Advances in Spectroscopic Analysis of Food and Drink

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Advances in Spectroscopic Analysis of Food and Drink

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To my parents

Contents

Preface

Quality analysis of food and drink is undoubtedly in everyone's interest. Accordingly, this field has consistently attracted the attention of the scientific community. The quality parameters of these items may be analysed using several approaches. This volume, titled Advances in Spectroscopic Analysis of Food and Drink, presents quality assessment applications based on different spectroscopic techniques. Fruits, fruit juices, coffee beans, and edible oil samples have been covered in particular. Case studies on grape fruit juice, pomegranate fruit juice, and apple juice have been presented among the fruit juice category. Similarly, quality analysis of varieties of coffee (espresso, traditional, and instant), mate tea, star anise, and their respective infusions have been presented. There are 12 chapters in this volume covering different molecular and atomic spectroscopy techniques, including Fourier transform infrared (FTIR) spectroscopy, near-infrared (NIR) and mid-infrared (MIR) spectroscopy techniques. Electron spin resonance (ESR) spectroscopy techniques have also been included. The chapters have mostly adopted a bottom-up approach and talk about the applications of these spectroscopic techniques combined with data analytics.

I sincerely thank John Navas, Senior Commissioning Manager at IOP Publishing, for giving me an opportunity to present this volume. I also wish to thank Phoebe Hooper, Editorial Assistant at IOP Publishing, for extending her support during different stages of this project. I thank the expert contributors for their quality contributions, which have made this volume a unique collection.

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Editor biography

Ashutosh Kumar Shukla

Ashutosh Kumar Shukla has more than two decades of physics teaching and research experience. He has published numerous articles and review articles in peer-reviewed journals. He has also authored textbooks and participated as an editor of more than two dozen edited volumes published by reputed publishers, often prepared in collaboration with experts from different countries. He intends to continue pursuing his academic interests, which include spectroscopy applications in different fields of societal importance.

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IOP Publishing

Advances in Spectroscopic Analysis of Food and Drink

Ashutosh Kumar Shukla

Chapter 1

Determination of fruit quality: a spectroscopic approach

Triveni Shelke, Nabamita Halder and Monalisa Mishra

The market price of fruit is significantly influenced by quality. Meanwhile, the quality of fruit may be improved by a variety of processes that concentrate on firmness, ripening, acidity, and soluble solid contents, among other factors. However, the different procedures that claim to improve the quality of fruit need to be examined. The parameters that are used in determining the quality of fruit can be assessed using spectroscopic analysis. Since existing techniques are labor-intensive and complicated, spectroscopy offers a superior way to ascertain the chemical and physical characteristics of fruit. In particular, the internal and external chemo-matrices of the fruit can be identified using the spectroscopic method. Adulterations of fruit products can also be an analyzed using spectroscopic methods. Fruits such as mango hold a strong place in the Indian market and spectroscopic approaches can help to improve the yield of better-quality fruits.

1.1 Importance of fruit in the human diet

Fruits can be classified based on their anatomical structures and origins as simple, complex, and accessory fruits. The simple fruits include dry and fleshy simple fruits [1]. On the basis of the region in which they grow, they are classified as temperate zone, sub-tropical and tropical fruits (figure 1.1). Fruits are nutritionally rich (table 1.1) and are a source of dietary fibers, vitamins, and minerals [2]. They are strong antioxidants, and act as detoxifiers of carcinogens and modifiers of metabolic processes. These properties make fruits beneficial supplements to avoid diseases such as heart disorders, chronic diseases, and cancer [3]. The dietary fibers form bulks in the intestine, and hence increase absorption of nutrients. The fibers when fermented to short fatty acids in the colon act as anti-carcinogens [4]. In addition, high fiber content helps in calcium absorption and decreases acid-load in the diet [5]. Several secondary metabolites, e.g., anthocyanins, procyanidins, and flavanols, reduce

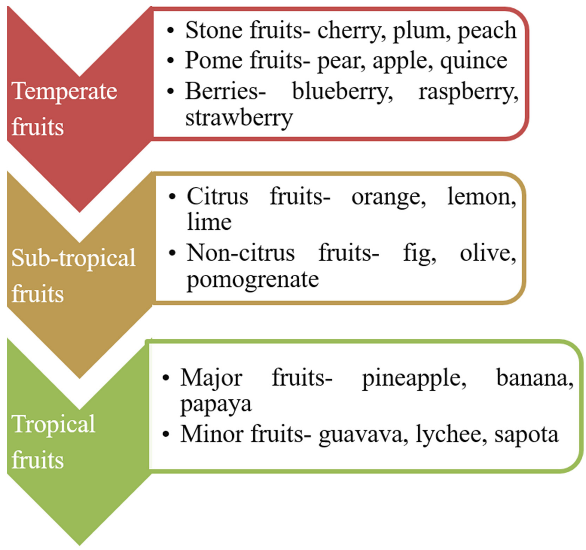

Figure 1.1. Classification of fruits based on their regions of growth.

Table 1.1. Nutritional qualities of fruits.

Nutrients	Examples	References
Carbohydrates	Fructose, glucose	Slavin, Lloyd [8]
Antioxidants	Carotenoids, phenolic compounds	
Dietary fibers	Cellulose, pectin, lignin	
Minerals	Calcium, iron, potassium	
Vitamins	Vit A, B6, C	
Others	Water, proteins, fats	

heart-related disease risks, and protect against lens damage and respiratory syndromes [6]. Carotenoid rich fruits maintain cholesterol and reduce oxidative damage [7].

Low consumption of fruits is associated with diseases such as hypercholesterolemia, blood pressure, osteoporosis, and pulmonary diseases [9], it also promotes obesity due to overgrowth of adipose tissues [10]. Fruits help in loss of body weight because the fibers create an environment in which the enzymes hydrolyzing fats, carbohydrates, and proteins have reduced activity [11]. The deteriorating quality of fruits is one of the reasons for increasing malnutrition [12]. The recommended level of fruit and vegetable intake is 400 g/person [13]. The 2015 data of GEMS/Food database shows the mean fruit intake of India was 158.2 g/d [14]. The quality of fruit deteriorates due to many factors that influence the production, ripening, and marketing of the fruits.

1.2 Factors affecting fruit quality

The quality of fruit is determined by various factors and is tested on several parameters (figure 1.2).

1.2.1 Pre-harvest factors

Pre-harvest factors include environmental and cultural factors.

1.2.1.1 Environmental factors

Temperature determines the rate of transpiration, and effects photosynthesis, uptake of nutrients, biochemical reactions inside the plant cells, and fruit setting [15]. Temperature affects the ripening of the fruits: some fruits when exposed to sunlight ripen faster, whereas others delay their ripening. Temperature also influences the sugar content and acidity [16]. The concentration of carbon dioxide is related to the stomata conduction and ozone uptake [17]. Optimum rainfall is essential for better-quality fruit: higher rainfall can cause mechanical damage to the fruits, whereas lesser rainfall can affect the growth of the plant [18]. Exposure to sunlight affects the size, weight, and anthocyanin production in fruits. In addition, the canopy light condition influences the time of ripening, and hence maturity [19]. Finally, humidity is related to the color, acidity, and also Salmonella outbreaks in fruits [20].

1.2.1.2 Cultural factors

The cultural factors take nutrition, growth regulators, and disease-causing pests into consideration. The appropriate amount of minerals such as nitrogen, calcium, phosphorus, boron, copper, magnesium, and potassium are essential for fruit development. The other compounds that are actively involved in the growth of the fruits are the growth regulators or phytohormones, which constitute auxin, cytokinins, ethylene, and gibberlins [21]. Pests such as Saltatoria, Dermaptera, Isoptera, and Hemiptera are widely responsible for fruit stock losses [22].

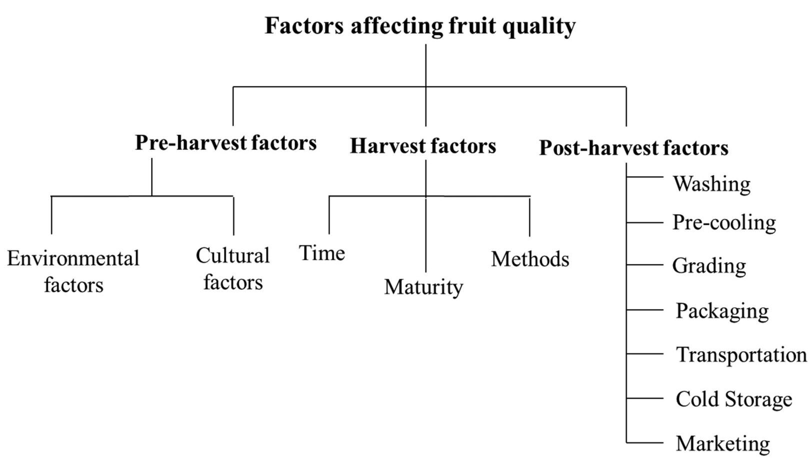

Figure 1.2. Factors affecting fruit quality.

1.2.2 Harvest factors

The harvest factors include the time and maturity at which the fruits are harvested, as well as the methods used for harvesting. The time of the day for harvesting, and the time lapse between harvest and transportation make the fruit susceptible to bruising. The damage done by bruising is more prominent when the harvesting is done at the heat prone time of the day. Bruising decreases the shelf life of the fruit because it promotes early senescence [23]. Meanwhile, an early or late harvest influences the fatty acid composition in the fruits [24]. Fruits are divided on the basis of maturity as fully mature, half mature, and immature. At the time of harvest, the fully and half mature fruits show good fruit quality upon ripening when compared to the immature fruits [25]. Berries are generally harvested at early maturity stages for their firmness [26]. The traditional methods of harvesting with hooks attached to bamboo may damage the fruit due to injuries and bruises [27]. Sun drying of the berries upon using impact force harvesting leads to a fading of fruit color and affects its appearance; therefore, the shade drying method is much preferred for berries [28]. Modified machine harvesters decrease the firmness and increase the probability of bruises in the berries [29].

1.2.3 Post-harvest factors

Post-harvest factors include packing house operations such as washing, pre-cooling, grading, packaging, transportation, cold storage, and marketing. The fruits are washed with chlorine water around the pH of 6.5–7.5 to maintain quality. Pre-cooling removes the heat acquired by the fruit when in the field, which enhances shelf life. Various types of pre-cooling methods are applied to the fruits based on their requirements. The grading of the fruits is based on their size and appearance. Instruments such as a size gauge and rings for circular fruits are used to grade them into a designated category. The type of packaging and the arrangement of the fruits in layers from top to bottom determine the fate of the fruit in the market. Generally, the fruits in the top layers do not suffer much damage whereas those in the bottom layers suffer bruises [30]. Packing materials such as double walled fibers, foam nets, and plastic trays to arrange the fruits in layers are chosen according to the texture of the fruit [31]. Temperature has to be monitored during the transportation of fruits to the storage houses, and eventually to the market. In addition, radiation treatment and fumigation are usually used to resist certain molds that can infect the fruits during transportation [32]. Cold storage can alter the fruit's softness, antioxidants, and biologically active compound levels depending on the pre-applicants used [33]. There are also many different stages of marketing that can affect the fruit's quality [34].

1.3 Spectroscopy in fruit quality determination

Fruit quality plays an essential role in customer satisfaction and fruit sales as a whole. Fruit quality is mainly attributed to ripeness, color, taste, smell, firmness, soluble solid contents (SSC), and size. These are common physical markers that are used to assess the condition of a fruit before purchase but they are greatly unreliable and do not give an absolute assessment of the fruit's quality, hence more competent parameters have been taken into consideration, such as acidity, sugar concentration, and starch content. The SSC, sugar concentration, acidity, and starch content measurements are estimated by conventional means such as refractometry, pH monitoring, and titration acidity [35]. However, these procedures are invasive, difficult to perform, and expensive [36]. This has prompted the demand for a reliable, non-invasive, and fast method for fruit quality assessment.

The most effective method for accomplishing this is spectroscopic analysis, which has many benefits: it is non-invasive, which allows for the acquisition of internal quality parameters in fruits without affecting their surfaces; the quantification processes are straightforward and fast because no time-consuming chemical treatments or reactions on fruit samples are needed; and it enables the simultaneous detection of multiple internal fruit attributes [37]. However, the disadvantage of the tiny point-source measurements frequently used in spectral assessment is that they do not provide spatial information, which is essential in many scenarios evaluating fruit quality [37]. To accurately quantify the internal parameters of fruit quality, the visual (Vis) and near-infrared (NIR) properties are typically used in the analysis of fruit quality. Hyperspectral imaging, a combined spectroscopic and imaging approach that produces a three-dimensional hyperspectral image with two-dimensional spatial information and one-dimensional spectral information, is another technique that is used to assess the quality of fruit [38]. The commonly used techniques for fruit quality analysis are explained in the following subsections.

1.3.1 Vis/NIR spectroscopy

Vis/NIRS spectroscopy has a lot of applications in determining fruit quality. It has been used to acquire fruit spectra from both climacteric fruits such as mango, apple, banana, plum, apricot, peach, nectarine, and kiwi, and non-climacteric fruits such as watermelon, mandarin, and cherry. The NIR region of the electromagnetic spectrum has a range of 750–2500 nm and measures internal parameters such as titrable acidity (TA), ripeness, SSC, pH, and other fruit quality parameters in a non-destructive way. The visible region of the electromagnetic spectrum has a range of 400–750 nm, and measures the color and pigments present in the fruit. Several studies of the assessment of these properties have been conducted, which have assessed attributes at a certain wavelength. For example, a portable Vis/NIR spectrometer with a range of 960–1700 nm has been used to determine the SSC and TA 'Tommy Atkins' mango [39]. This works on the principle that the Vis/NIR has the signals for almost all of the functional groups and structures of the compounds with a probable stable spectrum [40], and the varying wavelengths are compatible with specific compounds, such as organic compounds with –OH, –NH, and –CH, bonds, are more sensitive to wavelengths in the NIR range [41]. Wavebands found in the Vis/NIR range are frequently used in multispectral and hyperspectral imaging techniques to assess fruit quality [42–44]. The detection of pigments such as chlorophyll in immature canola seeds [45] and carotenoids in wheat [46] is made possible by spectrophotometric examination of absorbance at certain wavelengths associated with the pigments. Radiation that strikes a specimen can be reflected, transmitted, or absorbed, which generates a specific spectrum reflecting a physical property or chemical constitution of the material [37]. This makes it easier to sequester the comparable parameters for testing and quantifying. The Vis/NIR range includes wavelengths for most of the major functional groups, side chains, and chemical compounds. This region is also highly dominated by H_2O, which absorbs in the NIR region and leads to interference in the spectral data. This is further followed by chemometric techniques, which involve the quantification of the desired variable and removal of unrelated variables from the spectral data collected from the sample. Chemometrics aid in obtaining clearer information from the spectral data regarding the required characteristics of the fruit samples.

The Vis/NIR range also has the advantage of quantifying more than one parameter at the same time, hence replacing several tests while also reducing contact procedures and human effort. This method appears to be effective in assisting breeders with genotype screening in breeding operations. Additionally, it enables online fruit screening and fruit quality evaluation, creating new market niches and prospects for fruit commercialization in the raw or processed market [47]. Now that Vis/NIR technology is available in handheld devices, it is becoming increasingly common to apply Vis/NIR in fruit quality analysis techniques.

1.3.2 Hyperspectral imaging spectroscopy

Classification systems for fruits and vegetables use a color video camera to take photographs with three filters that mimic human vision by employing red, green, and blue (RGB) wavelengths [48, 49]. They are therefore limited to observing events and are frequently unable to learn much about the exterior or inside makeup of the items. They are also unable to distinguish outward damage that has a color comparable to the healthy fruit skin. As a result, the market's increasing demand for fruits of higher quality has contributed significantly to the development of methods that can extract both spectral and spatial data from a sample using spectroscopy and imaging techniques such as hyperspectral imaging (HSI) spectroscopy [50]. These techniques are similar to the Vis/NIR in terms of quick evaluation and non-invasive determination but they have distinct differences with regards to their spectral data output—Vis/NIR techniques obtain their spectral data from a point-source, which limits the scanning to a small area of the sample, whereas HSI scans over a larger area, which gives more inherent knowledge about the components of the sample and works with its heterogeneity [51].

Since it is a result of the physical and chemical characteristics of the individual substance examined, the spectral signature obtained through HSI is distinctive [52]. Hyperspectral images are three-dimensional cubes made up of one wavelength and two spatial dimensions [$I(\lambda, x, y)$] [53]. Four methods can be used to create three-dimensional hyperspectral image cubes. There are two spectral scanning methods and two spatial scanning methods: area and plane scanning, point scanning, and line scanning, respectively [54]. When compared to VIS/IR analysis, which examines the sample as a whole and calculates its average composition, HSI has the advantage of providing spatial dispersion of sample quality metrics [55]. HSI can detect several injuries. It can also detect decay in the fruit and vegetable samples with great accuracy, e.g., bruising of fruits is not as readily detected by other spectroscopic methods due to variance in the defects and lack of proper spectral data. For example, Xing *et al* tested the effectiveness of a hyperspectral imaging system for detecting apple bruises [56]. The HSI proves to be more accurate over NIRS because it provides a continuous evaluation in production with greater data of the variety of attributes of fruits. HSI calibrations are also faster due to their greater statistical data from a single sample, where NIRS assumes sample homogeneity which might not be the real case [57].

The only drawback of HSI is that its setup is quite costly and time consuming. In addition, the hyperspectral imaging system cannot be employed online or in real-time due to the redundant data. In addition, a multispectral imaging system's effective wavelengths are always determined by analyzing the data from hyper-spectral imaging [58].

1.4 Chemometrics analyzed through spectroscopy

The data that are usually obtained from various spectroscopy techniques are mostly obtained from the Vis/NIR region. This region (as discussed earlier) includes the wavelengths for almost all of the side chains. However, the presence of so much information leads to undesired complications in the spectrum. Hence, it is important to preprocess the spectral data to improve the results and reduce noise, so that it can be analyzed properly [59]. There are many techniques for spectrum preprocessing and calibration in chemometrics, including partial least squares (PLS), principal component regression (PCR), and others. Note that MLR represents multiple linear regression, LS-SVM represents least square support vector machine, and ANN represents artificial neural network [41, 60]. The different types of pre-treatment methods are discussed in table 1.2.

1.5 Parameters for fruit quality analysis

Fruit quality may be measured by analyzing various parameters through spectro-scopy (table 1.3). These parameters are applied to the types of fruits [37].

1.6 Determination of fruit quality

1.6.1 Determining the quality of mango

Mango (*Magnifera indica* L.) is one of the most widely popular climacteric fruits, and has a huge commercial impact on both Indian and foreign markets. The quality of mangoes is described mainly by their sweet and sour notes, and the ripe color of the pulp. Mangoes are best collected when they are mature-green and pre-climacteric [75]. The fruits are picked in two stages: the pre-harvest stage and the post-harvest stage. The post-harvest stage is when the ripening is complete, the quality of fruits differs on the basis of the picking time. The fruits that have reached

Table 1.2. Chemometrics in spectral data.

Spectral preprocessing methods	Function	References
Smoothing	Removes high-frequency disturbances from the spectrum and improves the ratio of signal to noise. The primary idea behind it is to 'average' or 'fit' a number of points inside a window in order to arrive at an ideal estimation value. The spectral resolution would be reduced the wider the window is. Therefore, picking the right window width is essential.	Wang *et al* [37]
Offset Correction	In this type of central processing, the average value of the first few wavelength points is taken out of each spectrum, e.?g., five. The baseline drift is the only thing that is modified by offset correction; the spectrum structure is left unaltered. Its major purpose is to lessen the impact of optical distance, instrument noise, and the detecting environment.	Wang *et al* [37]
De-trending	De-trending is a strategy to get rid of the spectrum's baseline drift, which is typically used along with traditional normal variate correction (SNV).	Wang *et al* [37]
Multiplicative scatter correction (MSC)	MSC is a modification technique that is used to account for additive or multiplicative effects in spectral data.	Barnes *et al* [61, 62])
Standard normal variate (SNV)	SNV is a row-oriented modification that may be able to eliminate multiplicative interferences from spectral data that are caused by scatter and particle size effects. SNV reduces the effects of dispersion by focusing and adjusting each individual spectrum.	(R. Barnes *et al* [63]; Barnes *et al* [61])
Spectral derivatives	Drifting and scattering are removed using the first and second derivatives, respectively. They can improve spectral resolution and sensitivity, eliminate background interference, and separate superposed peaks. Two frequently used methods for spectral derivatives are direct finite difference and Savitzky–Golay (S?-?G) derivatives.	Wang *et al* [37]
Net analyte preprocessing (NAP)	NAP is mainly used to extract spectral data of a specific component in a mixed spectrum.	Wang *et al* [37]

Wavelet transformation	The basic idea of wavelet transformation it is to combine sinusoidal waves with numerous different amplitudes, frequencies, and orientations from the original spectrum. The chemical signals from the sample are broken down into measurable components according to their frequencies by using a basic function.	Wang *et al* [37]
Optimal wavelength selection	**Function**	**References**
Successive projections algorithm (SPA)	SPA is a forward selection method that seeks out a wavelength with the least amount of duplicated information and collinearity by using simple operations in a vector space. SPA begins with one wavelength and keeps adding more until a certain number is reached. The bulk of the sample's spectral data could be accurately captured using the SPA-extracted wavelengths with the least amount of information overlap.	Araújo *et al* [37, 64, 65]
Regression coefficient (RC)	The RC value is indicative of how predictive the model's performance is. The absolute value of RC represents the characteristic wavelength.	Wang *et al* [37]
Loading weights (LW)	In LW, a particular wavelength is chosen, and these wavelengths are equal to the latent variables. The loading weight is obtained from the latent variables, which is predictive of the impact of wavelengths on the model.	Wang *et al* [37]
Genetic algorithm (GA)	GA is an algorithm that uses genetic operations based on a randomly selected generation, such as genetic selection, crossover, and mutations to obtain best outcomes. Through this, useless spectral data is removed and noise is significantly reduced.	Wang *et al* [37]
Competitive adaptive reweighted sampling (CARS)	CARS is a cutting-edge algorithm that chooses the best wavelength based primarily on Charles Darwin's concept of the 'survival of the fittest.' The adaptive reweighted sampling method of a PLS model is used to sequentially identify wavelengths with large absolute coefficients as CWs. Cross validation is used to create a number of variable subsets, and the one with the lowest root mean square error of cross validation (RMSECV) is chosen.	(H. Li *et al* [66]; Wang *et al* [37])

(*Continued*)

Table 1.2. (*Continued*)

Optimal wavelength selection	Function	References
Uninformative variable elimination (UVE)	UVE is a method for selecting variables based on an analysis of the PLS regression coefficient. Using calibration samples that are randomly selected, the technique first builds a large number of models and then evaluates each variable using the stability of the corresponding coefficients in these models. Variables with poor stability are eliminated.	Centner *et al* [37, 67, 68]
Calibration models	**Functions**	**References**
Multiple Linear Regressions (MLR)	MLR predicts the dependent variables as a linear combination of the spectral values at each wavelength point. The error between the predicted and measured values is diminished in a least squares sense. The effectiveness of MLR algorithms is reduced by multicollinearity between the variables in spectral analysis.	Wang *et al* [37]
Principal component regression (PCR)	In PCR, a small number of principal components (PCs) are found using principal component analysis (PCA). These PCs are used as predictors and to create an MLR model rather than using the original spectral data.	Wang *et al* [37]
Partial least squares regression (PLS)	PLS forecasts the dependent variables by sifting through the variables to find the smallest collection of orthogonal elements with the best predictive power. The importance for forecasting the dependent variables was used to order these orthogonal elements, also known as latent variables (LVs). PLS regression, which combines the ideas of MLR and PCA, is especially useful when there is multicollinearity between the variables and there are frequently fewer latent variables than in PCR regression.	Wang *et al* [37]

the ripening stage are of better quality than those that are preharvested [75]. However, the ripened fruits lack the lifespan required for long delivery distances. Thus, determining fruit quality is of utmost importance, and using spectroscopic methods is the best way to achieve it without destroying the fruit samples. Mangoes fit for export are usually rated based on their green stage [75]. However, the buyers

Table 1.3. Parameters used to assist the analysis of fruit quality.

Parameters	Uses	Spectral range	References
Acidity	Measures of organic acids.	5882–9900 nm	Bureau *et al* [69]
Soluble solids/ sugar contents (SSC)	Measures the total solid content in the given solution. In the case of fruits, it is mostly the sugar content.	800–1100 nm	Angra *et al* [70]
Firmness	Measures the crispness of the fruits.	500–1000 nm	Mendoza *et al* [43]
Bruise detection	The damage in the fruit's cell and tissues is noted.	380–1000 nm	Luo *et al* [71]
Total polyphenols	Measures polyphenols content in fruits.	400–2500 nm	Pissard *et al* [72]
Vitamin C content	Measures Vitamin C content in the fruits.	1333–1835 nm	Xia *et al* [73]
Pigments	Measures different families of pigments in fruits.	680 nm	Zude *et al* [74]

will eat mango fruits when they reach the maturity stage. In the interim, the employees will be able to assess the quality of the mango fruits solely based on their physical characteristics, such as color, firmness, size, and weight [76]. When the fruits are mature, such grading techniques at the green stage typically cannot ensure the quality of the flavors. Therefore, the categorization of quality is crucial.

Theanjumpol *et al* determined the quality of mangoes with the spectroscopic approach. The spectral data was collected at wavelengths of 700–1100. Total soluble solid (TSS) and TA were then calculated using a digital refractometer. Prior to calibration, the spectral data were translated using a number of mathematical methods and prediction models based on partial least square regression were produced. In an effort to identify physiological issues, mango fruits were kept in a chamber at a temperature of 5 °C–1 °C to mimic the symptoms of a chilling injury [77].

1.7 Conclusion

The quality of a fruit lies in its nutritional constituents as well as its appearance, which both play a major role in determining its market value and the costumer's preference. Although fruit quality can be evaluated using several techniques, spectroscopic methods have many advantages when compared to others. For example, spectroscopic methods are simple and do not damage the fruit during the process, they can also quantify more than one attribute at a time. However, even though they are quite useful techniques, they do not provide spatial information about the fruit. Many new technologies are being developed that use the basics of spectroscopy to build novel systems that are robust and able to evaluate quality more accurately.

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Chapter 2

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Chapter 6

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