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Application of infrared spectroscopy using Fourier transformation in the analysis of bioactive compounds of citrus fruits - systematic review

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KEY CONTRIBUTION
An overview of the application of FTIR spectroscopy as a fast, non-destructive method for the analysis of bioactive compounds in citrus fruits and their products is shown here. It highlights the advantages of combining FTIR spectroscopy with chemometric tools (e.g. PCA, PLSR) for accurate classification, authentication, and quality assessment of samples. The paper discusses the limitations of the FTIR method in the analysis of complex matrices and compounds in low concentrations and emphasizes the need for complementary techniques such as LC–MS and GC–MS. It emphasizes the potential of FTIR spectroscopy in sustainable food systems, especially in the valorisation of citrus processing by-products.

ABSTRACT

Citrus fruits (*Citrus spp*.) constitute a significant portion of global agricultural production due to their rich nutritional profile and the presence of bioactive compounds with positive health effects. Phytochemicals such as flavonoids, carotenoids, phenolic acids and terpenoids contribute to the antioxidant, anti-inflammatory and cardioprotective effects of citrus fruits and make them important and functional foodstuffs. Infrared spectroscopy coupled with Fourier transformation, or FTIR spectroscopy, is increasingly used as a rapid, non-destructive, and reliable method for analysing the chemical composition of fresh and processed citrus fruit samples, including juices, pulp, peel, and essential oils. FTIR enables the identification and quantification of bioactive substances by detecting characteristic vibrational bands. In combination with chemometric techniques such as principal component analysis (PCA) and the method of partial least squares regression (PLSR), it allows for the accurate classification and estimation of the content of bioactive compounds. The method has also proven useful for authentication, quality control, and the analysis of citrus waste and by-products. Despite its many advantages, FTIR spectroscopy has limitations in the analysis of complex mixtures and low concentrations of compounds, as well as poor selectivity compared to methods such as high-performance liquid chromatography (HPLC) or gas chromatography with mass spectrometry (GC–MS). Therefore, it is often used in combination with other techniques to increase analytical accuracy and specificity. Thanks to its simplicity, speed, and ability to analyse different matrices, FTIR spectroscopy is a valuable tool in food and agricultural science, especially in the context of quality control and valorisation of bioactive compounds in citrus fruits.

Introduction

The genus *Citrus*, which is part of the subfamily *Aurantioideae* within the family *Rutaceae*, is one of the most important genera of fruit species cultivated worldwide for their highly valued fruits, either for fresh consumption or for processing (Zhong and Nicolosi, 2020). This group of citrus fruits includes oranges, tangerines, lemons, limes, grapefruits, pomelo, citrons, etc., as well as a wide range of their hybrids (Richa et al., 2023). Many citrus species are cultivated in the Republic of Croatia, with the most intensive production being concentrated in the Dubrovnik-Neretva County (Kaleb, 2014). Among mandarins, the most common variety is the 'Satsuma', which includes cultivars such as 'Kawano Wase', 'Chahara', 'Zorica Rana', 'Owari', 'Kuno', 'Saigon' i 'Okitsu'. Of the lemon varieties, the most cultivated are 'Lisbon', 'Meyer', 'Meyer Improved' i 'Eureka'. As for oranges, the most common varieties are 'Washington Navel', 'Skaggs Bonanza Navel' and 'Tarocco' (Černi et al., 2020).

Citrus fruits and their juices have long been recognized as an important part of a balanced and healthy diet, primarily due to their rich nutritional profile and the presence of bioactive compounds with beneficial effects on health, which makes them extremely popular in global consumption and production (Lu et al., 2023). Scientific studies confirm the positive effects of citrus fruit consumption, including antioxidant, anticancer, anti-inflammatory and cardioprotective effects, which are largely attributed to diverse phytochemical compounds such as, vitamins, minerals, terpenoids and flavonoids (Yi et al., 2017; Munir et al., 2024). Analyses of the phytochemical composition of fresh and processed citrus products have indicated the presence of several bioactive compounds, among which polyphenols and carotenoids stand out and are considered to play an important role in reducing the risk of developing chronic diseases (Bamise and Oziegbe, 2013; Ozdemirli and Kamiloglu, 2024). In addition to polyphenols and carotenoids, they also contain other beneficial phytochemicals, such as limonoids, terpenes, and alkaloids (Liu et al., 2021; Nassarawa et al., 2024).

FTIR spectroscopy (Fourier Transform Infrared Spectroscopy) is a method of infrared absorption spectrum, and measurements are made in solid, liquid, or gaseous material. It collects and digitizes the interferogram followed by Fourier transformation and displays the spectrum. The technique finds wide application in food analysis, forensics, environmental research, and pharmaceuticals. It is a fast, easy to handle, non-destructive and precise method (Ahmad and Ayub, 2022; Van de Voort, 1992). FTIR spectroscopy is increasingly used in the food industry for the analysis of citrus fruits and their products, including juices, pulp, and peel. This technique allows reliable determination of the presence and quantity of valuable phytochemicals, such as carotenoids, flavonoids, phenolic acids and terpenoids, thus contributing to a better understanding of their nutritional and functional importance (Ernawita et al., 2017). In combination with multivariate statistical methods, such as Principal Component Analysis (PCA), and Partial Least Squares Regression (PLSR), FTIR has shown high efficiency in the characterisation of citrus fruits. These approaches enable differentiation between species and cultivars, as well as the identification of those with higher levels of targeted bioactive compounds, making this method a valuable tool for quality control and raw material selection (Song et al., 2018).

The aim of this systematic review is to demonstrate the presence and significance of bioactive compounds in citrus fruits and to explore the possibilities of their identification and quantification using FTIR spectroscopy. In this context, the paper provides an overview of the chemical composition of the major bioactive compounds present in citrus fruits, with particular emphasis on flavonoids, phenolic acids, carotenoids, and essential oils. Furthermore, it examines the application of FTIR spectroscopy as a modern, rapid, and non-destructive analytical technique for their identification and characterization.

This systematic review is based on a comprehensive literature search conducted to identify relevant studies on the application of FTIR spectroscopy in the analysis of bioactive compounds in citrus fruits. Relevant articles were identified through searches of Scopus, Web of Science Core Collection, PubMed, and Google Scholar using combinations of keywords related to FTIR spectroscopy and citrus bioactive compounds, including FTIR, citrus fruits, citrus peel, flavonoids, phenolic acids, carotenoids, and essential oils. The search included peer-reviewed articles published in English and Croatian between 2005 and 2024. Studies were selected based on their relevance to the topic and their scientific contribution. Conference abstracts without full text, non-peer-reviewed publications, and studies not directly related to citrus species or FTIR analysis were excluded. After screening titles and abstracts and removing duplicate records, the most relevant studies were selected for detailed analysis.

Bioactive compounds in citrus fruits

Citrus fruits are popular worldwide for their pleasant taste and richness in bioactive and nutritional substances. They are rich in nutrients, such as ascorbic acid (vitamin C), tocopherols and tocotrienols (vitamin E), and minerals (selenium, zinc, copper, iron, and manganese) (Zou et al., 2016; Lu et al., 2023). They are also an excellent source of bioactive compounds, mainly phenolic compounds (flavonoids, phenolic acids, and coumarins), terpenoids (limonoids and carotenoids), and pectin (Cebadera-Miranda et al., 2019; Lado et al., 2018; Nieto et al., 2021) (Figure 1). Collectively, these studies indicate that citrus fruits combine strong antioxidant capacity with structural polysaccharides and secondary metabolites, which together contribute to both their nutritional value and functional properties. The flavour characteristics and organoleptic quality of citrus fruits are greatly influenced by the types and proportions of organic acids, sugars, and phenolic compounds (Albertini et al., 2006). Glucose and fructose are the most important reducing sugars in citrus fruits, while sucrose is the most abundant disaccharide (Ladaniya and Mahalle, 2011). The most important organic acid in citrus fruits is citric acid. In addition, malic, oxalic, malonic and quinic acids are also present (Hussain et al., 2021).

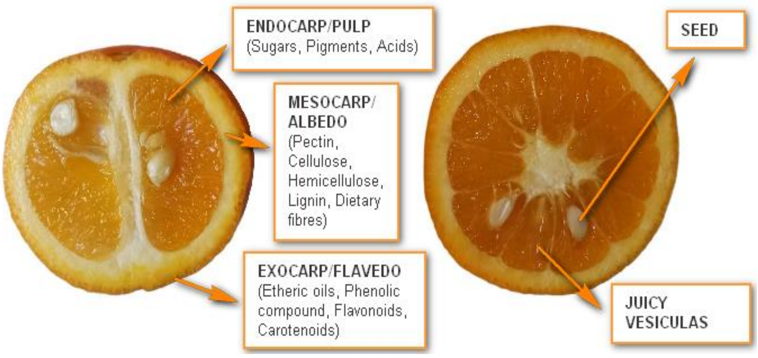

Figure 1. Cross-section of an orange fruit and its main compounds (author's photo)

The composition and content of individual bioactive substances vary considerably among citrus species, fruit parts, and degrees of maturity (Voća et al., 2022). Citrus fruits are a particularly rich source of polyphenolic compounds, with flavonoids dominating, which significantly contribute to the antioxidant compounds in the human diet (Ozdemirli and Kamiloglu, 2024). Chemically, flavonoids consist of a 15-carbon skeleton (C6-C3-C6) composed of two six-carbon phenyl rings connected by a heterocyclic ring containing an incorporated oxygen (Peng et al., 2021). In citrus fruits, flavanone-7-O-glycosides, such as naringin, eriocarpin, hesperidin and narirutin stand out, followed by flavones such as rhoifolin, vitexin and diosmin, and polymethoxylated flavones including nobiletin, tangeritin and 5-demethyl nobiletin. Also present are flavonols such as quercetin, rutin and kaempferol, as well as anthocyanins such as cyanidin- and peonidin-glucoside (Saini et al., 2022). Phenolic acids are present in smaller quantities in citrus fruits, mainly in the peel, and primarily include caffeic, p-coumaric, ferulic and sinapic acids (Singh et al., 2020; Ozdemirli and Kamiloglu, 2024).

Carotenoids are isoprenoid plant pigments of yellow to red colour, present in large quantities in citrus fruits, with an important role in photosynthesis, signalling and as precursors of vitamin A with pronounced antioxidant activity (Hasan et al., 2024). They are chemically divided into carotenes (e.g. α- and β-carotene, lycopene) and xanthophylls, i.e. oxygenated derivatives (e.g. lutein, zeaxanthin, violaxanthin, β-cryptoxanthin) (Britton et al., 2009). The occurrence of specific xanthophyll esters, as well as the total amount of carotenoids, largely depend on the type of citrus fruit, the degree of ripeness of the fruit and the analysed part of the fruit (Lux et al., 2019). Flavedo, that is, the outer layer of the peel, contains significantly higher levels of carotenoids compared to the pulp and juice, with lutein, zeaxanthin, β-cryptoxanthin and β-carotene being the most abundant (Wang et al., 2020). In the pulp of the orange variety ''Valencia'', the most abundant carotenoids are esters of violaxanthin, antheraxanthin, β-cryptoxanthin and mutatoxanthin. These compounds are mainly present as monoesters or diesters, together with fatty acids such as lauric, myristic and palmitic acids (Etzbach et al., 2020). A comparative study conducted on orange ('Washington Navel' and 'Tarocco'), lemon ('Akragas') and pomelo ('Chandler') varieties, demonstrated that the flavedo of ripe 'Washington Navel' oranges contains the highest concentration of total carotenoids, reaching a value of 159 mg/kg of dry matter (Multari et al., 2020).

Essential oil from the flavedo layer of citrus fruits has significant economic and health value due to the presence of terpenes, limonoids, and other bioactive compounds (Gao et al., 2020). In the essential oils of mandarin, grapefruit, orange, citron, and lemon, D-limonene accounts for almost 45–90% of the total terpenoids (Li et al., 2019; Denkova-Kostova et al., 2020; Paw et al., 2020). In lemon and tangerine essential oils, γ-terpinene and β-pinene constitute 8–20% and 0.3–11% of the total compounds, respectively (Raspo et al., 2020). Limonoids are a large group of oxygenated terpenoids, such as limonin, obacunone, nomilinic acid and deacetylnomilin, present in the seeds, pulp, and peel of citrus fruits (Gualdani et al., 2016). To date, more than 40 limonoids have been identified in citrus fruits, among which limonin and nomilinic acid predominate, especially in oranges and grapefruit. Together with naringin, these compounds contribute to the characteristic bitterness of these fruits (Shi et al., 2020; Gupta et al., 2023). Citrus peel contains 20–30% pectin in dry matter (Shan, 2016). The highest percentage of pectin is obtained by extraction from the peel of sweet orange and lemon. The percentage of pectin and the rate of its extraction depend on parameters such as pH, temperature, solvent, and extraction time (Patil et al., 2022).

Fundamentals and technological aspects of FTIR spectroscopy

FTIR spectroscopy is one of the key analytical techniques in the field of infrared spectroscopy, based on the vibrational transitions of molecular bonds (Hou et al., 2018). Due to this principle, molecules possessing a dipole moment absorb infrared radiation at specific wavelengths corresponding to energy differences between their vibrational levels, resulting in the formation of a characteristic absorption spectrum. Because substances differ in atomic composition and molecular structure, each compound exhibits a unique FTIR spectrum, which enables its identification and classification (Bunaciu et al., 2010; Tiernan et al., 2020). Functional groups are of particular importance in this spectrum, since their fundamental vibrations cause characteristic absorption bands within defined wavenumber regions (Griffiths and Haseth, 1986), a detailed overview of which is presented in Table 1. FTIR spectroscopy is based on the specific absorption of infrared radiation by molecules, with each compound having a unique vibrational pattern, which allows its identification and classification. With the development of FTIR technology, measurements can be performed in different modes, such as transmission, attenuated total reflection (ATR) or imaging, and diffuse reflectance infrared Fourier transform spectroscopy (DRIFT) (Szentirmai et al., 2020; Hafidi et al., 2005).

Table 1. Assignment of characteristic FTIR wavenumbers (cm^{-1}) to vibration types, functional groups, and indicated compound classes

Wavenumber (cm^{-1})	**Vibration Type**	**Functional Group / Bonds**	**Corresponding Compound Class**	**References**
4000–400	Stretching and bending vibrations (mid-IR region)	Various chemical bonds	General molecular vibrations detected in the mid-IR region	Smith, 2011
3200–3600	O–H stretching	O–H bond	Water, alcohols, phenols, pectins, cellulose	Mansur et al., 2004
2800–3000	C–H stretching	C–H bonds	Aliphatic chains, fatty acids	Smith, 2011
~1740	C=O stretching	Carbonyl (C=O) group	Carboxylic acids, esters, hemicellulose, pectins	
1600–1700	C=C stretching	C=C bonds	Aromatic compounds, lignin	Nandiyanto et al., 2019
900–1400	Mixed stretching and bending vibrations	C–O, C–C, O–C–H, C–C–H, C–O–H	Carbohydrates (glucose, fructose, sucrose)	Leopold et al., 2011
900–1153	C–O and C–C stretching	C–O and C–C bonds	Carbohydrates	
1400–1199	Bending and vibrational modes	O–C–H, C–C–H, C–O–H	Carbohydrates	
900–1200 (“Fingerprint region”)	Complex coupled vibrations	Various skeletal vibrations	Cellulose, starch, and specific compound identification	Guo et al., 2019

The selection of the appropriate measurement mode depends on the physical state and characteristics of the analysed sample, as FTIR spectroscopy can be applied to liquids, solutions, pastes, powders, films, fibres, and gases. FTIR spectroscopy, often combined with chemometrics, is used to study various quality attributes in many food samples, including fruits, vegetables, or beverages, e.g. apple wax (Veraverbeke et al., 2005), polymethoxylated flavones isolated from orange oil residues (Manthey, 2006), vitamin C in both powder and liquid form (Yang and Irudayaraj, 2002). The technique is also widely used for the analysis of musts and wines. FTIR enables the analysis of different types of fruit samples, including whole fruit, juices, and extracts, providing information on their chemical composition, such as carbohydrates, proteins, amino acids, fatty acids, and organic acids. To achieve optimal results, different measurement modes- such as transmission, ATR, and DRIFT- are applied, depending on the type of sample analysed (Song et al., 2018).

Application of FTIR spectroscopy in citrus fruit analysis

Previously, FTIR and near-infrared (NIR) techniques were used in combination with multivariate statistics to analyse various citrus products such as oils (Steuer et al., 2001), sugars and acids. These approaches have also proven useful in addressing authenticity and forgery problems (Kemsley et al., 1996).

Nowadays, FTIR spectroscopy is increasingly used as a fast, non-invasive, and non-destructive technique for analysing chemical composition, assessing authenticity, and identifying characteristic molecules in citrus fruits and their products (Song et al., 2018) (Table 2).

Table 2. Application of FTIR spectroscopy in citrus fruit analysis

Application		Analysed compounds	References
Analysis of the composition of citrus fruits	Citrus juices	Physical-chemical properties (pH, electrical conductivity, density), content of total and reducing sugars, organic acids (citric, malic), vitamin C (ascorbic acid)	Bichara et al., 2015; Clark, 2016; Goodner and Manthey, 2005; Aykas and Rodriguez-Saona, 2024
	Pulp and fruits	Functional groups (O–H, C–H), structures of cellulose, hemicellulose, and pectin	Andronie et al2017
	Pectin and waste materials	Pectin structure (–OH, C=O, carboxyl groups), degree of esterification	Kozioł et al., 2022; Kanmani et al., 2014; Zapata et al., 2024; Fadzil and Othman, 2024
Authentication of citrus fruits and their products	Analysis of essential oils	Volatile compounds (limonene, α-pinene, myrcene), terpenoids, spectroscopically identified groups (C=C, C–H, O–H)	Salamah et al., 2024; Latifah et al., 2023; Cebi et al., 2021; Boughendjioua and Djeddi, 2017; Toprakçi et al., 2024
Analysis of characteristic bioactive molecules and properties of novel biomaterials	Quantitative analysis of bioactive compounds	Carotenoids (β-carotene, lutein), flavonoids (hesperidin, naringenin), phenolic compounds (gallic acid, quercetin), antioxidant activity	Song et al., 2018; Kim et al., 2015; Sherazi et al., 2017; Senoretta and Sumathy, 2016
	Analysis of the polymeric form of flavanones	Naringenin and polymers: hydroxyl groups (–OH), aromatic methyl (Ar-CH_3), carbonyl (C–CO–C), epoxy groups; thermal, antioxidant and antimicrobial properties	Latos-Brozio et al., 2021

FTIR spectroscopy is often used to analyse the chemical composition of citrus fruits and their juices. Clark (2016) reported that FTIR spectroscopy can be used as a rapid method for determining the sugar and acid content of citrus juices, which facilitates the assessment of industry ripeness standards. An analysis of 1470 'Navel' orange samples showed that improved ATR-FTIR models, developed using juice samples from a single variety, achieved significantly better predictive results compared to generic models. This improvement was reflected in lower prediction errors: 0.12 °Brix for sugar content, 0.027% for total acids (TA) and 3.1 BRIMA units (an index based on the linear weighted difference between Brix and total acid rather than their ratio). Furthermore, FTIR spectroscopy combined with quantitative predictive modelling enablesearly and accurate assessment of citrus variety qualitybased on sugar and acid content. In the study by Song et al. (2016), modelling was performed using the PLS regression algorithm withFTIR spectra as input data. The results showed an extremely high correlation between predicted and measured values, with a regression coefficient (R2) of 0.99, confirming the effectiveness of this method in the quantitative analysis of the chemical composition of citrus fruits.

In recent years, FTIR spectroscopy has been increasingly used to determine the degree of methylation (DM) of pectin, as this technique does not require prior chemical treatment of the sample. Although it offers slightly lower resolution compared to some conventional methods, FTIR spectroscopy provides valuable information about the pectin structure. The DM values obtained by FTIR analysis showed good agreement with those from standard methods, as confirmed by the study by Kozioł et al. (2022). Therefore, the FTIR method is considered useful not only in the food industry, but also in the pharmaceutical industry. Studies also show that pectin isolated from citrus peel, especially orange, can be successfully analysed by this technique and compared with commercial pectin. In the study by Duwee et al. (2022), different acidic extraction media (acetic, nitric, hydrochloric, and citric acids) were used to isolate pectin from orange peel. The obtained FTIR spectra were similar, regardless of the solvent used, with characteristic bands confirming the presence of pectin. In the spectra, bands corresponding to –OH groups (3000–3700 cm^{-1}), –CH groups (2800–3000 cm^{-1}), carbonyl groups of methyl esters (1680–1810 cm^{-1}), and carboxylate groups (1490–1700 cm^{-1}) were detected. Comparison with commercial pectin showed a high degree of agreement in wavenumbers. FTIR analysis was also used for the identification and characterisation of pectin derived from Citrus limon peel waste, enabling optimised production of pectin from different citrus fruits and confirmed the desirable properties of lemon pectin for industrial applications (Kanmani et al., 2014).

FTIR spectroscopy, combined with multivariate statistical methods, has become a reliable tool for the authentication of citrus fruits and their products, enabling the differentiation of species, varieties and product origin based on their molecular spectra. In this context, Bichara et al. (2015) reported on recent studies of model orange juices that combined FTIR spectroscopy with the analysis of physicochemical properties at room temperature and during storage. The results showed that FTIR spectroscopy, together with physicochemical parameters, can be successfully used to distinguish natural juices of different origins. The study also proposed an interpretation of the observed absorption bands in the FTIR spectra of three varieties of bitter orange (*Citrus aurantium*), common orange (*Citrus bigardia Risso*), and sweet orange (*Citrus sinensis*) within the spectral range of 400–4000 cm^{-1}. In the study by Andronie et al. (2017), FTIR was applied to the analysis of lemon and mandarin pulp, where characteristic vibrational bands associated with O–H and C–H functional groups were identified in the spectral range of 1400–700 cm^{-1}. The obtained data enabled differentiation between varieties, thus confirming the usefulness of the FTIR method in the food industry for the authentication and quality control of citrus fruits. Salamah et al. (2024) used FTIR spectroscopy in combination with chemometric methods, including PCA and PLS, for the analysis and authentication of essential oils obtained from the peel of sweet orange, lime, and lemon. The results showed that sweet orange and lemon peel oils exhibited high quality indices- 958 for orange and 921 for lemon indicating strong similarity between their spectral fingerprints and the reference spectrum of limonene. These quality indices represent a quantitative measure of the similarity between the FTIR spectra of the tested samples with pure limonene, the dominant component of the mentioned oils. Furthermore, FTIR analysis combined with PLS modelling showed that the most informative spectral region was between 1450–1650 cm^{-1}, with an RMSEC value of 0.00553, indicating high model precision. RMSEC (Root Mean Square Error of Calibration) is a statistical measure that reflects the average calibration error of the model, with lower values indicating higher prediction accuracy. Subsequent PCA analysis enabled clear separation of the oil samples, confirming the ability of the method to distinguish citrus peel essential oils of different origins, and to assess their similarity to commercial products. This method also proved effective in detecting adulteration, such as the mixing of higher-quality oils with cheaper ingredients (e.g., turpentine oil), thereby supporting the verification of the authenticity of the product (Ledita et al., 2019; Salamah et al., 2024).

Although FTIR spectroscopy is recognised as a very useful and widely applicable analytical technique, certain limitations must be considered depending on the context of application. For example, in a study conducted by Goodner and Manthey (2005), focused on the differentiation of orange juices, FTIR analysis combined with multivariate statistical methods, such as Discriminant Function Analysis (DFA), enabled differentiation of juices; however, this separation was less distinct compared to other analytical approaches. PCA was also applied in this analysis, with 10 principal components selected based on combinations of signals from different wavenumbers. However, such a transformation makes it difficult to identify the specific functional groups responsible for the observed differences between samples.

Unlike conventional FTIR devices that are primarily used in laboratories for the analysis of bioactive substances in citrus fruits, portable FTIR systems have proven equally effective for product authentication, especially in the rapid and non-destructive field analysis of fruit juices. Their field application, without the need for sample preparation, enables the rapid, non-destructive, and simultaneous determination of multiple chemical properties. In one study, the analysis of 68 fruit juice samples from the US market using a portable FTIR device and PLSR achieved a high correlation with reference methods (cross-validation correlation coefficient, R^2CV ≥ 0.93), along with low prediction error. The study also revealed significant deviations between declared and measured values of of sugar (21%) and ascorbic acid (37%). These results confirm that, in addition to laboratory applications, FTIR technology, including portable systems, represents a reliable tool for rapid, accurate and on-site quality control of food products, such as fruit juices (Aykas and Rodriguez-Saona, 2024).

FTIR spectroscopy enables the detection of specific chemical compounds present in citrus fruits byidentifying their functional groups through characteristic vibrational bands in the infrared spectrum. The results of Song et al. (2018) showed that accurate quantitative predictions of total carotenoids, flavonoids and phenolic compounds can be obtained from FTIR spectra of citrus fruits and that the resulting quantitative prediction model may serve as a usefultool for the rapid selection of citrus fruits containing elevated levels of carotenoids, flavonoids, and phenolic compounds. Sherazi et al. (2017) applied FTIR spectroscopy to analyse the total phenolic content of liophilised lemon juices and compared the results with those obtained using the conventional Folin-Ciocalteu method. The comparison showed that the results of both methods are comparable, confirming that transmission FTIR spectroscopy can serve as a fast and economical alternative to classical, time-consuming chemical analysis of total phenolic substances in lemons.

Several studies confirm the application of FTIR spectroscopy in the analysis of citrus essential oils. For example, Latifah et al. (2023) analysed the quality of kaffir lime peel oil using FTIR spectroscopy to characterise the compounds present. Cebi et al. (2021) also successfully detected the presence of orange essential oil, isopropyl myristate, and benzyl alcohol in lemon essential oil using FTIR analysis combined with chemometric methods. The volatile compounds of lemon (*Citrus limon L*.) collected from the Colla region, Skikda city (Algeria), were identified by qualitative FTIR analysis, with ten volatile compounds detected. The spectrum revealed characteristic functional groups typical of essential oils, including C–H bonds of alkenes, C–H bonds of aromatic compounds, and C=C double bonds (Boughendjioua and Djeddi, 2017). In the studies by Auta et al. (2018), FTIR spectra revealed pronounced alkene bands corresponding to C=C stretching at 1642 and 1643 cm^{-1}, indicating the presence of limonene as the dominant component of lemon and orange essential oils. Similar results were confirmed by Pollard et al. (2016), who observed characteristic bands for C–H (~2900 cm^{-1}), C=O (~1700 cm^{-1}), a broad O–H stretching (~3400 cm^{-1}) and C–O vibrations (~1100 cm^{-1}) in the FTIR spectrum of pure lemon essential oil, associated with terpenoid compounds. Following these findings, Toprakçi et al. (2024) used limonene-rich mandarin peel to isolate essential oils, where FTIR spectroscopy confirmed the presence of characteristic functional groups associated with limonene. By optimising the extraction process, themaximum D-limonene yield (75 mg/g) was achieved. Gas Chromatography-Mass Spectrometry (GC-MS) analysis revealed that D-limonene was the dominant component (91.56%), accompanied by myrcene, α- pinen and sabinene. The obtained results were additionally supported by NMR spectroscopy. The content of carotenoids in citrus fruits can also be effectively evaluated using FTIR spectroscopy in combination with multivariate analysis, as confirmed by the research of Kim et al. (2015). Their results showed that the concentrations of individual carotenoids, such as antheraxanthin (R^2 = 0.9117), β-carotene (R^2 = 0.8816), β-cryptoxanthin (R^2 = 0.8856), and violaxanthin (R^2 = 0.7305) can be accurately predicted from FTIR spectral data using the PLS model. In addition, the Partial Least Squares-Discriminant Analysis (PLS-DA) enabled clear differentiation of metabolic variations during fruit development. These results confirm that FTIR spectroscopy, when coupled with appropriate statistical modelling, can not only identify chemical changes associated with citrus fruit ripening but also quantify the valuable bioactive compounds such as carotenoids. Additionally, the FTIR spectrum of β-carotene shows characteristic infrared bands between 1250 and 740 cm^{-1} associated with the 7-cis configuration, while the band at 780 cm^{-1} indicates the presence of the 15-cis isomers. Cis-isomers of β-carotene are also recognised by the double C=C–C stretches at 1720 and 1680 cm^{-1}. FTIR analysis of orange samples thus confirmed the presence of β-carotene, further emphasising the ability of the FTIR method to identify specific carotenoids (Senoretta and Sumathy, 2016). In the study by Latos-Brozio et al. (2021), the polymeric form of the flavonoid naringenin, a naturally occuring compound in citrus fruits, was examined, to obtain poly(naringenin) via a cross-linking reaction with glycerol diglycidyl ether (GDE). Formation of the polymeric products was carried out by FTIR spectroscopy, which revealed characteristic bands of polymeric flavonoids. Broad bands between 3700–3000 cm^{-1} indicated the presence of free -OH groups, while bands between 1370–1250 cm^{-1} and at 1061 cm^{-1} corresponded to aryl vibrations and ketone C-CO-C bonds. Signals of epoxy groups from GDE were also detected (750–900 cm^{-1}). In addition, the FTIR spectrum also showed bands characteristic of monomeric flavonoids, including aromatic vibrations and methyl groups attached to aromatic rings ($Ar-CH_3$). The conversion of naringenin into its polymeric form was estimated at 85% based on FTIR analysis.

FTIR spectroscopy has proven to be a highly effective tool for the analysis of chemical compounds extracted from the citrus waste materials. It enables the detection of specific functional groups, such as hydroxyl groups, alkyl chains, aromatic rings (from lignin) and carbonyl groups (from pectin). The results of the study by Fadzil and Othman (2024) confirmed that FTIR analysis can successfully identify key chemical groups (O–H, C=O, aromatic and alkyl) in citrus biowaste materials, further highlighting their potential for the development of sustainable bio-composites as alternatives to conventional plastics. There is increasing interest in the detailed characterisation of the chemical composition of citrus by-products, as confirmed by the study by Zapata et al. (2024). The study focused on the chemical characterisation of Citrus sinensis, Citrus paradisi and Citrus limon peel by-products using Fourier transform infrared spectroscopy (FTIR). The spectra show a similar trend, with pronounced differences in the spectral regions of 1600–1750 cm^{-1}, 1400–1440 cm^{-1} and 3200–3600 cm^{-1}. These differences correspond to the stretching vibrations of the C=O bond and the bending and stretching vibrations of the O–H bond (Pretsch et al., 2009), indicating the presence of phenolic compounds. Furthermore, PCA enabled a clear distinction of the studied species based on their chemical structure.

Advantages, challenges, and limitations of FTIR spectroscopy

FTIR spectroscopy has numerous advantages, including ease of use, internal calibration, fast analysis time, and the ability to obtain qualitative and quantitative information about compounds, including their behaviour at the cellular level. In addition, it is characterized by high sensitivity and speed, making it extremely suitable for rapid and precise analysis of biological samples (Table 3).

Table 3. Advantages and limitations of FTIR spectroscopy for the analysis of diverse sample type

Advantages	Disadvantages	Sample type	References
Rapid spectroscopic analysis with minimal or no sample preparation	Limited selectivity in the analysis of complex matrices	Fruit products, edible oils and fats	Mohamed et al., 2011; Rohman, 2017
Environmentally friendly and economically viable method, without the need for organic solvents and consumables	Insensitivity to homonuclear diatomic molecules without a dipole moment (e.g. O_2, N_2)	Citrus fruit and other food products	Workman, 2024
Non-invasive and non-destructive method suitable for preserving sample integrity	The presence of water can significantly interfere with infrared absorption bands.	Cosmetic products	Chophi et al., 2021
Possibility of simultaneous detection of a wide range of molecular vibrations in a single measurement	Limited quantification of analytes present in very low concentrations (in traces)	Food and beverage products, herbs (oregano)	Dasgupta and Ranjan, 2018; Wielogorska et al., 2018
High sensitivity and a favourable signal-to-noise ratio enable the detection of minor variations in sample composition	Analysing large sets of spectral data requires advanced algorithms and specialised software	Commercial food products containing nanoemulsions	Silva et al., 2012; Goodner and Manthey, 2005
Suitable for analysing samples in different states of aggregation (solid, liquid, gaseous)	Reduced ability to distinguish between similar patterns, such as different types of fruit juices	Citrus (orange juice) and other fruit products	Workman, 2024; Goodner and Manthey, 2005
Effective in combination with chemometric methods (e.g. PCA, PLS-DA) for the classification and authentication of food products	A complementary technique is often required for the precise identification of individual compounds	Honey samples (citrus honey), herbs (oregano), and edible fats and oils	Xagoraris et al., 2021; Rohman, 2017; Black et al., 2016

Unlike dispersive spectrometers, FTIR instruments do not use slits to limit the light and contain a minimal number of mirrors, which reduces reflection losses. This results in increased optical throughput, allowing more energy to reach the sample and detector, thereby producing a stronger signal and an improved signal-to-noise ratio, which enhances sensitivity to small absorptions and improves spectral clarity. One of the key features of FTIR is its ability to simultaneously record all peak frequencies corresponding to the vibrations of different metabolites. This provides detailed insight into the chemical composition of the sample without the need for multiple measurements. In addition, thanks to increasingly sophisticated software solutions, the interpretation of the obtained data is becoming increasingly efficient and reliable (Dasgupta and Ranjan, 2018). FTIR enables the identification of different materials, quantification of compounds by measuring the size of absorption peaks, determination of the number of compounds in a mixture, and assessment of sample quality and consistency. Therefore, it can be used as a rapid and sensitive analytical technique (Mohamed et al., 2011; Silva et al., 2012). One of the greatest advantages of this technique is its ability to analyse almost all types of samples, regardless of their aggregation state.

FTIR spectroscopy offers numerous advantages, but differs in approach and application compared to other analytical techniques, such as High-Performance Liquid Chromatography (HPLC) or GC-MS. Unlike HPLC, which requires the use of solvents and extended separation times, FTIR enables spectra to be obtained almost instantly (Dong, 2013). GC-MS is a widely used technique for the qualitative and quantitative analysis of volatile and semi-volatile substances in food (Wang et al., 2020). Compared to GC–MS, FTIR is less selective but significantly faster, making it a practical tool for rapid qualitative and semi-quantitative analysis (Rohman, 2017; Workman, 2024). While HPLC and GC–MS are more suitable for the analysis of complex mixtures and trace compounds, FTIR excels in the qualitative characterisation of pure substances and rapid identification without destroying the sample (Chophi et al., 2021). In addition, FTIR analysis does not require consumables to the same extent as chromatographic methods, which makes it more economical for routine use (Workman, 2024). This is confirmed by a study of Greek citrus honey of different botanical origins, in which ATR–FTIR spectroscopy combined with chemometrics showed comparable accuracy to solid-phase microextraction, combined with gas chromatography and mass spectrometry (Solid Phase Microextraction-Gas Chromatography-Mass Spectrometry (SPME-GC-MS), but with a significantly simpler, faster, and more cost-effective application (Xagoraris et al., 2021).

Despite its many advantages, FTIR spectroscopy faces certain limitations and challenges that may affect the accuracy and reliability of the obtained results, especially when analysing complex mixtures or low analyte concentrations. Although FTIR provides rapid metabolite detection and simultaneous acquisition of spectral information, it is less suitable for the analysis of aqueous solutions due to the strong water absorption in the infrared region. Furthermore, it cannot detect molecules that do not exhibit a change in dipole moment during vibration (e.g., homonuclear diatomic molecules such as N_2 and O_2) (Workman, 2024) (Table 2). In addition, information about individual compounds or compounds in a complex mixture cannot be extracted. Therefore, FTIR spectroscopy is often complemented by other analytical techniques, such as liquid chromatography (Liquid Chromatography- Polymerase chain reaction (LC–PCR) that is related to high-resolution mass spectrometry (Liquid Chromatography–Mass Spectrometry (LC–MS), to enable precise identification and quantification of specific biomarkers (Black et al., 2016; Wielogorska et al., 2018). The combination of FTIR spectroscopy with chromatography enables the separation of compounds in complex biological matrices, such as food, according to their physicochemical properties (Hird et al., 2014). When coupled with mass spectrometry, this method becomes particularly powerful because it enables the identification and quantification of compounds based on their mass and ion charge ratio (De Hoffmann and Stroobant, 2007).

Analytical approaches focusing on volatile compounds, such as electronic nose (e-nose) technologies based on pattern recognition and mass spectrometry (MS)-based methods that enable compound identification and quantification, as well as complementary physicochemical analyses, demonstrate clearer and more precise discrimination of orange juice samples compared to FTIR analysis. In addition, the FTIR approach faces challenges, including demanding software management and longer processing times for very large datasets. Although FTIR spectroscopy can serve as a useful tool for basic juice differentiation, the results clearly indicate that alternative methods are more sensitive and efficient for this type of analysis (Goodner and Manthey, 2005).

Conclusion

FTIR spectroscopy has proven to be a valuable analytical technique for the identification and quantification of bioactive compounds in citrus fruits, due to its speed, simplicity, non-invasiveness, and ability to simultaneously measure a wide range of functional groups. By applying FTIR in combination with chemometric modelling, it is possible to reliably distinguish between types, varieties, and quality levels of citrus fruits and to identify key bioactive compounds such as flavonoids, carotenoids, phenolic acids, and pectins. However, FTIR spectroscopy has certain limitations, particularly when analysing complex matrices and low concentrations of compounds, which can make data interpretation challenging without additional statistical or instrumental processing. Therefore, FTIR is increasingly complemented by high-resolution methods, such as LC–MS or GC–MS, to improve the specificity and quantification of target analytes. Despite these challenges, FTIR remains an extremely useful tool for rapid quality control, authentication and compositional research of citrus fruits and their products, with considerable potential for the sustainable analysis of waste and secondary raw materials from the food industry.

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