucial consideration in the food system. A sustainable food system shown in Figure 1 is one that ensures food security and nutrition for everyone in terms of economic, social, and environmental dimensions. This creates food security and nutrition for future generations that is profitable (economic sustainability), has significant positive effects on society (social sustainability), and has a favorable or neutral impact on the environment (environmental sustainability) [9,10]. It involves responsible resource management, waste reduction, and the preservation of the environment for future generations. In the context of food, sustainability encompasses various dimensions, such as sustainable agricultural practices, waste reduction, and the conservation of biodiversity. Prominent international organizations and reports have highlighted the urgent need for sustainable food systems. The Food and Agriculture Organization of the United Nations (FAO) categorized the effects of sustainable food systems as social, economic, and environmental effects. The FAO also highlighted the significance of sustainable

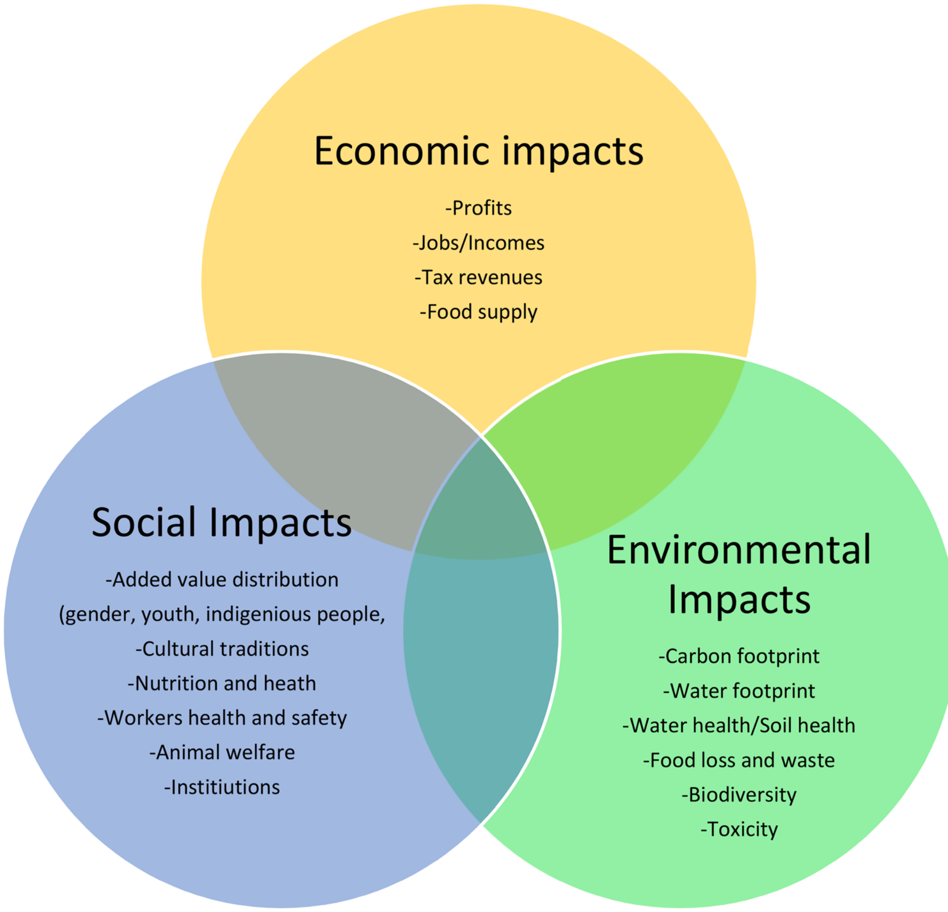

Figure 1. Sustainability in food systems [10].

agriculture in addressing issues, such as food security, biodiversity loss, and climate change [10]. Ensuring food quality and safety is crucial for safeguarding public health, maintaining customer confidence, sustaining economic stability, and complying with legal and regulatory standards. It is possible to lessen the amount of food that is lost or wasted and enhance both the quality and the level of safety of the food that is available to consumers by improving the management of the information flow associated with food logistics. By implementing robust quality control measures, safety standards, and effective monitoring systems, the risks associated with foodborne illnesses can be minimized, fostering a healthier and more sustainable food system [9].

Vibrational spectroscopic methods like Fourier-transform infrared (FTIR), infrared (IR), near-infrared (NIR), mid-infrared (MIR), Raman, and surface enhanced Raman (SERS) spectroscopy are crucial for analyzing the vibrational modes of molecules across the electromagnetic spectrum. Among all vibrational spectroscopic methods, IR and Raman are the primary techniques used in various scientific fields for the analysis and characterization of molecules [11,12]. In IR spectroscopy, molecules are irradiated with infrared radiation, causing the vibrational modes of the molecule to absorb energy. The absorption of IR radiation results in the excitation of these vibrational modes, providing information about the molecular structure and functional groups present in the sample. IR spectroscopy is commonly used in organic and inorganic chemistry, biochemistry, pharmaceuticals, and materials science for identification, quantification, and structural analysis of compounds. It's particularly useful for detecting functional groups, such as -OH, $-NH_2$, -COOH, etc.. On the other hand, Raman spectroscopy relies on the inelastic scattering of photons when they interact with the vibrational modes of molecules [11]. Unlike IR spectroscopy, Raman spectroscopy does not rely on the absorption of photons, but rather on their scattering. This technique provides complementary information to IR spectroscopy and is often used to identify molecules that may not have strong IR absorption bands or to differentiate between different structural isomers. Raman spectroscopy finds applications in materials science, pharmaceuticals, forensic analysis, and environmental monitoring. The methods provide an in-depth knowledge of molecular structures, compositions, and interactions [12]. Vibrational spectroscopy allows for quick and non-intrusive analysis throughout the agricultural process to the final product, assisting in quality assurance, safety assessment, and verification of authenticity [1,2].

Over the last several years, it has been widely implemented across the whole food production chain, from the farm to the fork. Although the literature has examined the fundamental principles, and practical implementations of vibrational spectroscopy in modern analytical chemistry and food science, it has not sufficiently discussed the transformative capacity of these methods in the food industry. This review stands out for its innovative application of vibrational spectroscopy to monitor food safety and quality specifically during transportation—a phase often overlooked in previous research. Unlike earlier studies that typically focus on static environments or single food types, this paper conducts a comprehensive analysis across various food categories, such as fruits, dairy, meat, and seafood, demonstrating broad applicability. It uniquely emphasizes real-time, nondestructive, and on-site testing using portable spectroscopic devices, which contrasts with the traditional laboratory-based or stationary equipment highlighted in earlier studies. Additionally, the integration of advanced data analysis techniques, such as chemometrics and machine learning, sets this work apart by enhancing accuracy and predictive capabilities for detecting food adulteration and spoilage during transit. These advancements offer a practical and immediate solution for ensuring food safety and quality in dynamic and high-risk environments, distinguishing this paper from the more theoretical or limited applications explored in previously published papers.

Thus, the present review aims to provide a comprehensive analysis of vibrational spectroscopic methods and their applications in various fields, with a focus on food processing. In addition, the technological advancements and capabilities of FTIR, NIR, Raman, and related techniques are summarized, emphasizing their significance in identifying molecular composition and elucidating chemical reactions.

Role of farm-to-fork applications in tracking food journeys from farm to consumer's fork

Processing, packaging, distribution, and retail sales are all examples of activities that are included in the definition of food systems as chains of activities that stretch from the point of food production (also known as "the farm") to the point of food consumption (also known as "the fork"). Numerous political, economic, sociocultural, and environmental factors all have an impact on these activities to varying degrees [13]. The capacity to track the origin of food is crucial for assuring its high quality and safety in today's world. The ability to track an animal, commodity, food item, or component from its origin to its final destination in the supply chain, and vice versa [11,14,15].

By implementing robust quality control measures and safety standards throughout the food supply chain, the risk of microbial contamination, chemical hazards, and foodborne outbreaks can be minimized. Farm-to-fork applications refer to technological tools and systems that enable the tracking and tracing of food journeys from the consumer's fork back to the farm where the food was produced. These applications provide transparency and visibility into the entire food supply chain, allowing consumers, producers, and regulators to gather information about the origin, production practices, and transportation of food items. Blockchain technology, Radio Frequency Identification (RFID), quick responds Codes and Mobile Apps, IoT (Internet of Things) Sensors and Data Analytics and Data Sharing Platforms are some of the farm-to-fork applications used for tracking [16–18].

It is critical to develop and apply the idea of sustainable diets in various contexts (industrialized and transition nations) in order to assure food security and quality, particularly in the Mediterranean region. In contrast to the common "farm-to-fork" approach (from production to consumption) for improving food systems in terms of food safety and nutrition, the MEDINA research project "Promoting sustainable food systems in the Mediterranean for good nutrition and health" proposed a "fork-to-farm" conceptual framework. The group identified issues that could be incorporated into the initial framework, such as nutrient bioavailability and exposure to contaminants and agriculturally active substances, and that could help with the creation of ambitious agricultural, food, and health policies as well as the prioritization of actions [13].

The application structure for food traceability employing RFID and blockchain technology is shown in Figure 2. Blockchain is a decentralized and transparent digital ledger that enables the secure recording and tracking of transactions. It can be applied to food supply chains to create an immutable record of each stage, from fork to farm. This technology allows stakeholders to trace the movement, storage conditions, certifications, and other relevant data of food products. To guarantee the safety of agri-food tracking data, the best possible decisions about food production were made using a blockchain-based agriculture security chain framework [19]. RFID tags

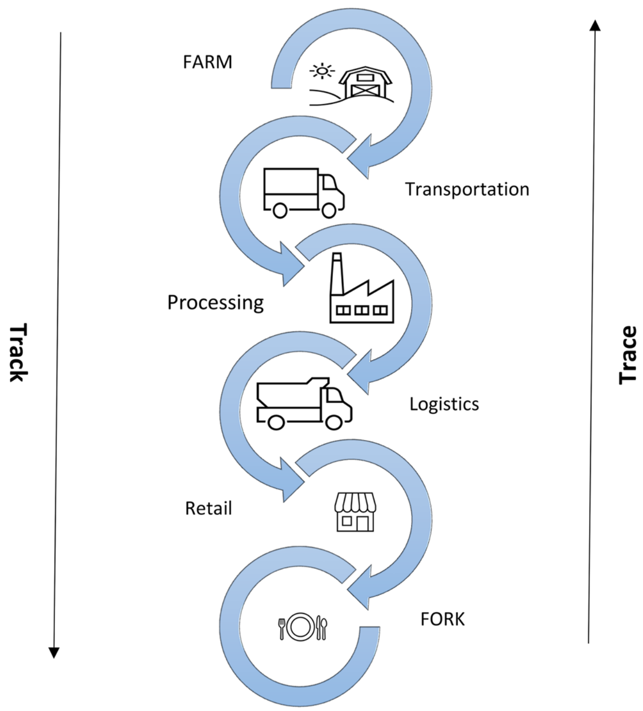

Figure 2. Farm to fork traceability approach.

are small electronic devices that use radio waves to identify and track objects [12]. They can be attached to food packaging or pallets to provide real-time data about the location and movement of products throughout the supply chain. These intelligent RFID devices have the ability to detect changes in food qualities, such as pH, conductivity, dielectric constant, humidity, temperature, gas, etc., and then send the recorded information to the central control system [12]. RFID systems facilitate rapid and accurate identification, reducing manual labor and improving traceability [9]. RFID is used in different areas, such as food freshness monitoring, tracking and monitoring the differences between RFID and wireless sensor networks and the possibility of combining the two technologies [12,14,15].

The IoT is a network of dedicated sensors connected to the Internet that can detect and prevent problems in the food industry [1]. IoT sensors can be embedded in food packaging or storage facilities to monitor temperature, humidity, light exposure, and other environmental factors that affect food quality and safety. Real-time data from these sensors can be collected and transmitted to a centralized system, enabling stakeholders to track the conditions in which the food has been stored and transported [15]. Quick response (QR) codes are scannable barcodes that can be printed on food packaging. Consumers can use their smartphones to scan the code, which directs them to a dedicated mobile application or website providing detailed information about the food's journey, including its source, production methods, and quality certifications [20].

Advanced analytics and data sharing platforms enable the aggregation and analysis of vast amounts of data collected throughout the supply chain. These platforms provide insights into food traceability, allowing stakeholders to identify bottlenecks, optimize processes, and ensure compliance with food safety and sustainability standards. In addition to all of these technologies, DNA barcoding, isotope analysis, chemical analysis, and biological analysis that are determined using vibrational spectroscopic techniques are also utilized in the food traceability process [21].

Use of vibrational spectroscopy in the farm

Identifying potential problems with crops

It is expected that within 25 years from now, the global population will reach over 10 billion people. In order to accommodate the growing population, there has been a significant surge in food production that has been increasing at an exponential rate. Although the goal of sustainable agriculture is likely to be seriously threatened by the scarcity of land and water and climate change, one of the Sustainable Development Goals of the United Nations is to provide food security [22]. Diseases in growing plants reduce a considerable portion of the productivity, and this situation drives attention to find effective methods in the detection of plant disease. An early diagnosis of the type of plant illness is necessary to give efficient procedures for detection and avoidance of destruction. Nowadays, significant efforts have been made to specify plant defects that impact various crops, such as viruses and fungus infections. When the root cause is unknown, before it has spread to a critical manufacturing area, this becomes a serious problem [23] (Figure 3).

Up to 50% of global agricultural yield can be prevented with prompt diagnosis of plant pathogens. There are numerous limitations in common molecular and imaging techniques to diagnose and characterize diseases seen in plants [24]. The agriculture and food sector has been interested in using nondestructive methods, such as vibrational spectroscopy and spectral imaging techniques. Vibrational spectroscopy-based methodologies have been advanced, making it possible to test multiple parameters quickly and easily without causing any damage. Recent reports have shown, how well vibrational spectroscopy and spectral imaging methods can be used in conjunction with data analytics (Figure 4), such as chemometrics [25–29]. Chemometrics is the qualitative and quantitative

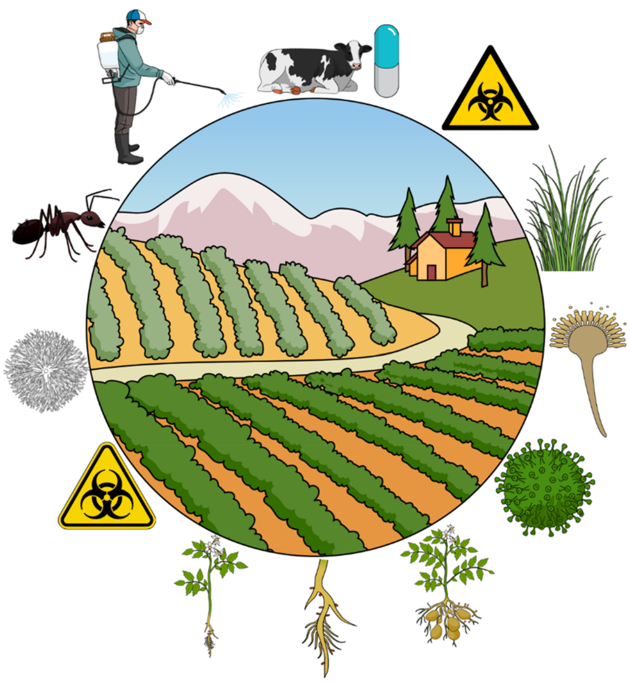

Figure 3. Serious problems of crops and products occurred in a farm. (created by Mind the Graph)

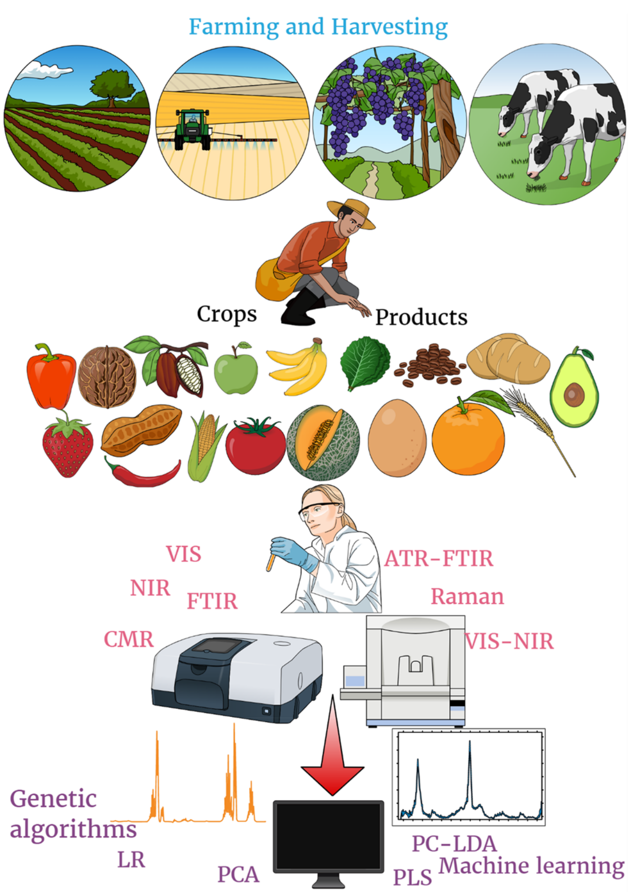

Figure 4. General view of vibrational spectroscopy applications in farm. (created by Mind the Graph)

extraction of relevant information from spectroscopic data and can provide a statistical context and confidence for the precise identification of compounds of interest, which can help researchers make decisions and gather evidence for further studies. Pre-processing is essential for statistical analysis, and changes are required for data obtained by FTIR and Raman spectroscopy. Unsupervised methods like principal component analysis (PCA) do not have user-defined tags, even though supervised ones (for instance linear discriminant analysis, LDA and partial least squares-DA, PLS-DA) use a user-defined data tag algorithm to process the collected data and give excellent segregation and identification capabilities [30]. Figure 3 visualizes the general flowsheet of vibrational spectroscopy combined with chemometrics in farming and harvesting applications.

According to Table 1, several diseases, such as canker [31–33], huanglongbing [34,35], late blight [36,37], leaf blight [38], wilt [39,40] and wheat blight [38,41] were diagnosed, as well as pathological disorders [37,42–50], and insect/weed infestation [51–53] by different spectroscopic techniques. Raman spectroscopy has emerged as a prominent analytical technique that employs nondestructive laser-based methods. It has shown remarkable potential in detecting plant diseases, identifying abiotic stressors, enabling label-free phenotyping, and facilitating digital plant selection in breeding programs, as evidenced by Table 1 [54]. Visible-near infrared (VIS-NIR) spectroscopy is the second reliable method for identifying stress and disease in plants (Table 1), but it contains some restrictions and challenges. One of the biggest challenges that researchers encounter when collecting data is the environmental component. While collecting data outside, variation and noise can skew the results of spectral reflectance measurements, leading to mistakes and unneeded information. Checking, controlling, or taking into account environmental elements including temperature, humidity, and light intensity are significant for preventing these situations [55]. On the other hand, intelligent technology can be used in smart agriculture to monitor the distribution of weeds precisely in the field and undertake weed control operations in specific regions, while increasing both economic benefits of agricultural goods and efficacy of pesticides. Convolutional neural network (CNN), support vector machine (SVM) and artificial neural network (ANN) are just a few machine learning (MAL) techniques, that have been used for data processing [56]. K-nearest neighbors (KNN) [42] and soft independent modeling by class analogy (SIMCA) [34,35,57] algorithms are

Table 1. A comparative overview of vibrational spectroscopy techniques for monitoring several crop defects.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/ or accuracy	Reference
Apple	60	*Valsa mali Miyabe* et Yamada	NIR, Raman	NIR: 900–1700 nm Raman: 0–2000 cm^{-1}	PCA, CARS, air-PLS, LS-SVM	Methods were promising for detecting apple valsa canker disease in an early period.	NIR Classification: 94.67 and 97.33% Raman Classification: 89.33 and 89.33%	[31]
Banana	27	*Fusarium* wilt	Raman	350–2000 cm^{-1}	PLS-DA	*Fusarium* disease can be diagnosed fast by Raman spectroscopy.	76% ≤Accuracies≤ 100%	[39]
Citrus	96–168	Huanglongbing	Raman	600–1800 cm^{-1}	OPLS-DA, SIMCA	Suggested also for other crops	Grapefruit Accuracy: 100% Orange Accuracy: 94%	[34]
Coffee bean (Robusta)	200	*Aspergillus ochraceous*	NIR	900–1700 nm	PCA, LDA, SVM, KNN, DT, NB, QDA	Early monitoring of fungal contamination, and DT gave optimal results.	PCA score: 85.99% Accuracy_{DT}: 97.5% Classification rate_{DT}: 100%	[42]
Kiwi	504	Canker	HSI	325–1075 nm	FDA, GLM, PLS, SVM	Helpful for diagnosis of *Pseudomonas syringae* pv. *actinidiae*	Overall accuracy: 85%, Kappa score: 0.70, F-measure: 0.84	[32]
Milk (raw)	28	Whey	Raman	700–4000 cm^{-1}	PCA, PLS	Enabled quality control of milk.	PCA score: 79.86%, R^2: 0.992, RMSEP: 0.777, RPD: 13.894, Bias: 0.557	[61]
Maize	892	Fungi	HSI-NIR	1150–1700 nm	PCA, SPA, SVM	Spatial data about infected grains were obtained by pixel-wise (PW) classification.	PW-PCA-SVM Accuracy: 92.00–99.32% PW-SPA-SVM Accuracy: 100%	[62]
Maize	–	*Colletotrichum graminicola*	Raman	375–1698 cm^{-1}	PLS-DA	Viable tool	Leaf-based Accuracy: 73% Stalk-based Accuracy: 92%	[43]
Orange	48–84	Huanglongbing	Raman	350–2000 cm^{-1}	OPLS-DA, SIMCA	Raman was able to detect canker with great accuracy levels.	87.7% ≤Accuracies≤ 96%	[35]
Potato	154	Pathogen	HSI	350–2500 nm	PCoA, PLS-DA	Early detection of *Phytophthora infestans* and *Alternaria solani*	Internal CV Accuracy ≥ 91.3%	[44]
Potato	270	Late blight	VIS-NIR	350–1000 nm	PLS, SVM, KNN, DT, CARS	Early and on-line screening of potato disease	Best accuracy: 99%, $R^2_{prediction}$: 0.961–0.997	[37]
Potato	200	Late blight	VIS-NIR	400–2400 nm	PCoA, PLS-DA, RF, NDSI	Enabled better understanding of interactions between host and pathogen.	PcoA score: 93% PLS-DA Accuracy: 65.09–83.10% RF Accuracy: 61.68–71.13%	[36]
Potato	60	Verticillium wilt	NIR	1596–2396 nm	ANN	High potential for detection	Model 1 R: 0.76–0.89 Model 2 Accuracy: 84–94%	[40]

(*Continued*)

Table 1. Continued.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/ or accuracy	Reference
Rice	287	Weed, grass	HSI	380–1080 nm	RF, SVM	415–1007 nm wavelengths were suitable for designing an optical sensor for *Echinochloa crusgalli* and *Oryza sativa f. spontanea*.	Recognition rate: 92–100%	[51]
Rice	2376	Leaf blight, rice blast, rice sheath blight	HSI	400–1000 nm	PCA, SVM, CNN	Data fusion can be applicable for detecting rice diseases.	Accuracy > 93%	[38]
Rice	842	Rice sheath blight	NIR	1348–2551 nm	PLS-DA, SVM	Promising tool for diagnosing diseases in field	PLS-DA Total performance: 0.642–0.643	[41]
Sorghum grains	108	Insect	NIR	4000–10 000 cm^{-1}	PCA, PLS-DA	Fast, cheap and non-invasive detection of *Sitophilus zeamais* Motschulsky	Accuracy: 97.1–100%	[52]
Sugarcane	590	Monocotyledons, dicotyledons	VIS-NIR	450–2500 nm	SIMCA, RF	New approach can enable weed mapping.	SIMCA Accuracy: 97.4%, Sensitivity: 81%, Specificity: 99.4% RF Accuracy: 97.4%, Sensitivity: 88.2%, Specificity: 98.3%	[57]
Tomato	300	*Liberibacter*	Raman	350–2000 cm^{-1}	PLS-DA	A portable diagnostic device was recommended for detecting structural changes arising from related bacterial disease in several crops.	*Candidatus Liberibacter solanacearum A* Accuracy: 70% *Candidatus Liberibacter solanacearum B* Accuracy: 78.8%	[45]
Tomato	40	*Botrytis cinerea, Solanum lycopersicum*	ATR-FTIR	900–1800 cm^{-1}	PC-LDA	Great accuracy rates were observed by this automatic decision-making platform.	Accuracy: 100%, Sensitivity: 100%, Specificity: 100%	[46]
Tomato	–	Virus	Raman	400–3100 cm^{-1}	PCA, PLS-DA	Disease monitoring can be conducted effectively by Raman spectroscopy.	Tomato yellow leaf curl virus PCA score: 59.88% Tomato spotted wilt virus PCA score: 95.90%	[47]
Tomato	60	Bacterial canker	Raman	800–1800 cm^{-1}	PCA, PC-MLP, PC-LDA	Raman was reliable to detect *Clavibacter michiganensis* subsp. *michiganensis*.	Accuracy: 0.97–0.99, Sensitivity: 1.00 Specificity: 0.88–0.95	[33]
Wheat	180	Fungi	VIS-NIR	VIS: 380–1050 nm, NIR: 950–1690 nm	PC-LDA, PLSR	Rapid prediction of toxic fungal infections	Accuracy: 91.7%, R_p^2: 0.89, RMSEP: 0.369, RPD: 3.03	[48]
Wheat	1400	Sunn pest	VIS-NIR	VIS: 400–813 nm, NIR: 950–1636 nm	PLS, DA	A more powerful model was required for assessing single kernel model.	R^2: 0.25–0.89, SECV: 2.75–10.9, Average accuracy: about 85%	[53]

(*Continued*)

Table 1. Continued.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/ or accuracy	Reference
Wheat	105	Mold	VIS-NIR with colorimetric sensor	350–1000 nm	PCA, PLS, Si-PLS, GA-Si-PLS	HBDP sensor was the most effective, and Si-PLS model was the superior.	RMSECV: 0.612–1.190, RMSEP: 0.709–1.140, $R_{prediction}$: 0.7957–0.9297, $R_{calibration}$: 0.7853–0.9762 Optimum bands RMSECV: 0.411 RMSEP: 0.709 R_p: 0.9387, R_c: 0.9762	[49]
Wheat	41	Wheat streak mosaic virus, barley yellow dwarf virus, *Triticum mosaic* virus	Raman	500–1700 cm^{-1}	PLS-DA	Raman technique was helpful for diagnosing wheat viral diseases.	Accuracy: 90%	[50]

suitable for pattern recognition, however nonlinear iterative partial least squares (NIPALS) [58] is used for PCA [59]. Furthermore, PLS regression weights are calculated and normalized by the competitive adaptive reweighted sampling (CARS) [31,37] method to select the best features [60]. The quantity of preserved features is determined by exponential decreasing function, and they are selected through adaptive reweighted sampling [60]. Examples of successful uses contain detecting weeds in vegetable crops, such as tomato and lettuce, and in grain crops like maize and wheat, with supervised or unsupervised learning [56].

Aflatoxins [63–69], ochratoxins [67,70] and deoxynivalenol [71–74] are the most important mycotoxins, which can be available in crops (Table 2), and they are poisonous substances that some species of fungi naturally create. Mycotoxins have the ability to contaminate a variety of foods, such as cereals, nuts, and spices, and pose a serious concern to humans and animals by having toxic impacts that can be acute and long-lasting. In this context, there is an urgent need for trustworthy methods for the precise and sensitive identification of mycotoxins in food and agricultural goods [75]. Although IR spectroscopy is utilized for inspecting the safety and quality of food crops, its low sensitivity and overlapping absorption characteristics preclude the detection of food contaminants directly, in small quantities. The indirect assessment has been made possible by observing fungal-induced matrix alterations with hyperspectral imaging (HSI) [73,76], besides NIR [66,69,71,74,77,78] and middle infrared (MIR) [79] (Table 2). HSI was initially created for remote sensing and satellite-based earth observation. With recent technological developments in sensing and data analysis, HSI has become well-known as a nondestructive and quick analytical method for quality assessment in crop field. Real-time photos are used to provide pertinent information regarding crop disease, enabling farmers and agronomists to remotely manage their crops [80]. Moreover, a rapidly developing analytical method is near-infrared (800–2500 nm) spectroscopy, and the data provided on the anharmonicity of molecular vibrations and intermolecular interactions have greatly helped physical chemistry. The complexity of the near-infrared spectrum has proven to be a significant obstacle. Theoretical near-infrared spectroscopy is now possible thanks to developments in anharmonic theories and computer technology [25].

In the farming of crops and cattle, pests and insects are typically controlled with pesticides and veterinary medications. Remaining residues are thought to be potentially dangerous for the health of both the environment and humans; thus, ongoing monitoring is necessary for the evaluation and regulation of pesticides and veterinary antibiotics [82,83]. Maximum Residue Limit (MRL) for several pesticides has been established by the Commission of Codex Alimentarius in order to safeguard consumer health and promote global trade. MRL is the amount of pesticide residue that is permitted by law to be present in an agricultural product, and the objective is to establish MRL values that keep pesticide residues found in food as low as is practical and safe for consumers. The MRL makes sure that pesticides are applied to commodities in line with accepted Good Agricultural Practice standards, including application rate and technique,

Table 2. Vibrational spectroscopy applications for detecting mycotoxins or mycotoxicogenic species.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Barley	107	Deoxynivalenol	NIR	4000–10 000 cm^{-1}	PCA, PLS, PLS-DA	Green technology	PCA score: 72.1% PLS RMSEC: 101.94 RMSEP: 160.76	[71]
Cocoa bean	1500	Aflatoxin B_1, Ochratoxin A	SER	550–1950 cm^{-1}	PLS, CARS	Rapid quantification of mycotoxins	Recovery: 96–110% CoV: 2.12–8.07% Linearity > 95%	[67]
Corn kernels	480	Aflatoxin	VIS-NIR	304–1086 nm	RF	Aflatoxin < 20 ppb in 374 kernels, ≥ 20 ppb in rest, and considerable classifying model potential	Accuracy: 95%, Sensitivity: 86%, Specificity: 97%	[68]
Corn silage	115	*Fusarium* and *Penicillium* toxin	NIR	1100–2500 nm	RF	Silage was discriminated according to the level of contamination.	*Fusarium* Accuracy < 90%, *Penicillium* Accuracy: 95.1%,	[77]
Maize	102	Aflatoxin	NIR	400–2500 nm	KNN, SVM	Detection of versicolorin A, was performed in a fast, cheap and practical way, without solvent and pre-treatment.	KNN Validation: 58.06–67.47% SVM Validation: 80.65–90.32% Specificity: 66.67–75%, Sensitivity: 84.21–100%, Accuracy: 80–85%	[69]
Maize	676	Fumonisins, zearalenone	NIR	400–2500 nm	PCA, PLS	In mycotoxin testing, a confirmed methodology was provided.	R: 0.809–0.991, R^2: 0.899–0.984, RMSEP: 69.4–659, SEP: 69.8–682, RPD: 2.71–3.33	[78]
Maize	15	*Fusarium verticillioides, Fusarium raminearum*	HSI-NIR	1000–2500 nm	PLS-DA	Non-destructive and non-invasive measurement	Accuracy: 100%, Sensitivity: 100%, Specificity: 100%	[76]
Maize	244	Aflatoxin	VIS-NIR, SNIR, Raman, HSI	VIS–NIR:419–1007 nm SNIR: 1007–2472 nm Raman: 374–2814 cm^{-1}	LSVM, QSVM, QDA	Cheap tools for monitoring aflatoxins fast	$Classification_{VIS-NIR}$: 82.6% $Classification_{SNIR}$: 95.7% $Classification_{Raman}$: 87%	[81]
Oat	119	Deoxynivalenol	HSI-NIR	900–1700 nm	PLS, RF	Promising tool	Accuracy: 78%, R^2: 0.75 RMSEP: 403.18	[73]
Peanut kernel	180	Aflatoxin B_1	VIS-NIR	410–1070 nm, 1120–2470 nm	PLS-DA, RF	VIS-NIR technique had potential in capturing the aflatoxin signals.	PLS-DA Accuracy: 88.57–92.86% RF-PLS-DA Accuracy: 90.00–94.29%	[63]
***Pistachiavera* nuts**	45	Aflatoxin	DRIFT	1061–1260 cm^{-1}, 1481–1570 cm^{-1}, 1721–1770 cm^{-1}, 2821–3035 cm^{-1}	PCA, DA	Useful methodology	PCA score: 84.5% DA score: 100%	[64]
Rice	105	Aflatoxin B_1	SNIR	950–1650 nm	PLS-DA	Method enabled rapid detection.	External validation R: 0.952, RMSEP: 3.362, Bias: -0.778, Most predictive models R: 0.966–0.967, RMSECV: 2.689–2.691, Bias: 0.008–0.015, Accuracy: 90%	[65]

(*Continued*)

Table 2. Continued.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Rice (brown)	120	Aflatoxin	NIR	800–2500 nm	PLS	Rapid and practical method	RMSEC: 594–673, RMSEP: 415–520, $R^2_{prediction}$: 0.9171–0.9473, $R^2_{calibration}$: 0.8627–0.8933 RPD: 3.47–4.39	[66]
Wheat	229	Ochratoxin A	FT-NIR, FT-MIR	FT–NIR: 4000–7500 cm^{-1}, FT–MIR: 400–4000 cm^{-1}	PC-LDA, PLS-DA	Related methods were reported as rapid and inexpensive.	TDR > 94%, FCR = 6%	[70]
Wheat	1266	Deoxynivalenol	NIR	950–1650 nm	Pearson, PCA, DI	DI had potential to develop accuracy and consistency of fusarium damaged material phenotyping.	Accuracy: 0.404–0.594 R: 0.588–0.594 R^2: 0.63–0.76	[74]
Wheat bran	94	Deoxynivalenol	FT-MIR, FT-NIR	FT–MIR: 350–4000 cm^{-1} FT–NIR: 10 000–4000 cm^{-1},	PC-LDA, PLS-DA	The combination of methods was effective for visualising lots of contaminated wheat bran	FT-MIR TDR: 87–91% FT-NIR TDR: 86–87%	[72]

number of applications, and cultural practices [84]. Traditional sample preparation for detecting harmful chemicals involves labor-intensive work, expensive instrumentation, and calls for much dangerous organic solvent (e.g., mass spectroscopy, liquid chromatography and capillary electrophoresis), and there is a possibility that a molecule will break down before the experimental procedure(s). Current technologies, such as SER spectroscopy [85–92] (Table 3), are straight-forward, portable, environmentally friendly, efficient, and fast [82,83]. It is possible to detect and identify molecules and chemical structures at incredibly low quantities, even in complicated sample matrices, using highly sensitive technique of SER spectroscopy. The collected spectrum information naturally comes from domains of nanometer size, since a substrate surface is necessary for the increment of Raman scattering, turning it into a nano spectroscopic technique by overcoming the diffraction limit of light [93]. SER spectroscopy substrates could be divided into three categories; nano-colloidal (e.g., gold and silver), rigid (e.g., glass and silicon) and flexible (e.g., paper and sponge) [94]. Logan et al. [88] benefited from colloidal nanogold particles for SER spectroscopy tests of pesticides in rice. After 2018, apple [85,86,92], bok choi [95,96], cabbage [97], chickpea seed [98], cherry tomato [86], eggplant [92], green pepper [92], hami melon [99], lettuce [95], mustard [95], orange [87], pear [90], rice [88,100,101], strawberry [89,102], tea [90,91,103] and tomato [92,104] have been investigated with respect to different pesticides by many vibrational spectroscopic techniques combined with chemometrics and/or MAL algorithms (Table 3).

An important technique to preserve the health of farm animals is the use of antibiotics as veterinary medications. Animal producers' unethical behavior, when administering medications has grown to be a significant contributor to the contamination of animal products [105]. This review paper explored several antibiotics which were used as veterinary drugs; florfenicol [106], tylosin [58,106–108], doxycycline hydrochloride [108], nitrofuran [109], oxytetracycline [110], tetracycline [111], fleroxacin [112], ofloxacin [113], pefloxacin [112], ciprofloxacin [113] and norfloxacin [113], diagnosed in animal products, through vibrational spectroscopy protocols, during 2019–2023 (Table 4). It is crucial to employ promising techniques like SER spectroscopy in the animal farming industry, because infractions including excessive dosage, prolonged use, and the utilization of illegal medicines during administration, are highly widespread [114].

Table 3. Vibrational spectroscopy applications for detecting pesticides.

Crop/product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Apple	–	Insecticide, Herbicide	SER	300–1800 cm^{-1}	LR	Accurate detection of Chlorpyrifos (CPF) and 2,4-Dichlorophenoxyacetic acid (2,4-D)	CPF R^2: 0.96–0.98, Recovery: 89.30–96.21 2,4-D R^2: 0.96–0.98, Recovery: 87.97–97.06	[85]
Bok choi	120	Chlorpyrifos	NIR	908–1676 nm	PCA, PLS-DA, SVM, PC-ANN	Residue of pesticide was able to be detected by portable NIR device.	Best model (SVM, PC-ANN) Accuracy: 100%	[96]
Cabbage	–	Carbendazim, chlorpyrifos	VIS-NIR	350–2500 nm	PLS, SPA, LS-SVM	LS-SVM was better, compared to PLS, and combined method was efficient.	PLS $R_{calibration}$: 0.9991, $R_{prediction}$: 0.9997, RMSECV: 1.39, RMSEP: 0.82 LS-SVM $R_{calibration}$: 0.9998, $R_{prediction}$: 1.0000, RMSECV: 0.66, RMSEP: 0.31	[97]
Chickpea seed	640	Flumioxazin, glyphosate, diquat, saflufenacil, glufosinate ammonium-	FT-NIR	4000–10 000 cm^{-1}	PC-LDA	Harvest aid chemicals can be determined accurately.	PCA score: 28.8–98.9% Specificity: 0.995–0.999, Sensitivity: 0.933–0.997, Accuracy: 0.935–0.997	[98]
Fruit (apple, pear, cherry tomato)	–	Thiabendazol (TBZ), Thiram	SER	400–2000 cm^{-1}	LR, ALS, SMA	SER with SMA may be useful for determining various analytes.	TBZ (water) R^2: 0.9740–0.9786, Thiram R^2: 0.9764–0.9961, TBZ (surface) R^2: 0.9775–0.9777	[86]
Hami melon	120	Pyraclostrobin, chlorothaloni, imidacloprid	VIS-NIR	348.45–1141.34 nm	PLS-DA, SVM, 1D-CNN	Pesticides can be identified by VIS-NIR methodology.	1D-CNN Accuracy: 95.83%	[99]
Orange	–	Thiram, malathion, phoxim	SER	500–1900 cm^{-1}	LR	A promising tool for screening pesticides	R^2: 0.9665–0.9891 Recovery: 96.5–118.9%	[87]
Pear	14	Chlorpyrifos	Raman	200–800 nm	PLS, RF	Accurate and fast detection by Raman coupled with RF	PLS R^2: 0.6985–0.8622 RMSE: 0.1193–0.1765 RF R^2: 0.8495–0.9003 RMSE: 0.1015–0.1247	[90]
Rice	85	Chlorpyrifos	SER	0–1600 cm^{-1}	PLS, SPA, SVM	Characteristic peak monitoring technique with SER was a good option.	Recovery: 97.45–103.96% $R^2_{prediction}$: 0.97 RMSEP: 2.89 RPD: 4.26	[100]

(*Continued*)

Table 3. Continued.

Crop/product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Rice	1980	Chlorpyrifos	NIR	950–1650 nm	PLS	Chlorpyrifos-methyl residues were detected both qualitatively and quantitatively by NIR method.	Rough rice R^2: 0.702–0.839 SEP: 1.763–2.374 Brown rice R^2: 0.722–0.800 SEP: 0.953–1.168 Millet rice R^2: 0.693–0.789 SEP: 0.131–0.164	[101]
Rice (basmati)	21	Pesticide	SER	400–1600 cm^{-1}	LR	Rapid detection of multiple pesticides can be performed by handheld SER spectroscopy device.	Recovery: 83.4–115.0% RSD: 3.6–23.8%	[98]
Strawberry	60	Boscalid, pyraclostrobin	NIR	4000–11 000 cm^{-1}	PCA, PLS	Promising and successful tool for rapid determination of pesticides.	PCA score: 98.1%, SEC: 0.73–3.25, SECV: 0.77–3.47, SEP: 0.83–3.22, RPD: 2.28–2.31	[102]
Strawberry	–	Endosulfan, thiabendazole, malathion thiram	SER	400–2000 cm^{-1}	PCA, PLS, FEM	Successful determination of each pesticide	Recovery: 90–122%, RSD: 1.6–6.1%,	[89]
Tea	44	Chlorpyrifos	CMR	491–2184 cm^{-1}	PLS, SVM, ANN	High potential for determining pesticide	$R^2_{calibration}$: 0.396–0.998, $R^2_{prediction}$: 0.298–0.922, RMSEC: 0.0031–0.0393, RMSEP: 0.0305–0.0821	[103]
Tea (oolong)	–	Flusilazole	SER	200–2000 cm^{-1}	PLS	Detection limit: 0.5 mg/kg, novel nanoparticle was effective.	R: 0.957–0.970, RMSEP: 0.859–0.962, RPD: 2.45–2.70, Recovery: 87–93%	[90]
Tea (oolong)	–	Phosmet	SER	200–2000 cm^{-1}	PLS	Detection limit: 0.1 mg/kg, silver nanoparticle was effective.	R: 0.927–0.934, RMSEP: 1.001–1.157, RPD: 3.79–4.20, Recovery: 94–95%	[91]
Tomato	180	Profenofos	VIS-NIR	400–1050 nm	PLS-DA	VIS-NIR was an applicable tool.	PLS R_{CV}: 0.7778–0.9295 RMSECV: 4.1379–7.6328 PLS-DA $Accuracy_{calibration}$: 84.0–90.3%, SECV: 4.1566–7.6652 $Accuracy_{prediction}$: 85.88–91.66%	[104]
Vegetable (Lettuce, mustard, bok choi)	308	Emamectin-benzoate, chlorantraniliprole and indoxacarb, carbendazim	VIS-NIR	380–840 nm	MULR	Handheld spectrophotometer can be generalized for estimation of other agrochemicals.	Emamectin-benzoate $R^2 \leq 0.80$ Chlorantraniliprole and indoxacarb $R^2 \leq 0.90$ Carbendazim $0.80 \leq R^2 \leq 0.90$	[95]
Vegetable (green pepper, tomato, eggplant) and apple	–	Thiram	SER	200–1600 cm^{-1}	LR	Detection limit: 140 pg/cm^2 for tomato and green pepper, and 2 pg/cm^2 for apple	$0.87 \leq R^2 \leq 0.96$	[92]

Ensuring the quality of the food produced

Consumers and food processors prioritize swift quality monitoring techniques prior to processing, marketing, and other post-harvest operations. Analytical methods, such as imaging and spectroscopy, which do not cause damage, are now valuable in evaluating the quality of various horticulture and food products. Generally, both internal and external properties are taken into account, when evaluating the quality of agricultural products [114].

The nutritional importance of horticultural goods as natural sources of active ingredients, such as vitamins, minerals, and fiber (can be classified under internal quality indices), makes it difficult to assess their quality and safety. They are not stable over time and develop via a series of maturation and ripening phases, before eventually becoming bad. Appearance (including color, shape, surface texture and size, actually external quality attributes) can serve as a good indicator of quality and safety characteristics. While human inspection has traditionally been relied upon for rapid and nondestructive evaluation of these products, its limitations have spurred the development of automated sorting systems that utilize machine vision. These advanced systems replace the fallibility of human perception with cameras, computers, and automated ejectors, thus providing more accurate and efficient evaluations [116].

The identification of the point at which crops reach maturity is a crucial factor in determining the ideal time for harvesting. Farmers are particularly concerned with ascertaining the optimal time to harvest their crops, as failure to do so in a timely manner, may result in significant financial losses. This is because, the optimal harvest time is determined by the moisture content of the crops at the conclusion of the growing season [117]. In addition to this, the differentiation between maturity and ripeness in fruits holds significant value. Maturity refers to the state of readiness for consumption or the potential to attain such a state after further ripening, whereas ripeness denotes the ideal state when the fruit's flavor, texture, and color have reached their maximum potential. Certain fruits, particularly those that are soft (e.g., cherries), are harvested, when they are mature but not yet ripe to avoid damage during the picking process. Moreover, various fruits continue to ripen even after being picked, leading to over-ripeness, if harvested at their peak ripeness [118].

Numerous computational techniques have been found to be efficacious in anticipating the maturity and ripeness of fruits. Certain methods necessitate the implementation of feature engineering using MAL algorithms, whereas others utilize deep learning algorithms to process unprocessed data. Each approach is predicated on a distinct feature representation of the fruit specimen for grading aims. Discriminatory features are gathered using low-cost and straightforward sensors, such as a consumer camera, or specialized and typically expensive sensors, such as an acoustic vibration detector. Nondestructive evaluations of fruit ripeness/maturity, while still on the plant are generally preferred and have garnered growing interest owing to their benefits over conventional and destructive methods [119]. Various nondestructive tools and technologies have been developed, mostly visible near infrared (VIS-NIR) spectroscopy [120,121], apart from IR [122], NIR [123], attenuated total reflection Fourier transform infrared (ATR-FTIR) [124–126], raman [125,127] and confocal micro raman (CMR) [128,129] spectroscopy, and HIS [130–134] for both maturity and ripeness identification (Table 5). FTIR spectroscopy is a vital form of IR spectroscopy utilized for acquiring detailed IR spectra encompassing a broad spectrum range. The system comprises of various essential elements, such as a radiation emitter, an interferometer, a compartment for the sample, a detector, an amplifier, an analog-to-digital converter, and a computing device. The source emits radiant energy that travels through the sample via the interferometer and reaches the detector. The amplifier strengthens the signals and translates them into digital signals that are subsequently conveyed to the computer for Fourier transformation [135]. To address limitations associated with FTIR, a novel approach known as ATR mode, involving a sampling technique based on internal reflection spectroscopy, has emerged as a potential solution [136]. Besides FTIR, the methodology of Raman spectroscopy has also been developing year by year. Raman microscopy is achieved by utilizing Raman spectroscopy in conjunction with an optical microscope. In the process of CMR spectroscopy, a focused light source originating from a point is directed through a source pinhole and splitter beam. This light is then concentrated by an objective lens onto a precise area of the specimen, limited by diffraction. The scattered or emitted light is collected and collimated by the same objective lens, then passed through a detector pinhole and sent to a spectrometer for analysis [12].

The apple is one of the most popular fruits studied in research papers focused on quality attributes diagnosed by vibrational spectroscopy in the farm. The advantages of IR and VIS-NIR spectroscopy were taken in the band range of 726–1008 nm and 300–1100 nm, respectively [120,137]. PCA (for clustering) and linear regression (LR, supervised learning) [161] were chosen

Table 4. Vibrational spectroscopy applications to specify veterinary antibiotics.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical/ computational model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Chicken meat	225	Florfenicol	SER	400–2400 cm^{-1}	LR	There were no significant differences between the results of SER and LC/MS/MS.	R: 0.9890–0.9904 R^2: 0.8534–0.9967	[106]
Chicken meat	400	Tylosin, doxycycline hydrochloride	SER	400–1800 cm^{-1}	PCA, PC-LDA, Air-PLS	Good potential of monitoring antibiotic residues	Accuracy: 100%	[107]
Duck meat	478	Tylosin, doxycycline hydrochloride	SER	50–3000 cm^{-1}	Air-PLS	SER was helpful for detecting antibiotics.	Accuracy: 100%	[108]
Honey	39	Nitrofuran	SER	0–2340 cm^{-1}	PLS	SER can be implemented in order to detection of antibiotics fast.	$R_{calibration}$: 0.9744, $R_{prediction}$: 0.9760, RMSECV: 1.0353, RMSEP: 0.9987	[109]
Honey	7	Oxytetracycline	Raman, SER	400–2000 cm^{-1}	DFTG	Perfect agreement between SER data and DFTG calculations	–	[110]
Milk (raw)	115	Tylosin	ATR-FTIR	1000–3000 cm^{-1}	PLS, MLP, NIPALS	Residues were quantified cheaply and efficiently.	R: 0.9941, R^2: 0.9882, RMPRESS: 0.1077	[58]
Milk (raw)	10	Antibiotic	Raman, FT-MIR	350–4000 cm^{-1}	PCA	Successful isolation	Raman PCA score: 57.38%, FT-MIR PCA score: 83.15–85.13%	[115]
Milk (raw)	5	Tetracycline	SER	0–2000 cm^{-1}	LR	In 10 min, in-site detection of related antibiotic was ensured.	Recovery: 98.87–112.61% RSD: 1.341–2.503% R: 0.987	[111]
Pork	–	Fleroxacin, ofloxacin, pefloxacin	Raman	400–1800 cm^{-1}	–	New method 2.5 times faster and 1/60 times cheaper, compared to gold immunochromatography.	Recovery: 86.6–95.3%	[112]
Poultry egg yolk	20	Ciprofloxacin, norfloxacin	DRIFT	400–4000 cm^{-1}	LR	Linearity range: 0.05–0.50 ng/mL, Detection limit: 0.032–1.551 ng/mL, Quantification limit: 0.028–0.194 ng/mL for ciprofloxacin and norfloxacin, respectively.	Recovery: 83.1–102.3%	[113]

as statistical tools, and dry matter content was attributed to maturation degree in the article of Toivonen and Lannard [137]. The score of PCA was absolutely agreeable (91.8%), and determination coefficient (R^2) was greater than 0.8, that is an indicator of a good fit. In other research, LDA, random forest (RF), least square-SVM (LS-SVM), and RF-successive projection algorithm (RF-SPA) were used for chemometrics purpose [120]. RF, SVM and LDA are categorized under supervised MAL algorithms, however LDA can also reduce dimensionality by unsupervised learning approach. RF and SVM are useful for regression and classification [161]. A combination of RF-SPA and LS-SVM was mentioned as more powerful than LDA method, and accuracy of superior combined MAL algorithm was nearly 90% [120].

The maturity and ripeness of grapes were investigated by Schorn-Garcia et al. [126], Pampuri et al. [122], Benelli et al. [123] and Costa et al. [144], and despite being used commonly VIS-NIR method among them, diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy was also found as applicable. DRIFT spectroscopy, a technique that nondestructively reveals the chemical and structural essence of metabolites, requires minimal sample preparation in contrast to traditional transmission geometry. This method possesses the unique ability to assess both surface and volume of sample before re-emitting it, thus enhancing the acquisition of spectral information [162].

The internal quality of fruit cannot be improved by postharvest treatments, so it is necessary to have reliable and accurate information on the influence of preharvest factors on fruit quality. Common methods in measuring: dry matter, firmness, titratable acidity and total soluble solids (TSS)s of fruit crops are time-consuming, labor-intensive, and fruit-damaging. This technique is not suitable for obtaining large-scale data or for real-time assessment and understanding of the impact of different preharvest parameters on fruit maturity and internal quality of fruit trees in the field [163]. Several papers have focused on prediction and/or assessment of internal quality attributes like firmness [147,157], TSS [122,124,126,131,138,140,141,143,144,150,153,154,156] and nutrient content [142,143,151,152,157] of crops especially fruits, with the aid of vibrational spectroscopy, as such in maturity. Also, handheld and portable spectroscopic instruments have been implemented for on-site applications to evaluate crop quality [131,140,143,149,154,155] (Table 5). Nowadays, the reduction in size of spectrophotometers while maintaining high performance has emerged as a topic of interest. Numerous commercial spectrophotometers have been created, and novel approaches have been implemented to produce more compact spectrophotometers. Particularly, NIR spectrophotometers with Fourier transform, array detection, scanning grating, filter, Hadamard transform and acousto-optic tunable filter type have been used, and advanced detection, advanced microelectro-mechanical and internet of things technique have been utilized for miniaturization of NIR spectrophotometer [164]. On the other hand, the effectiveness of SER spectroscopy in conducting on-site analyses has been enhanced through the utilization of portable Raman instruments (consists of a Raman probe, a small laser and tiny spectral system), SERS substrates (flexible, hydrophobic/superhydrophobic, liquid and with internal standard), and the integration of other advanced technologies (electrochemical and microfluidics) [165].

Use of vibrational spectroscopy in the processing facility

Analysis of ingredients to ensure their quality

Determining the quality characteristics of foods plays a critical role in the maintenance of the desired quality of products in the food industry. However, routine quality analyzes in food plants take a great amount of time with current techniques and increased cost. Chemical analyses accentuate the problems of disposal of these chemicals and infer environmental concerns. NIRS and FTIR spectroscopy, demonstrated rapid advances for the past thirty years. Accordingly food plants have been using these techniques for routine quality analyzes by directly utilizing on food itself without the use of chemicals. Raman spectroscopy has also become widely used in the food industry for more than ten years [166].

The major advantage of FTIR and NIR, which are designed to measure food chemical composition in accordance with full automation, is to provide simultaneous sample analysis during industrial production, hence, any change in quality parameters that may occur during production can be detected quickly, on-site without the need for laboratory staff. One advantage of using vibrational spectroscopy in food plants is that it allows quick action against manufacturing defects, since detection of the errors accelerated in these techniques compared to traditional methods. Another advantage of using vibrational spectroscopy in food plants is that it avoids human-induced errors that may result from traditional methods. A major problem with the traditional methods for quality analysis in production plants is that there is no chance to analyze the whole batch which results in lower accuracy. Vibrational spectroscopies offer an effective way of quality analysis simultaneously and homogeneously during production within seconds, thereby prompt action can be taken against possible quality losses in the final product.

Carbohydrate, fat, protein, and water analysis, which are the basic components of food materials, can be easily performed with FTIR and NIR as routine analyzes in processing plants. In these analyzes, food functional groups were associated with characteristic absorption bands, allowing fingerprint analysis of specific food components. For instance, carbonyl ester and C-H signals are associated with fat, amide signals are associated with protein, C-O-H bands are associated with carbohydrates, and H-O-H bands are associated with water [167].

The proliferation of spectral library data has allowed fingerprint analysis of food contaminants to be easily detected. On the other hand, it is possible to analyze the sample directly or close to its original state, without changing its structure, and without requiring intensive and complex sample preparation. Considering the rapid analysis of the sample or food ingredient through industrial production eliminates the risks that

Table 5. A comprehensive review of vibrational spectroscopy techniques for product quality.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Apple	400–500	Maturity	IR	726–1008 nm	PCA, LR	The lower dry matter was related to faster maturation in-field.	PCA score: 91.8% Dry matter R^2: 0.94 RMSE: 0.35	[137]
Apple	846	Maturity	VIS-NIR	300–1100 nm	RF, RF-SPA, LDA, LS-SVM	A reference was provided for testing apple maturity.	RF-SPA-LS-SVM Accuracy: 89.05% LDA Accuracy: 77.63–80.95%	[120]
Apple	80	TSS, dry matter	NIR	300–1100 nm	PCA, PLS	In external validation, poor results were obtained.	Internal/external validation TSS R^2: 0.50–0.82/0.06–0.81 RMSE:0.41–0.67/0.49–1.32 Dry matter R^2: 0.58–0.89/0.01–0.71 RMSE: 3.97–4.68/5.31–12.81	[138]
Avocado	690	Dry matter	NIR	720–975 nm	PLS	PLS was a useful guide.	Calibration R^2: 0.59–0.89 RMSEC: 0.85–1.72% Validation R^2: 0.31–0.88 RMSEP: 1.37–3.08%	[139]
Banana	450	Maturity, TSS	NIR	600–870 nm	MULR	NIR device had potential of testing fruit quality.	Accuracy: nearly 100%	[140]
Banana	384	Quality, ripening	VIS-NIR	350–2500 nm	RF, SVM, MP	VIS-NIR with MAL was a successive tool.	TSS R_{cv}^2: 0.90 RMSECV: 2.31 Ripening Accuracy: 74.22%	[141]
Bananito	90	Ripeness	VIS, HSI	VIS: 360–740 nm, HSI: 400–1000 nm	PCA, PLS-DA, SIMCA, K-NNR	HSI enabled accurate classification.	Classification PLS-DA: 93.3%	[130]
Bell pepper	80	Ripeness, freshness	VIS-NIR	420–2520 nm	PCA, PLS-DA, SVR, MULR	Independent from ripening status at HT, freshness can be determined.	Non-error rate PLS-DA Calibration: 80.7% CV:78% SVR Calibration: 84.7% CV:82.6%	[121]
Berry	144	Ripeness	HSI	100–400 nm	PLS	On-the-go HSI system was suitable for in-field measurements.	R^2 (Validation) TSS: 0.82 pH: 0.61 Titratable acidity: 0.81 Tartaric acid: 0.62 Anthocyanin: 0.88 Malic acid: 0.84 Polyphenols: 0.55	[131]
Chili pepper	105	Ripeness	ATR-FTIR, Raman	ATR–FTIR: 485–4000 cm^{-1} Raman: 800–1700 cm^{-1}	PCA	Effective monitoring of samples	PCA score: 81.16%	[125]
Grape	90	Ripeness	ATR-FTIR, DRIFT	650–4000 cm^{-1}	PCA, PLS, KS, ONION	A chart was prepared in order to decide the correct HT.	TSS RMSEP: 0.3–0.4 R^2: 0.962–0.986 pH RMSEP: 0.06–0.07 R^2: 0.591–0.687	[126]

(*Continued*)

Table 5. Continued.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Grape	743	Sugar content	VIS-NIR-SWIR	350–2500 nm	PLS, RF, SVR, CNN	CNN model was the best, and highest accuracy was observed in Syrah. The methodology was valuable for deciding real HT.	R^2: 0.46–0.87 RPIQ: 1.76–4.26 RMSE: 1.76–2.94	[142]
Grape	80	Maturity	VIS-NIR	450–860 nm	PLS	Optical tool gave beneficial information about real maturation level.	<u>TSS</u> RMSECV: 1.84 RMSEP: 1.90 RPD: 2.81 <u>pH</u> RMSECV: 0.18 RMSEP: 0.14 RPD: 1.85 <u>Total acidity</u> RMSECV: 3.59 RMSEP: 3.94 RPD: 2.25	[122]
Grape	429	Maturity	HSI, VIS-NIR	400–1000 nm	PCA, PLS-DA	HSI had a potential for HT prediction.	PCA score: 87% <u>Classification rate</u> Calibration: 89–91% CV: 89–91% Prediction: 86–91%	[123]
Grape	144	Composition	VSNIR	570–990 nm	PLS	TSS, anthocyanins and total polyphenols were monitored succesfully n vineyard.	<u>Calibration</u> R^2: 0.54–0.93 RMSEC: 0.607–1.119 <u>Cross-validation</u> R^2: 0.42–0.92 RMSECV: 0.664–1.248 <u>External-validation</u> R^2: 0.43–0.95 RMSEP: 0.618–1.011	[143]
Grape	432	Maturity	VIS-NIR	450–1800 nm	PCA-LDA, PCA-LDA Mahalanobis, PLS, MULR	VIS-NIR was a powerful tool.	$Accuracy_{PLS\text{-}DA}$: 93.15% $R^2_{TSS} \geq 0.90$ $R^2_{anthocyanin} \geq 0.90$ $R^2_{flavonoids} \geq 0.70$	[144]
Grape bunch	338	Maturity	FT-NIR	800–2500 nm	PLS	Internal maturity was investigated by a contactless method.	RMSEP: 0.21–19.86 $R^2_{calibration}$: 0.27–0.92 $R^2_{prediction}$: 0.07–0.71 R^2_{cv}: 0.06–0.83	[145]
Grape berry	137	Maturity	HSI, VIS-NIR	400–1000 nm	RoBoost-PLS	Roboost-PLS regression method was better.	<u>Prediction</u> Syrah R^2: 0.971–0.990, RMSE: 3.14–5.36 Fer-servadou R^2: 0.788–0.848, RMSE: 10.20–11.69 Mauzac R^2: 0.690–0.927 RMSE: 7.58–15.61	[132]
Kadam fruit	45	Ripeness	LIF, CMR	LIF: 400–800 nm, CMR: 0–2000 cm^{-1}	PCA	For both minimizing postharvest losses and maximizing quality, CMRS tests can be helpful by analyzing chlorophyll and carotenoid.	PCA score: 87.14%	[146]

(*Continued*)

Table 5. Continued.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Kiwifruit	200	Ripeness	VIS-NIR	540–800 nm	LR, Pearson	Kiwi-meter suggested a successful measurement of chlorophyll and color.	Pearson's test (r) Firmness: 0.64–0.87 TSS: -0.68, -0.91 Dry matter: -0.23, -0.75 Flesh color: 0.75–0.89 Total chlorophyll: 0.76	[124]
Mango	50	Ripeness, firmness	VIS-NIR	400–1130 nm	PLS	Firmness prediction can contribute to consumer demand.	Calibration R^2: 0.75 RMSEC: 6.02 Validation R^2: 0.75 RMSEC: 5.92	[147]
Mango	156	Ripeness	HSI	400–1100 nm	MAL, SVR, LR	Genetic algorithms was the best solution.	Best performance R^2: 0.74 Four-sensor device $R^2 \leq 0.69$	[133]
Mung bean	90	Growth	NIR	900–1700 nm	PCA, PLS-DA	Reliable option for the quality of mung bean sprout	Accuracy: 100% Ascorbic acid $R^2 > 0.90$	[148]
Olive	1000	Ripeness	VIS-NIR	670–970 nm	LR	Better absorbance difference index (I_{AD}) was calculated in color, rather than the contents of fruit oil, water and pulp oil, also pulp firmness. I_{AD} was useful for rapid screening of suitable HT.	Kiwi-meter (validation) DRMSECV: 0.574–0.810 R^2: 0.500–0.752 RPIQ: 2.018–3.044 Standard DA-meter (validation) DRMSECV: 0.622–0.861 R^2: 0.311–0.661 RPIQ: 1.068–2.827	[149]
Oriental melon	91	Quality	Red-NIR, VIS, HSI	Red–NIR: 600–860 nm, VIS: 460–600 nm	SVR, RR, KNN, RF	SVR model was the superior to predict solid solution and moisture contents.	TSS content (validation) R^2: 0.68–0.87 RMSE: 0.95–1.50% Moisture content (validation) R^2: 0.61–0.79 RMSE: 0.99–1.19%	[150]
Papaya	15	Ripening, maturity	VIS, CMR	VIS: 200–800 nm CMR: 0–2000 cm^{-1}	PCA	Effective monitoring	PCA score Mezocarp: 95.71% Pericarp: 96.05%	[128]
Pomegranate	210	Maturity	HSI	720–1050 nm	PCA, PLS-DA, PLS-R	HSI had great potential for screening color, chemical properties, total polyphenols and antioxidant activity.	PCA score: 93.6–98.1% Accuracy: 95–100%	[134]
Pomegranate	100	Tannin	Raman	100–3000 cm^{-1}	PLS, PCA, SMA	Well detection of tannin on subsurface	Validation R^2_{aril}: 0.9253 R^2_{rind}: 0.9603 $R^2_{white\ tissue}$: 0.9227	[151]
Potato	474	Chlorophyll	VIS	200–1000 nm	PLS, CARS, CWT	Important method for chlorophyll pigment of potato	$R^2_{calibration}$: 0.93 $R^2_{validation}$: 0.85 RMSECV: 2.77	[152]
Spinach	128	Quality	NIR	1600–2400 nm	MPLS, PLS-DA	The pre-harvest screening tool had capable of evaluating ascorbic acid, TSS and nitrate levels.	Fresh samples Classification: 73.08–76.92%	[153]

(*Continued*)

Table 5. Continued.

Crop/ product	Number of specimens	Attribute	Spectroscopy	Band range	Statistical model and/or algorithm	Remarks	Performance and/or accuracy	Reference
Sweet cherry	54	Ripening	CMR	0–2000 cm^{-1}	PCA, HCA	CMRS with PCA and HCA was a good option for screening quality characteristics and ripening of sweet cherry.	PCA score: 81.52%	[129]
Tomato	319	Quality	NIR	1295–2611 nm	PLS	NIR tool was able to specify many characteristics of tomato fast and practically.	$R_{prediction}$ TSS: 0.87, Citric acid: 0.86 Ascorbic acid: 0.81, Fructose: 0.87 Glucose: 0.83	[154]
Tomato	90	Ripeness	ATR-FTIR	900–1800 cm^{-1}	PC-LDA, SVM	For supply chain, MIR was recommended.	Sensitivity ≥ 99% Specificity ≥ 99%	[155]
Tomato	250	Maturity, TSS	VIS-NIR	600–1160 nm	PLS, ELM, MSC	Full transmittance mode was recommended.	Classification rate Total: 80.08%, Stages: 62.69–94.62% Accuracy Total: 91.31%, Stages: 89.23–95.38%	[156]
Tomato	1000	Firmness, antioxidant	NIR	285–1200 nm	PCA, LR	NIR was helpful in order to estimate quality during both HT and post-harvest stage.	R^2: 0.919–0.984 RMSEC: 0.163–2.506 RMSECV: 0.64–1.82	[157]
Tomato	600	Maturity	SR	550–1650 nm	SVMDA	Emerging spectroscopy methodology gave valuable information about tomato maturity.	Accuracy: 75–100% Sensitivity: 0.750–1.000 Specificity: 0.970–1.000	[158]
Watermelon	63	Maturity	VSNIR	200–1100 nm	PCA, PLS	Successful, portable and cheap method was suggested for determining TSS level.	Overall accuracy: 85% RMSEC Unmatured: 0.49 Matured: 0.30 Over-matured: 0.48 RMSEP Unmatured: 0.69 Matured: 0.34 Over-matured: 0.64	[159]
Watermelon	48	Maturity	Raman	400–2000 cm^{-1}	PLS-DA	A versatile tool was proposed for effective monitoring of carotenoid variances on surface	Accuracy > 85%	[127]
Watermelon	96	Quality	VIS-NIR, NIR	VIS–NIR: 475–1075 nm NIR: 950–1650 nm	PLS	The development of maturity can be monitored by NIR spectroscopy.	Calibration R^2: 0.47–0.87 RMSEC: 0.12–4.87 Cross validation R^2: 0.31–0.78 RMSECV: 0.13–6.77 Prediction R^2: 0.32–0.78 SEP: 0.14–6.81 RPD: 1.19–2.15	[160]

may occur during chemical analysis since it allows analysis of food without preparation dilutions or chemical interaction. Since the functional groups of the molecules move in various ways at unique frequencies, it allows for their identification with high accuracy, allowing the examination of any contaminants and detection of adulteration, as well as the classification of foods for their geographical origin [168]. Moreover, due to the developments in vibrational spectroscopy technology, portable spectroscopy devices allow simultaneous analysis both in processing facilities and in the field [169].

On the other hand, there are certain problems with the use of sensory analysis as a routine analysis of production plants. One of these is that there is a need for panelist training, the calibration of trained panelists over time, the exposure of the human factor to environmental and psychological variables that adversely affects the results, and a long-time requirement of these analyses. In this respect, vibrational spectroscopy can be more useful for identifying and characterizing sensory indicators in food material that has huge potential to be a substitute for traditional sensory analysis methods in production plants [166].

Today, vibrational spectroscopy devices are widely used in the food industry around the world, both manually and in automation. These devices, which only have initial investment and sometimes calibration costs, are advantageous in terms of economic losses through manufacturing defects, as well. Much of the current literature on vibrational spectroscopy pays particular attention to grain analysis [170–175] since the grain processing plants are most widely using vibrational spectroscopy in the food industry. NIR, which is used for the analysis of solid and semi-solid foods, gives results through measuring the radiation absorbed and reflected by the food which is used in the grain production line with full automation. Chemical composition analysis, sedimentation test, and black spot analysis is performed with NIRS for every second, giving instant data collection.

Vibrational spectroscopy is employed especially for monitoring humidity within the grain production line. When the humidity surpasses the predetermined limit value, it is rapidly detected within seconds, which enables prompt action to ensure the quality of the final product. Thus, necessary measures are taken to regulate the humidity value to the set point which provides production under optimum process conditions. Rapid and on-site analysis of humidity has resulted in a lower staff requirement, reduction in chemical analysis time, prevention of production errors and, consequently, economic losses. Moreover, incorporating a precision-measured camera with the device, facilitates the analysis of L* value of the grain which has been used for the quality assessment.

The detection of cultivation defects, referred as embryo burn or black spot diseases, plays a crucial role during production to obtain products with high quality which are separated by sieves in traditional production methods. However, in the case of sieve rupture, black dot separation was a failure that resulted in low quality flours, until this issue was identified through the attention of the employees. The NIR spectroscopy device can count black dots based on microns with the incorporated camera and when the number of pikes exceeds the predefined threshold, the system automatically pauses and sieves are changed. Moreover, through portable NIR devices, quality analyzes can be conducted in the field before the grain harvest, thus these devices provide benefits in the grain industry comprising every stage of production process, from farm to table.

FTIR, which allows the analysis of liquid and semi-liquid food products, is utilized in the dairy industry for quality control and adulteration detection purposes. In this system, spectroscopic analysis is performed by drawing the food into the device, which enables the use of the same sample for multiple analyzes without the need for sample preparation. The most important quality parameters of milk, namely fat and protein content, are determined within a matter of seconds with FTIR. FTIR, enables the analysis of various quality characteristics, such as chemical composition and conductivity, as well as calculation of adulteration in percentage for raw and processed milk and dairy products. Therefore, prior to the acceptance into the processing facility, raw milk, which is highly susceptible to microbial spoilage, is analyzed to detect common milk adulterants, such as hydrogen peroxide, formaldehyde, and phosphate salts, thus allowing rejection of raw milk that includes such contaminants, before they enter the production plant. Vibrational spectroscopic analysis is also utilized for determining rennet coagulation, the formation of skimmed milk powder, and monitoring the changes in lactose-free milk [174]. Moreover, portable FTIR devices enable on-site raw milk analysis obtained from farmer and collection centers.

The database of spectroscopic instruments is quite extensive and is continuously improving. This enables generating and recording results for geographically marked dairy products. Device calibration is performed by comparing the device reading with those R&D units for newly introduced milk or dairy product types to obtain accurate results which are consequently integrated to the data library. For instance, to illustrate the minute definition of a single cheese type, thousands of cheeses are analyzed, and the determined precise parameters are introduced to the database. Thus, proper and reliable measurements can be obtained for unique food types.

Quality analyzes based on spectroscopic measurement are becoming increasingly common in the meat industry. NIRS, which provides swift results, plays an effective role for the quality control of meat and other muscle foods. NIRS, primarily used for protein analysis of meat, enables quality classification and meat can be processed into suitable products depending on its quality [169]. Besides, in the poultry industry, zero tolerance was granted for certain contaminants, such as septicemia and toxemia, and to prevent their contamination into the product and processing such place measurements are demanded [175]. However, tens of thousands of chickens are processed daily and during the breeding phase of these chickens in integrated production facilities, biosafety assessments are performed by manual and visual health checks conducted by veterinarians and inspectors. This manual control of large-scale daily processing facilities is time-consuming and labor-intensive. To address these issues Chen et al. developed a portable Visible/Near-Infrared Spectroscopy (Vis/NIRS) system to classify chickens as normal, infected, and dead with 93% accuracy [169,176]. Implementation of these developed techniques in poultry enterprises might decrease animal deaths and minimize contamination risk, which, in turn, prevents economic losses while ensuring food safety.

The composition of meat emulsions and water in oil emulsions (such as margarine) is subject to some legal limitations, regarding the amount of fat and protein. In this regard, FTIR spectroscopy paves the way for rapid results in 5 min with an accuracy of ±0.2% considering emulsion composition that is practical before production. Vibrational spectroscopy is commonly used in the oil industry for determination of saturated and unsaturated fat for quality analysis and adulteration detection as well as possible adulteration owing to the mixtures of vegetable oil and animal fat. Control of trans fatty acid formation, peroxide number and iodine value have significant importance for the oil industry which are control parameters and now extensively analyzed via infrared spectroscopy along with the method described by American Oil Chemists' Society. Developed FTIR method is more advantageous compared to the traditional chemical methods in terms of accuracy and enables it to give results in a short time, mostly around 2.5 min [167].

Raman spectroscopy also has growing interest in the food industry. Although, it has limited use due to the inability to provide sufficient signals for the specific molecules at low concentrations, it offers results with high accuracy for identification of food pathogens and their species [12–178]. In this regard, Raman spectroscopy has high potential for detecting microbial contamination in food production and supply chain. On the other hand, its applicability to both solid and liquid foods has importance in the food industry as this grants the analysis of a wide range of food stuff. Raman spectroscopy is frequently utilized for the analysis of products, such as liquid foods, juices, wines, beer, milk and dairy products, plant extracts, spices, oils, flour and starch, and it enables analysis of the amount and distribution of food components, such as fatty acids, proteins, and water, with a rapid response. This technique allows the analysis of various proteins with diverse structures, properties, and functions, and enables the predication of quality assessment within the meat industry upon any protein alterations [179]. Moreover, Raman spectroscopy is employed for various intentions across diverse food operations, such as detecting fraudulent wines and beverages, analyzing wine composition, determining wine origin [180,181], analyzing milk composition, detecting milk adulteration [182–185], examining components in plant extracts for the spice industry [12], etc..

In conclusion, Raman spectroscopy is a versatile tool used by the food industry in a wide range of applications, and its development and widespread use can meet numerous needs of the food industry. Due to the increase in consumer awareness and their desire to know really what they consume contributed to the rise of clean labels and accurate labeling approaches. Clarifying the changes in the chemical structure of food has become very important for producers to meet consumer demands since food undergoes multiple processing stages until it is consumed, from farm to fork. Detailed analysis of the food components will also enable consumers to be protected against adulteration. Therefore, verification of food components with molecular-level analysis is the current issue, therefore, building legal regulations for detailed labeling has become the focus of international food authorities [174]. Through the vibrational spectroscopy technique, compound-specific bands as well as multiple bands, identification of various components within a given sample is possible [186].

One of the main restrictions for widespread usage of vibrational spectroscopy is the necessity of generated analytical methods to be officially recognized, as well as taking part in any official methods literature. Common applied chemical analysis methods utilized for legal quality classification of oil, such as antioxidant activity, fatty acid composition, peroxide value etc., could be assessed through vibrational spectroscopy. The inclusion of these methods in official analytical methods with standardization and high accuracy rates may enable widespread use of these methods in industrial applications [187]. On the other hand, the heterogeneous and complex structure of given food components, as well as the presence of various organic components within several food types, lead to some drawbacks with respect to the application of vibrational spectroscopy in the food industry. Thereby, applying statistical techniques to identify intended food components is a powerful tool to explain the possession of certain food components to complex spectral responses. In addition, the comparison of the results obtained from spectroscopic analysis with the data obtained from instrumental analysis is necessary to calibrate the spectroscopy devices to achieve responses with high accuracy [166]. The use of vibrational spectroscopy is increasingly feasible in the food industry, principally for quality analysis, contaminant detection and compositional analysis. Current studies on vibrational spectroscopy focus on ensuring high accuracy results for further chemical analysis by detecting distinct chemical bonds energy [168,179]. The detection of chemical changes in food during production that may impact human health would be possible with the ongoing efforts that aim to optimize and promote this technique, through the production of more healthy food products.

Prevention of contamination in food

Foods can be contaminated in a variety of ways throughout the processing. There may be physical, chemical, and/or biological contamination. Food pollution may be caused by several processing steps, including cleaning, conditioning, heating, and packaging [188]. Furthermore, equipment, employees and environmental conditions may act as potential contamination sources in food processing facilities [189]. Physical contaminants that may occur during food processing contain the presence of some undesirable materials, such as glass or metals, insects, as well as rodent droppings [190]. On the other side, one of the main food processing techniques, namely thermal treatment, leads to the formation of several chemical contaminants or the conversion of some contaminants into more toxic compounds. Acrylamide, polycyclic aromatic hydrocarbons, heterocyclic aromatic amines, chloropropanol esters, *N*-nitroso compounds, and oxidation products like aldehydes are the most common chemical food contaminants formed as a result of thermal treatments [191]. Residues of disinfectants and detergents used in food processing facilities and the migration of toxic substances from food packaging materials, such as phthalates, bisphenol A, and melamine are other contributors to chemical contaminants [192]. Microbial contamination may arise from the improper hygienic practices of food handlers, the utilization of polluted water, low-microbial-quality indoor air, and equipment without efficient cleaning and disinfection applications [193,194]. The review published by Møretrø and Langsrud [195] comprehensively covers process-related spoilage microorganisms or pathogens in foods. Beyond these, food products may be intentionally adulterated with a wide range of substances [196].

Food contaminants have been detected using different methods. These may be categorized into three main groups: (1) physical techniques (macroscopic or microscopic visual evaluation), (2) chemical techniques (high-performance liquid chromatography (HPLC), gas chromatography (GC), thin layer chromatography (TLC), inductively coupled plasma mass spectrometry (ICP-MS), nuclear magnetic resonance (NMR), electrophoresis, immunoassays), and (3) molecular methods mainly polymerase chain reaction [197,198]. Regarding drawbacks of some of these conventional techniques, such as complicated sample preparation steps, long analysis duration, the need for qualified analysts, and high investment costs, alternative simple approaches (sensing methods, ion mobility spectrometry) have been developed [199–204]. Nondestructive vibrational spectroscopic techniques, including NIR, MIR, Raman, and surface enhanced Raman, and SERS have stood out among all of these procedures due to their low cost, simplicity, high sensitivity, absence of reagents, and rapid detection [205,206]. These are appropriate for both online/in-line process control as well as at-line (laboratory) analyses [207].

IR has been widely used by the food and beverage industries for quality and process control as well as monitoring the cleanliness of equipments [208,209]. Food residues on food contact surfaces considerably promote biofilm formation and reduces the efficiency of cleaning and disinfection operations [210]. The formation of biofilms by microorganisms, including pathogens such as *Bacillus cereus, Campylobacter jejuni, Escherichia coli, Listeria monocytogenes, Salmonella enterica, Staphylococcus aureus, Geobacillus stearothermophilus, Anoxybacillus flavithermus, Pseudomonas* spp., and *Pectinatus* spp. on food contact surfaces are of great concern for food safety [211]. About 80% of persistent bacterial infections are associated with biofilms [212]. Vis-NIR (400–1000 nm) hyperspectral imaging technique with deep learning was successfully applied for the detection of organic residues of potato and spinach juices on stainless steel food contact surfaces [209]. A well-known biofilm- and histamine-forming bacterium, *Lentilactobacillus parabuchneri,* that adheres to stainless steel surfaces in cheese manufacturing factories was detected using *in situ* infrared attenuated total reflection spectroscopy (IR-ATR) with a spectral window of 1700–600 cm^{-1}. Significant changes in amide II and II bands, which are specific to extracellular polymeric substances that enclose biofilm populations enabled the detection of progress in biofilm formation by IR-ATR [213]. Fecal or ingesta contamination of meat and poultry products within processing facilities is a serious food safety issue [169]. In poultry processing plants, pathogen *Enterobacteriaceae* contamination through poultry fecal residues was rapidly detected by means of visible/NIR reflectance spectroscopy [214]. The combination of NIR with hyperspectral imaging was reported to be a promising and effective tool to predict *Enterobacteriaceae* on chicken fillets [215]. As the feces contained several pigments from undigested feed as well as bile fluids, they exhibited stronger spectral absorbance than uncontaminated chicken skin at 475 nm. The dominant oxymyoglobin content on the skin was represented by higher absorbance at 545 and 570 nm [216]. It was reported that, coupling of Vis-IR with variable combination population analysis/genetic algorithm enabled the detection of *E. coli* O157 and *S. aureus* on fresh longissimus pork muscles due to their effects on oxygenated (peaks at 414, 543, and 577 nm) and deoxygenated hemoglobin (peaks at 433 and 556 nm) concentration as well as lipid fingerprints of bacteria [217]. Similarly, some foodborne pathogens (*E. coli* ATCC 25922, *E. coli* O157: H7 ATCC 35150, ampicillin-resistant (AMPr) *E. coli*, *L. monocytogenes* ATCC 19115, *S. aureus* ATCC 25923, methicillin-resistant *S. aureus* T34, *Salmonella enteritidis* CICC 21482, and *Salmonella typhimurium* CICC 22956) were successfully differentiated using Vis-NIR hyperspectral imaging depending on the differences in bacteria fingerprints as a result of various combinations of acyl arms and head classes in lipid structures [218]. Furthermore, microbial loads in rainbow trout fillets were rapidly and precisely quantified using short-wavelength NIR in combination with multivariate statistical methods [219]. IR produces particular spectral peaks, like a fingerprint of any microorganism, that provide insights about bacteria's genetic-related structure in terms of proteins, lipids, nucleic acids, and carbohydrates [220]. Several successful attempts indicate that IR is a promising approach to minimizing microbial contamination in meat, poultry, and seafood processing facilities. In contrast to the detection of microbial contamination, although their sensitivity is lower, hand-held and portable NIR devices coupled with robust classification techniques or chemometrics are successfully used for the quantification of adulterants in various food products, including extra virgin olive oil, honey, yogurt, milk, spices, and dairy powders [221–223]. NIR, along with computer vision, is also a powerful technique to detect physical contaminants, like metals, hair, and plastic, in toasted bread [224].

MIR spectroscopy provides a spectral range from 2500 to 50 000 nm, whereas NIR ranges between 780 and 2500 nm [225]. These instruments have been mostly used in wineries for the early detection of spoilage processes induced by lactic acid or acetic acid bacteria during the alcoholic fermentation of white wine. This is accomplished by quantifying L-malic acid or lactic acid throughout fermentation [226,227]. FTIR, another common vibrational technique, has a wavenumber range from 4000 cm^{-1} to 400 cm^{-1} [228]. On the other side, FT-MIR spectroscopy, along with multivariate analysis, allows for fast characterization and categorization of foods by identifying compounds in a well-defined spectra even at ppb concentrations within milliseconds [229]. As the NIR region's multiple overtone and combination bands lead to lower structural selectivity than that of MIR spectra, spectrometers running in the MIR, generally known as "FTIR", region have been mostly preferred in the food industry [230,231]. One of the most recent applications of FTIR in the food industry is the determination of 3-monochloropropanediol (3-MCPD), a chemical heat-induced process contaminant, in refined vegetable oils. In palm-based cooking oil, 3-MCPD was detected through bands at 990–900 cm^{-1} and 800–700 cm^{-1} due to $–CH{=}CH_2$ or $CH{=}CH$ stretching and C-Cl bonding, respectively, using MIR-ATR-FTIR coupled with chemometrics, including consensus approach, cubist, RF, ANN, and partial least squares regression (PLSR) [232]. The content of another high temperature-induced process contaminant, acrylamide, was effectively predicted in commercial potato chips by handheld NIR-FTIR and portable MIR-FTIR devices along with PLSR models [233]. FTIR is considered a convenient, rapid, and inexpensive way to detect numerous gram(-) microorganisms, including *E. coli, S. enterica, Klebsiella pneumonia, Klebsiella oxytoca, Acinetobacter baumannii, Legionella pneumophila*, *Burkholderia cepacian*, *Campylobacter* spp., *Xanthomonas oryzae*, and gram(+) bacteria, such as *S. aureus, Streptococcus pneumoniae, L. monocytogenes, B. cereus, Enterococcus faecium, Streptococcus agalactiae, Corynebacterium ulcerans*, and *Alicyclobacillus*spp [220,234]. This is accomplished through certain peaks observed at FTIR spectra such as amide III between 1314 and 1205 cm^{-1}, C–N stretching from amines/amino acids at 1240 cm^{-1}, C=O symmetric stretching of COO^- groups at 1401 cm^{-1}, C-N bonding from amides at 1405–1413 cm^{-1}, amide 1 at 1600–1700 cm^{-1}, which are considered indicators of the proteolytic activity of microorganisms and/or strain-specific structural composition differences [220,235]. Although FTIR is commonly utilized and it provides reliable results for various food analyses in laboratories, its in-line applications to control microbial contamination are still scarce in the food industry. In addition to these, FTIR was reported to be a promising approach for detection of microplastics (polystyrene, polyethylene, polyethylene terephthalate, poly-(methyl methacrylate), polypropylene, and polyvinyl chloride) in packaged meat and rice as a result of migration from packaging materials [236,237].

As with other nondestructive vibrational spectroscopic methods, Raman spectroscopy also provides specific information about the chemical composition of any liquid, solid, or gaseous sample at the molecular level [238]. In a study, common meat spoilage and pathogen microorganisms, including *Micrococcus luteus, Brochothrix thermosphacta, E. coli, Bacillus subtilis, Pseudomonas fluorescens,* and *Bacillus coagulans,* were successfully discriminated based on their chemometrics-analyzed unique spectra obtained through Raman microscope or portable Fiber-optic Raman spectrometers. For instance, *M. luteus* displayed characteristics peaks at 1157 cm^{-1} and 1529 cm^{-1}, which were attributed to carotene-like pigments particular to this strain [239]. Similarly, *B. thermosphacta*, *P. fluorescens*, *M. luteus*, *E. coli*, *B. cereus*, *S. aureus*, *Bacillus thuringiensis israelensis, Cronobactersakazakii, Vibrio parahaemolyticus, Shigella flexneri, Shigella bogdii, Salmonella typhimurium, Salmonella cholerae-suis, Salmonella paratyphi-A, Salmonella enteritidis,* and *Salmonella Aberdeen* were discriminated at strain and genera using their distinct Raman spectral profiles that were analyzed by proper PCA methods [240–242]. All these findings are impressive in terms of replacing the labor-intensive, and time-consuming traditional microbiological analyses with simple, rapid, adaptable to processing lines, and nondestructive, spectroscopic ones in the food industry. Additionally, biofilms of *Shewanella putrefaciens* occurred on the food contact surfaces were clearly identified depending on their Raman spectra bands at: 880–980 cm^{-1} for polysaccharides, 1020–1080 cm^{-1} for carbohydrates, 1075–1125, 1235–1260, and 1300 cm^{-1} for proteins [243]. Another emerging contaminant, microplastics, is becoming a more serious issue for food safety. The most common way of microplastic contamination for food processing facilities is the water used in the equipment during various processes or for cleaning. A study carried out by Kniggendorf et al. [244] demonstrated that, polyethylene, polyamide, polypropylene, polystyrene, and polymethyl-methacrylate microplastics, with average particle sizes around 0.1 mm could be identified using an attachable-to-tap Raman spectroscopy-based flow cell in tap water flowing at a rate of 1 L/h. The strength of Raman signals can be improved, when a noble metal (e.g., copper, gold, silver) nanostructure is used for adsorption of the sample to be analyzed, which is known as SERS [245]. Allergens are considered the top food safety hazard worldwide [246]. The cross-contamination of allergens like lysozyme (a major egg allergen) from food handling surfaces can be avoided through utilization of SER spectroscopy with proper nanoparticles [247]. Accordingly, SER spectroscopy based lateral flow assay strips with gold-silver nanoparticles were developed to provide a fast and reliable detection of main milk allergens, namely casein and *α*-lactalbumin. The strips enabled the identification of the allergens in chocolate, milk, jelly, and biscuits in 5–10 min [248]. A very recent study showed that, SERS spectra coupled with $AgNO_3$ particles and a SVM classification machine enabled the rapid detection of *Salmonella typhimurium* in chicken rinse solutions [249]. Similarly, a paper-based SER spectroscopy with gold nanoparticles was developed for the early detection of *S. enteritidis* and *L. monocytogenes* [250]. Moreover, the efficiency of industrial disinfection process of chicken carcass against *E. coli* O157:H7 could be tested with silver nanoparticles enhanced SERS [251]. Unlike bacteria, several viruses (norovirus, coronavirus, adenovirus, parvovirus, herpesvirus, paramyxovirus) that can be transmitted to food processing facilities via raw materials or water were successfully differentiated using SER spectroscopy coupled with gold substrates along with SIMCA and PCA [252]. These are encouraging findings for in-plant applications of SERS for monitoring foodborne/waterborne pathogens and viruses in food processing plants. In addition to microorganisms, the application of SER spectroscopy with gold or silver colloids for on-site monitoring and prevention of *S. aureus, E. coli* O157:H7, *Vibrio parahaemolyticus*, and *Listeria innocua* biofilms, on food contact surfaces [253,254].

In summary, proper nondestructive vibrational spectroscopy techniques allow the rapid and sensitive detection of several foodborne contaminants, including physical, chemical, and microbiological hazards, in food processing facilities. Nevertheless, they still have many drawbacks and challenges that hinder their in-line implementation in the food industry [171]. For instance, they require the application of suitable processing and analysis techniques such as multivariate statistical tools for the extraction and interpretation of spectral data [255]. Furthermore, the presence of water in most biological samples and IR-inactive compounds restricts IR applications. On the other hand, Raman spectroscopy is limited due to its low sensitivity and the effects of several factors, including particle size, color, and fluorescence of samples on Raman spectra [205]. Therefore, further studies should be done to address these issues and improve the feasibility of these techniques on an industrial scale.

Use of vibrational spectroscopy in the distribution center

Detection of potential problems with food during transportation

It is essential for sustaining life and encouraging public health to have access to safe, adequate, and nutritious food [256]. Therefore, it is necessary that all available and delivered products are produced under stringent hygienic conditions and are free of hazardous and pathogenic substances for food safety, which involves a broad range of operations, including farm practices, processing, storage, manufacturing, transportation, and distribution [257,258]. Furthermore, the vast quantity and diversity of foods transported, as well as the wide range of containers, temperature, and processing specifications for each food item, demonstrate the susceptibility of the food industry to contamination throughout storage and transportation [259,260]. Contamination risk factors involve inappropriate production methods, temperature changes, unsafe cargo spaces, incorrect loading or offloading operations, damaged packaging or containers, poor behaviors of staff, and road conditions [259]. As a result, the need for the implementation of detection or monitoring techniques increased for the regulation of food safety and quality [261]. However, traditional food analysis techniques are generally laborious, expensive, destructive, and time-consuming, as they involve the preparation of samples and pre-processing steps prior to or throughout analysis [262,263]. Consequently, the application of nondestructive methods, such as those based on spectral imaging and vibrational spectroscopy methodologies, has become a highly desirable analytical instrument for the food value chain [26,29,264]. In addition, these techniques provide advantages, including rapid analysis, portability, versatility, and sensitivity. This section discusses the uses of vibrational spectroscopy during food transportation, with an emphasis on the characteristics of foods.

Automation in agriculture and food processing makes online monitoring crucial throughout the food supply chain, which involves logistics operations. The circumstances under which food is transported and stored influence its quality and safety. The post-harvest quality of the foods greatly depends on their freshness and microbiological safety throughout handling, storage, transport, and marketing. Among nondestructive methods, vibrational spectroscopy technologies like Raman, MIR, and NIRS have been well adopted in scientific and commercial practice for monitoring sustainable food systems [29,265]. In-line implemented NIRS units can investigate each item passing on the line (i.e., in the packing line); on the other side, the hand-held counterparts can be employed at any other points [28] such as in the fields, distribution, transportation, retail, and even markets, although they are based on lot-sampling.

The freshness of the food is one of the most critical challenges encountered during transportation. As citrus fruits are sensitive to several spoilage germs, monitoring the compositional alterations caused by spoilage (particularly by fungi) is worthwhile, and this is possible by Raman scattering microscopic imaging, in which fresh and spoiled samples can be distinguished [266]. The freshness of citrus fruits like mandarin, clementine, and tangerine, could be tracked with a developed portable monitoring system that takes advantage of the resonance Raman effect of carotenoids in fruit peels [267], fruit's characteristics and color, and as a result, the contents of carotenoids in the peel, were connected to the freshness of the fruit. Furthermore, the degradation of carotenoids due to aging and mold activity was tracked in Raman spectra through the declining intensities of their signals. The intensity of the carotenoid resonance Raman signal, obtained throughout twenty days, was determined to be a valid indicator of the freshness of the intact fruit. Also, the authors suggested that, different types of lasers in hand-held, portable spectrophotometers can be used for this aim. In particular, lasers with wavelengths of 532 nm (which is used in this study), 514.5 nm, and 488 nm can be operable. These lasers work well because, they match the electronic absorption of the carotenoids in fruits. Moreover, in the study of Wang et al. [268], Fourier transform-near infrared spectroscopy (FT-NIRS) combined with chemometrics was used to detect the freshness of kiwi fruit, and researchers reported that the proposed method could be utilized by food regulatory organizations, companies, and retailers to observe the freshness of kiwi fruits during production, transportation, and sales processes. Such discoveries pave the way for practical applications in quality monitoring during handling and transportation. As a bonus, the noninvasive character of the control method stands to boost both market dominance of producers and customers' confidence and security.

In global supply chains, fruits are often transported across the world to regions where they do not grow naturally, which can result in partly ripe or overripe fruits at the end of the transportation period. Further evaluation may be required during transportation or in repacking units to assess the remaining time for ripening and shelf life. This information can help the management make decisions on how to handle the fruit, such as whether to store it for longer, help it ripen, or distribute it for sale. Vibrational spectroscopy applications present a prediction of future attributes like storage time, susceptibility to spoilage, ripening, or eating quality [269,270]. For example, they enabled rapid determination of sensory and texture parameters in Bahri dates [271] and the oil content in macaw fruits, indicating maturity [272]. Therefore, during storage, transportation, or distribution, improved vibrational spectroscopic techniques (particularly portable ones) can serve as a decision-support tool and provide rapid and nondestructive measurements of important quality attributes. In this context, hand-held or portable NIRS or Raman Scattering instruments are getting attractive at various points in the food chain [223,273,274]. Because they pose various advantages, such as *in situ* investigation of the moisture content in palm oil [275], stage of maturity of whole fruits [276], or ripening attributes of dairy products [277]. Researchers explored the use of miniature portable spectrophotometers for online evaluation of strawberry shelf life and quality (including soluble solid content, pH, and firmness) to be adapted to supermarkets [278]. While diode-array or FTIR instruments yielded slightly superior results, hand-held Vis/NIR spectroscopy showed potential as a time-saving, cost-effective, and movable alternative. This suggests that, similar hand-held spectrophotometers could be employed in transportation settings to assess the quality of perishable foods, such as fruits and vegetables, without destructive testing.

In a more recent study, Vega-Castellote et al. [279] demonstrated that a portable NIRS device (MicroNIRTM Pro 1700) with a linear variable filter sensor connection could be used at supermarkets to measure color, soluble solid content, and the antioxidant activity in half-watermelons. It was suggested that, the NIRS analysis (in the spectral range 908–1676 nm) be performed in the dynamic mode so that the entire surface of the product may be examined. The nutritional properties detected at the point of sale without harming the food can be attractive to the consumer. On the other hand, a low-cost wireless optical sensing system based on NIR measurement, combined with ANN, showed promising results for screening the quality of grapes [280]. The system is cost-effective, making it feasible to install numerous sensing devices throughout the logistics system to collect average values representing the grapes' freshness. However, further improvements in model accuracy are necessary. As a result of these findings, portable NIRS instruments can offer several advantages in monitoring food products' maturity, sweetness, color, and antioxidant activity, when used for transportation or logistics operations. Real-time monitoring can help prevent spoilage, reduce costs, and improve overall efficiency, while nondestructive testing can preserve the integrity and shelf life of the products. In addition, portable NIRS instruments can provide important data for labeling and traceability, including nutritional information and origin. Overall, using portable vibrational spectroscopy in food product transportation can help ensure quality, save money, reduce waste, and improve consumer satisfaction.

The spoilage of milk will result in significant economic loss and severe damage to consumer health. During transportation, milk is susceptible to spoilage due to its high nutrient and water content, which makes it an optimal medium for the proliferation of microorganisms. Detecting milk freshness thus becomes a crucial stage in the dairy manufacturing industry [281,282]. Alhamdan [283] developed a quality index (Q_i) to determine the physicochemical properties of fermented milk drink (laban) and predicted it using the NIR spectrum. According to the results, it can be deduced that nondestructive NIR can anticipate Q_i and can be applied with great efficacy throughout the entire processing, production, storage, transportation, and retail chain to determine the "shelf life" and "quality" of a food product. An earlier study used Raman spectroscopy and chemometrics to determine milk acidity as a robust method. As a result of the study, the proposed method was a rapid and effective technique for observing milk adulteration by illegal neutralization, mostly attempted during transportation or storage periods [281]. Similarly, NIRS was successfully used to determine water adulteration, which is a common adulterant during production, transportation, and storage stages, in cow milk samples [284].

Fish and meat products, unless cured, canned, or fermented, mostly require cold-chain conditions. Structural deterioration, biological changes, microbial spoilage, and autolytic reactions during frozen storage and transportation are critical problems jeopardizing their quality and shelf life. The quality of fish muscle tends to decline during frozen storage, primarily leading to the loss of desirable texture and the development of deterioration with odor in fish [285]. These changes play a crucial role in determining the overall stability of the fish. Raman spectroscopy was utilized to investigate the impacts of frozen storage, freeze-thaw cycles [286], and the addition of cryoprotectants and antioxidants [287] on fish. This method provides information regarding the fish protein denaturation, in particular its secondary structure (α-helix and β-sheet, or random coil), derived from the amide I vibrational modes. Also, it can characterize the SH-groups and aromatic side chains in the structure [288]. According to the studies mentioned, ice crystal formation and lipid oxidation products are affecting factors in protein denaturation in frozen fish. Comparisons of Raman spectra revealed that the addition of cryoprotectants (sorbitol, sucrose, lactitol, and Litesse) or antioxidants (vitamin C and vitamin E) might stabilize fish proteins. This helps minimize hardening and deterioration, which is possible during logistics.

Usually, conventional Raman spectroscopy has restrained detection sensitivity due to the low cross-section of scattering (from 10^{-28} to 10^{-30} cm^2 by molecule) [289], which affects precision. On the other hand, Spatially Offset Raman Spectroscopy is the recently evolved technique to figure out the interior chemical composition of bulk food samples. It works by gathering Raman signals from deep layers along with spatially offset distance. Additionally, the use of SERS substrates allows for the detection of target analytes in complex matrices, such as food samples, which can be challenging using conventional techniques [261]. These noninvasive emerging approaches allowed determinations of the internal composition, quality, and freshness of intact prawns [290] or the volatile amine molecules in various meat samples as an indicator of spoilage [291]. Significant temperature fluctuations or abuse in vehicles expose products to thawing and re-freezing, which can have detrimental effects on their structure, safety, quality, and shelf life [292]. In this regard, Raman spectroscopy has the potential to measure textural characteristics and distinguish between frozen and thawed meat texture with the help of PLS models [293]. For estimating the shelf life or spoilage of meats, Raman and FTIR have been exploited to convert biological alterations (as a result of microbiological activity) into signals [294,295]. Several studies have demonstrated that Raman spectra can indicate the protein breakdown related to meat spoilage; consequently, investigations on estimating meat freshness (such as pork chops, minced beef, and chicken breast) by using the Raman spectroscopy technique have been presented in rapid succession [238,295–297].

In comparison to other vibrational spectroscopic practices, such as NIR, FTIR spectroscopy has a higher absorption intensity, whereas Raman spectroscopy is less sensitive to water [261]. Recent exploration revealed that both Raman and FTIR spectroscopy, individually or combined, can quickly predict beef spoilage under dynamic temperature conditions, which represent the alterations along the distribution chain [298]. Raman and FTIR spectra recognize amide regions, amino acids, and inorganic salts. Total viable counts and total volatile basic nitrogen were successfully estimated; however, there was a need to enhance the accuracy of the prediction model (PLSR) with further machine learning approaches or extended sample size. Zhong et al. [299] focused on developing the accuracy of the spectroscopic technique in the prediction of freshness. According to their study, Raman spectroscopy equipped with a novel Long Short-Term Memory (LSTM) neural network model was proven to be a rapid, precise, and non-damaging mechanism to predict salmon storage time at various temperature settings (−18 °C, 4 °C, or 20 °C), depicting the possible exposure conditions along transportation and house storage. Normalization as pre-processing and band region of 1000–1500 cm^{-1} produced the best results.

High protein content, polyunsaturated fatty acids, and water activity make fresh meat and marine products prone to spoilage through logistic stages. Similar to meats, fish and fish products may putrefy or become stale throughout transit, wholesale, and retail periods [300]. Temperature fluctuations along the cold chain can cause partial or full thawing and re-freezing, which produce a poor-quality product consisting of high free fatty acids and peroxide value [301], disrupted muscle tissue, and reduced water holding capacity [285]. NIR has been shown that, it can identify the repeated frozen-thawed cycles [302], predict microbiological spoilage [303], and ascertain the difference between fresh and frozen-thawed structures in fish fillets [304]. Lately, Asefa et al. [305], proved that NIR spectroscopy coupled with chemometrics was 100% efficient in classifying salmon based on the degree of temperature fluctuations encountered under simulated loading, transportation, and unloading conditions. Furthermore, the fast detection of oxidative impairment of pork myofibrils in the frozen state without thawing was possible by NIR/HSI (hyperspectral imaging) system [306]. HSI is a new technology that combines spectral and imaging methods. Once improved on a commercial scale, this combination can be an effective pointer for the deterioration prior to cold chain transportation. It is important for the handlers in the market to estimate the storage time of food products as it is a critical factor for food safety and consumer acceptance. These studies show that the use of vibrational spectroscopy in food transportation can offer the opportunity to prevent the deterioration of fish and meat products, thus improving their quality and extending their shelf life. However, portable devices provide unrealistic findings in some applications, highlighting the need for diverse, more extensive sample databases and measurement methods to enhance performance and build stronger models [169].

Consolidation of spectral analyses with advanced computer algorithms, networking tools, and data analytics enables the development of technologies such as real-time monitoring of transport and storage conditions of food products. For instance, in the period of transportation, temperature increases can lead to unfavorable results, such as the unintended heating of honey. Rapid evaluation of the changes caused by thermal exposure without any sampling requirement is possible with the combination of FTIR spectroscopy with chemometric methods like PCA and LDA. The combination enables 90% accuracy in distinguishing raw honey from thermally affected ones for evaluating its quality [307].

One of the potential problems during food transport and distribution is the risk of oxidation in edible oils [308]. Integration of a mesh cell (an accessory to load samples) into the FTIR spectroscopy mechanism enabled the interpretation of the stability of virgin olive oil stored at different temperatures (from 23 to 65 °C) and lightning settings (from 400 to 7000 lx), which simulate the actual conditions in supermarkets and transportation means [309]. Primary and secondary oxidation products formed were monitored within the spectrum gathered between 5000 and 400 cm^{-1}. The results obtained were valuable for optimizing the handling, storage, and transport settings of oils. In addition, long-term and unfavorable transportation processes also affect the final quality of sensitive foods, such as eggs. Therefore, hand-held measuring devices that determine the freshness of the egg without damaging it serve a similar purpose [310]. Likewise, Liu et al. [311] also reported a significant correlation between egg freshness and the Raman spectrum, and they demonstrated it is a novel, fast, and basic method for the nondestructive application to evaluate egg freshness.

Throughout post-harvest processing, storage, and transport of agri-food products, mycotoxins are readily formed in environments with favorable temperatures and humidity [312]. Consequently, the development of fast and reliable methods for identifying the presence of mycotoxins is crucial for ensuring food safety [313]. Wu et al. [313] reported that, SER spectroscopy is a sensitive and efficient method for screening trace mycotoxins. Nevertheless, the production of high-performance SER spectroscopy samples for on-site quantitative evaluation of actual food samples remains a difficult scientific problem. Furthermore, the results of Tao et al. [314] indicated the effectiveness of line-scan Raman imaging technology for distinguishing between uninfected control maize kernels, corn kernels contaminated with aflatoxigenic fungi, and corn kernels infected with non-aflatoxigenic fungi. As a result, continuous crop monitoring during production, storage, and transportation stages would enable fast disease detection and response, which could save billions of dollars by minimizing damage to cereals [238,315].

Furthermore, metabolites of chemical residues may develop during food manufacturing and transportation; thus, it may be necessary to further explore the effects of metabolic reactions in foods [316]. The surface-enhanced Raman spectroscopy SERS is a promising method for determining hazardous chemical residues, such as antibiotics and pesticides [317,318]. In addition, the migration from packaging substances has been a significant concern in food and health science for years. For example, plastics, such as polyethylene, are frequently used as food packaging materials for preservation and ease of use throughout food storage and transport [319]. In a previous study, the migration of low-density polyethylene (LDPE) was studied in Kefalotyri, Edam, and Parmesan cheeses using Raman and ATR-FTIR spectroscopy techniques. According to their results, the migration of LDPE was demonstrated for each cheese type during cold storage by these two vibrational spectroscopy methods. Therefore, a straightforward and effective vibrational spectroscopy technique is shown, which allowed them to obtain rapid and reliable results for the determination of LDPE migration from packaging materials [319]. Similarly, micro-Raman spectroscopy was used to observe the migration of microplastics from LDPE packaging to the external layer of cured meat samples, such as salami, mortadella, and bacon. According to their results, microplastics were initially determined on day 9 for bacon samples, followed by salami samples and mortadella on days 15 and 28, respectively. It has been reported that, Raman spectroscopy can be an efficient, rapid, and robust method to evaluate the migration of microplastics from foods [320].

In the field of food trading, there is a growing need for nondestructive evaluation of various quality characteristics of food products. This is even more important, if the product is rare and expensive. In the transportation and logistics industry, vibrational spectroscopy can be useful for the rapid analysis of complex mixtures, especially when dealing with remote locations or sensitive samples. However, environmental factors may interfere with the accuracy of the analysis. Therefore, the successful implementation of vibrational spectroscopy models in transportation and distribution systems would necessitate the development of further calibration models that encompass a variety of environmental variables, samples from various origins, extended sampling amounts at different conditions, and suitable spectral pre-processing.

Prompt action to prevent further issues

The use of vibrational spectroscopy in distribution centers is quite common, just as in production centers particularly in milk collection and distribution centers where raw milk quality analyzes are employed, and adulteration is detected. Also, quality classification is performed during the grain harvest, and the chemical quality parameters are determined in olive distribution centers by examining the protein and moisture of olives. Compliance with legal thresholds and contaminants are tested through analyzes performed at distribution centers, thus, possible deterioration and damage during transportation would be prevented by implementing solutions. Moreover, the advent of portable spectroscopy devices eliminates the need for various specific analysis appliances in distribution and collection centers.

Vibrational spectroscopy is a very useful tool for dairy collection and distribution centers especially in developing countries since the adulteration of milk and dairy products is a critical issue for these countries. The risk of spoilage of milk possesses significant challenges in collection and distribution centers due to the lack of effective cooling systems and inefficient maintenance, especially in summer season. Adulterants, such as sodium bicarbonate, caustic soda, calcium hydroxide, which are being used to prevent spoilage are rapidly detected in collection and distribution centers through FTIR [321]. Similarly, fish is also a highly perishable food and requires prompt chilling immediately following fishing and persistent frozen storage until reaching the final consumer. However, if the temperature exceeds the freezing point, postmortem changes begin within a few hours leading to microbial and chemical deteriorations. Determination of microbial and chemical quality safety with spectroscopic methods during fish collection, distribution and transportation stages is significant in terms of obtaining rapid results for estimating possible deterioration [322]. Moreover, microplastic existence in fish is yet another health concern and determining the amount and variety of microplastics in sea, and fish is also growing problem. Vibrational spectroscopy is a useful tool for identification of unknown microplastics even for low molecular weight plastic particles with high accuracy [323].

On the other hand, while the use of this technology highly depends on expertise, to obtain reliable results with high accuracy requires specialized knowledge. In this respect providing training for individuals working in distribution centers is essential. Moreover, verifying the results with the actual laboratory analysis occasionally is also critical for device calibration which brings dependency on the device distributor companies and quality assurance laboratories [29]. By comparing the results from chemical analysis with the reading from a spectroscopy device, adjustment can be made to upgrade precision by determining a margin of error (bias adjustment) for the value read by the device. Furthermore, the presence of device noise which is specific to each device must be evaluated individually for each device to receive accurate results [324].

Currently available portable devices find wide applications in field and distribution centers, but low data processing capacity of these on-site devices is restricted to its grateful utilization [325]. Existing portable devices have challenges with perception of multi-dimensional spectral data and complex signal sensation in remote locations. Therefore, it would be substantially beneficial to integrate data transfer systems into existing portable devices that would enable remote data storage, and so maintain records for food traceability [326,327].

Future prospects of vibrational spectroscopy in food science

The future prospects for vibrational spectroscopy hold great promise across various domains, including food science, where it stands poised to revolutionize quality control, safety assurance, and nutritional analysis. In the realm of food science, vibrational spectroscopy techniques offer unparalleled potential for rapid and nondestructive assessment of food quality, authenticity, and safety. Advancements in instrumentation and data analysis are expected to further enhance the sensitivity, specificity, and speed of these techniques, enabling more comprehensive and efficient analysis of food samples. Additionally, the integration of vibrational spectroscopy with other analytical methods, such as mass spectrometry and chromatography, holds potential for addressing complex food-related challenges, such as identifying foodborne pathogens, detecting adulterants, and assessing nutritional composition. Furthermore, the development of portable and on-site spectroscopic devices could facilitate real-time monitoring of food processing operations, supporting optimization of production processes and ensuring compliance with regulatory standards. Overall, the future of vibrational spectroscopy in food science is bright, with continued innovation expected to drive advancements that enhance food quality, safety, and sustainability.

Conclusion

The application of vibrational spectroscopy throughout the entire value chain, from farm to fork, holds tremendous promise for improving food quality, safety, and sustainability. This powerful analytical technique has proven its efficacy at various phases of the food production and processing spectrum, allowing for the rapid and nondestructive analysis of complex samples. Vibrational spectroscopy has proven useful for monitoring crop health, optimizing nutrient management, and assessing soil quality at the farm level. This technology assists farmers in making informed decisions regarding irrigation, fertilization, and pest management by supplying real-time insights into plant physiology and metabolic processes. By optimizing these factors, agricultural productivity can be increased while the environmental impact is minimized.

Researchers often select vibrational spectroscopy techniques for their ability to provide detailed insights into the molecular composition and structure of samples. These techniques offer unique advantages, including nondestructive analysis, high sensitivity, and the ability to characterize a wide range of materials, from solids to liquids and gases. Vibrational spectroscopy methods, such as FTIR, NIR, and Raman spectroscopy, offer distinct advantages over other analytical techniques. For example, they typically require minimal sample preparation, reducing time and resources needed for analysis. However, vibrational spectroscopy also has its limitations, including susceptibility to interference from sample matrices and the need for expertise in data interpretation. Compared to other analytical methods, such as chromatography or mass spectrometry, vibrational spectroscopy techniques may have lower resolution or depth penetration in certain applications. Nonetheless, the versatility, speed, and nondestructive nature of vibrational spectroscopy make it a valuable tool in various fields, from chemistry and materials science to biomedical research and food analysis.

Vibrational spectroscopy offers significant advantages in post-harvest management and food processing on the route up the value chain. It enables rapid identification and quantification of key constituents, such as moisture, protein, fat, carbohydrates, and micronutrients, thereby ensuring the nutritional and quality integrity of the product. This technique also enables the detection of contaminants, adulterants, and allergens, thereby ensuring food safety and protecting consumer health. In the domain of food authentication and traceability, vibrational spectroscopy is an effective method for confirming the origin, authenticity, and quality of food items. By comparing spectral signatures to extensive databases, it becomes possible to detect fraudulent practices such as mislabeling or adulteration, thereby protecting consumer confidence and promoting fair trade.

In addition, vibrational spectroscopy allows for real-time monitoring of culinary processes, such as fermentation, brewing, and drying, ensuring consistency and quality control. Its nondestructive nature enables continuous analysis, reduces sample preparation and waste production, and ultimately results in cost savings and environmental advantages. In conclusion, the incorporation of vibrational spectroscopy throughout the entire food value chain provides numerous benefits, such as increased productivity, enhanced food safety, increased sustainability, and increased consumer confidence. Its nondestructive, rapid, and adaptable nature makes it an indispensable instrument for both researchers and industry professionals. Vibrational spectroscopy will become a cornerstone technology in the realms of food production, processing, and quality assurance as a result of continued advancements in this field and the development of comprehensive data analysis techniques.

NOMENCLATURE

Air-PLS:	Adaptive iterative reweighting partial least squares
ALS:	Alternating least squares
ANN:	Artificial neural network
ATR-FTIR:	Attenuated total reflection Fourier transform infrared
CARS:	Competitive adaptive reweighted sampling
CMR:	Confocal micro raman
CNN:	Convolutional neural networks
CoV:	Coefficient of variation
CV:	Cross validation
CWT:	Continuous wavelet transform
DA:	Discriminant analysis
DFT:	Density functional theory with Gaussian09 code
DI:	Digital imaging
DRIFT:	Diffuse reflactance infrared Fourier transform
DRMSEC:	Dimensionless root mean square error of calibration
DRMSECV:	Dimensionless root mean square error of cross validation
DT:	Decision tree

ELM: Extreme learning machine
EV: External validation
FAO: Food and Agriculture Organization of the United Nations
FCR: False compliant rate
FDA: Flexible discriminant analysis
FEM: Finite element method
FT-MIR: Fourier transform mid-infrared
FT-NIR: Fourier transform near-infrared
FT-NIRS: Fourier transform-near infrared spectroscopy
GA-Si-PLS: Genetic synergy interval partial least square
GLM: Generalized linear model
HCA: Hierarchical cluster analysis
HSI: Hyperspectral imaging
HSI-NIR: Hyperspectral imaging-near infrared
HT: Harvest time
IoT: Internet of Things
KNN: k-nearest neighbors
KS: Kennard–Stone algorithm
LDA: Linear discriminant analysis
LDPE: Low density polyethylene
LIF: Laser induced fluorescence
LR: Linear regression
LS-SVM: Least square-support vector machine
LSVM: Linear support vector machine
MIR: Mid-infrared
MAL: Machine learning
MLR: Multiple linear regression
MLP: Multilayer perceptron network
MULR: Multiple linear regression
MP: Multilayer perceptron
MPLS: Modified partial least squares
MRL: Maximum residue limit
MSC: Multiplicative scatter correction
NB: Naive bayes
NDSI: Normalized difference spectral index
NIPALS: Nonlinear iterative partial least squares
NIR: Near infrared
OPLS-DA: Orthogonal partial least squares-discriminant analysis
PCA: Principal component analysis
PC-ANN: Principal component-artificial neural network
PC-LDA: Principal component-linear discriminant analysis
PC-MLP: Principal component-multilayer perceptron network
PCoA: Principal coordinates analysis
PLS: Partial least squares
PLS-DA: Partial least squares-discriminant analysis
QDA: Quadratic discriminant analysis
Qi: Quality index
QR: Quick response
QSVM: Quadratic support vector machine
R: Correlation coefficient
R^2: Determination coefficient
RF: Random forest
RFID: Radio frequency identification
RF-SPA: Random forest successive projection algorithm
RMPRESS: Root mean predicted residual error sum of squares
RMSE: Root mean square error
RMSEC: Root mean square error of calibration
RMSECV: Root mean square error of cross validation
RMSEP: Root mean square error of prediction
RPD: Relative percent difference
RPIQ: Ratio of performance to interquartile range
RR: Ridge regression
RSD: Relative standard deviation
SEC: standard error of calibration
SECV: Standard error of cross-validation
SEP: Standard error of prediction
SER: Surface-enhanced Raman
SIMCA: Soft independent modeling by class analogy
Si-PLS: Synergic interval partial least-squares
SPA: Successive projections algorithm
SR: Spatially resolved
SMA: Self modeling mixture
SNIR: Shortwave near infrared
SVM: Support vector machine
SVMDA: Support vector machine discriminant analysis
SVR: Support vector regression
SWIR: Short-wave infrared
TDR: Total discrimination rate
TSS: Total soluble solid
VIS: Visible
VIS-NIR: Visible-near infrared
VSNIR: Visible shortwave near infrared
1D-CNN: One-dimensional convolutional neural network
3-MCPD: 3-monochloropropanediol

Disclosure statement

No potential conflict of interest was reported by the author(s).

Funding

Dr. Ravi Pandiselvam would like to thank Indian Council of Agricultural Research (ICAR)-AICRP on PHET, Ludhiana [Project No: 1000767018], for funding.

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