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The combination of ATR-FTIR and chemometrics for rapid analysis of essential oil from Myrtaceae plants – A review

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ABSTRACT

Essential oils are widely used in a variety of industries, including food, chemicals, cosmetics, and pharmaceuticals. Like all commercial products, essential oils must pass a stringent quality control procedure established by the industry. Unfortunately, quality control of essential oils has become a difficult task due to the content of biosynthetic conditions and their complexity. The Myrtaceae family is the most well-known essential oil-producing plant in the community. The plants of the Myrtaceae family used for medical and commercial purposes include myrtle, guava, cloves, *Eucalyptus*, and tea tree, which consists of 140 genera and about 3,500–5,800 species that are scattered in tropical and subtropical areas. Essential oils obtained from this family, *Eucalyptus, Melaleuca*, *Syzygium*, and *Eugenia*, can be rapidly analyzed using Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR) and chemometrics. This review article aims to investigate the role and use of ATR-FTIR and chemometric methods as a rapid analysis for essential oils from Myrtaceae plants. The literature search was conducted and accomplished from January to October 2021 using an electronic database such as Scopus, PubMed, Web of Science, Directory Open Access Journal, and Google Scholar. This narrative review highlights various pieces of literature on FTIR, ATR-FTIR, chemometrics, analysis of essential oils, essential oils from Myrtaceae, application of ATR-FTIR, and chemometrics in essential oil from Myrtaceae plants and their prospects.

INTRODUCTION

Essential oils are commonly used in various industrial sectors such as the food, chemical, cosmetics, and pharmaceutical industries. The high economic value of essential oils has led to the emergence of various strategies to enhance the yield and production process of essential oils by developing new plant cultivars and optimizing techniques, including variations of different plant treatments (Haghighi *et al.*, 2017; Lourenço *et al.*, 2019). In these conditions, the chemical profile of essential oils usually deviates from the standard product quality and develops sustainable quality control methods (Xiong *et al.*, 2019).

Quality control is crucial in the production process before the product is marketed to the general public. All commercial products must pass an industry-mandated quality control test. Due to the content of biosynthetic conditions and the complexity of essential oils, quality control has become highly challenging. Among many essential oil-producing plants, the most well-known plant from the Myrtaceae family (Myrtle family), which consists of 140 genera and about 3,500–5,800 species, is scattered in tropical and subtropical areas (Farag *et al.*, 2018; Frauches *et al.*, 2016; Johnson and Briggs, 1984; Wilson *et al.*, 2001). Some studies have proven that myrtle family extract helps treat gastroenteritis, dysentery, and diabetes (Azevedo *et al.*, 2012). Essential oils from the myrtle family, such as myrtle, guava, cloves, *Eucalyptus*, and tea tree, are used for medical and commercial purposes (Siddique *et al.*, 2017). The Myrtaceae genera discussed in this review include *Eucalyptus*, *Eugenia*, *Melaleuca*, and *Syzygium*. The analysis of this essential oil information, both in terms of characterization of the classification model based on chemical composition and other

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information obtained from the analysis, can control the quality of essential oils in similar studies.

Gas chromatography (GC) combined with mass spectroscopy (MS) or flame ionization detector (FID) is a standard method and is often used to analyze the chemical composition of essential oils from natural products, mainly plants (Farag *et al.*, 2018; Khanh *et al.*, 2020). However, this method has feebleness, namely, the use of large amounts of organic solvents, sample preparation, and analysis time, requiring a relatively long time and high temperatures to cause sample damage (Shi *et al.*, 2020). Recently, vibrational spectroscopy methods have been developed using infrared (IR) spectroscopy, which is more efficient (Baranska *et al.*, 2005, 2006; Schulz *et al.*, 2004, 2005; Schulz and Baranska, 2007; Wang and Sung, 2011).

IR spectroscopy has been successfully used in analyzing the authenticity of herbal medicines (Laasonen *et al.*, 2002), detecting impurities or adding chemicals to the sample (adulteration context) (Dong *et al.*, 2012), measuring a single sample (Schulz and Baranska, 2007), and sample mix (Chan *et al.*, 2007; Escamilla *et al.*, 2013) in the plant matrix. Fourier Transform Infrared Spectroscopy (FTIR) is a measurement technique by collecting IR spectra formed due to vibrations in the atoms in a molecule. In spectrum measurement using FTIR spectroscopy, several techniques for measuring samples are standard: Attenuated Total Reflectance (ATR) (Beasley *et al.*, 2014).

ATR is a sampling technique that is connected to the FTIR device. Today, in many fields, ATR-FTIR spectroscopy is preferred over transmission FTIR spectroscopy (Manheim *et al.*, 2016; Özgenç *et al.*, 2017; Parhizkar *et al.*, 2017; Peets *et al.*, 2017). The ATR-FTIR technique allows a sample to be directly used in solid and liquid form, so there is no need to do sample preparation in advance, and it is a fast technique in the initial steps to characterize samples or materials. Other advantages are that it is easy to prepare samples, there is no need to grind potassium bromide (KBr), a broader spectrum of variation, and negligible difference in particle size (Thompson *et al.*, 2009). Therefore, ATR-FTIR can be an effective, fast, simple, reliable, sensitive, and nondestructive method for identifying and also analyzing essential oils and analyzing physical and chemical parameters in quality control (Bittner *et al.*, 2016).

The absorption spectra of the molecules in the sample usually overlap as spectroscopy presents the output data (IR spectrum) in high dimensional (HD) space. This condition makes it harder for visual and direct interpretation. Hence, the chemometric method is used to facilitate the data interpretation process. In the last few decades, chemometrics has been successfully applied in building regression or classification models using HD data, including the IR spectrum (Gad *et al.*, 2013; Muro *et al.*, 2015). The addition of chemometric techniques to the analysis of the spectrum has been proven effective in displaying specific differences between plant chemotypes (Baranska *et al.*, 2005; Schulz *et al.*, 2004; Schulz and Baranska, 2007). Combining ATR-FTIR spectroscopy with chemometric methods is widely used to classify and quantify various science and technology fields (Stöbener *et al.*, 2019).

This narrative review aims to investigate the role and use of ATR-FTIR and chemometric methods as a rapid analysis for essential oils from Myrtaceae plants. This article provides a comprehensive overview of various literature on FTIR, ATR-FTIR, chemometrics, analysis of essential oils, essential oils from Myrtaceae, application of ATR-FTIR, and chemometrics in essential oils from Myrtaceae plants, and their prospects.

METHODS

This current narrative review of the search literature for this study was accomplished from January to October 2021 using electronic databases such as Scopus, PubMed, Web of Science, Directory Open Access Journal, and Google Scholar. During the literature search, the following keywords were used: "Myrtaceae Plants," "Essential Oil from Myrtaceae," "ATR-FTIR Spectroscopy," and "Chemometric Analysis."

Fourier Transform Infrared Spectroscopy (FTIR)

IR spectroscopy is a technique that uses the interaction between electromagnetic radiation in the IR region to investigate the scattering, reflection, absorption, or transmission of IR radiation that occurs during the interaction process. From the results of the IR absorbance of a sample, researchers can determine the structure and chemical information (Glassford *et al.*, 2013). IR spectroscopy has been used successfully in authenticating herbal medicines (Laasonen *et al.*, 2002), detecting impurities or adding chemicals to the sample (adulteration context) (Dong *et al.*, 2012), and measuring both a single sample (Schulz and Baranska, 2007) and sample mix (Chan *et al.*, 2007; Escamilla *et al.*, 2013) in the plant matrix.

The IR region is divided into three wavenumber regions: far-IR at 400–10 cm^{-1}, mid-IR at 4,000–400 cm^{-1}, and near-IR at 14,285–4,000 cm^{-1}. This regional difference varies depending on the type of instrumentation used to measure the IR spectrum and depends on the radiation nature (Lin *et al.*, 2009). There are two instruments, namely, the dispersive IR spectroscopy and FTIR instrument. However, dispersive IR spectroscopy has limitations in sample handling and the inability to combine with precise spectral readings and processing to provide valuable quantitative information (Rohman, 2019). FTIR spectroscopy has become more commonly used to replace IR-dispersive instruments' limitations by providing higher energy yields, significantly scanning speeds, multiplexing capabilities, increasing accuracy, and stabilizing wavelength. FTIR spectroscopy is emerging as a technique for identifying, confirming, and quantitative analyzing (van de Voort *et al.*, 2008).

FTIR is a measurement technique by collecting IR spectra formed due to periodic vibrations of the atoms in a molecule. The principle of this technique is to shoot a beam of IR radiation at a sample so that the molecules in the sample absorb energy and vibration occurs. The absorption of this energy can be captured or detected at various wavelengths or frequencies. The difference in the absorbance patterns absorbed by each compound causes the compounds to be quantified and differentiated (Karoui, 2018; Sankari *et al.*, 2010).

FTIR uses an interferometer to separate wavelengths (Karoui, 2018). The most commonly used interferometer is the Michelson interferometer (Karoui *et al.*, 2008). The detector used in FTIR is made of materials that can receive high-speed signals, such as a mercury cadmium telluric detector or a pyroelectric lithium tantalate detector ($LiTaO_3$). There are two kinds of optical configurations in FTIR, namely, single beam and double beam. FTIR spectroscopy reading begins when the energy released from the source passes through the interferometer before the energy passes through the sample, then proceeds to the detector,

computer, and reading section. The interferometer radiation source will be divided half by the beam splitter towards the stationary mirror and the mobile mirror, which constantly moves (Karoui, 2018; Karoui *et al.*, 2008). The beam splitter is usually made of KBr coated with germanium (Ge) between the mirrors (Karoui *et al.*, 2008). The beam splitter reunites the two separated lights (Karoui, 2018), producing a constructive/destructive interference pattern caused by the variance between the two beam components' distance traveled. The part of the light that comes back together then reaches the detector (Ismail *et al.*, 1997; Prieto *et al.*, 2017).

In spectrum measurement using FTIR spectroscopy, there are three techniques for measuring samples that are commonly used, namely, ATR, Diffuse Reflectance Infrared Fourier Transform, and Photo Acoustic Spectroscopy. Each of these techniques has different characteristics in the molecular vibration spectrum (Beasley *et al.*, 2014).

Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR)

ATR is a relatively fast technique in the initial steps of the characterization of samples. Other advantages are that it is easy to prepare samples, there is no need for KBr grinding, a broader spectrum variation, and a negligible difference in particle size (Thompson *et al.*, 2009). The ATR principle is based on the phenomenon of total internal reflection. It measures the changes in IR reflected light internally in interaction with the sample via zinc selenium (ZnSe), crystals, or diamonds. When the sample is placed on the ATR crystal, the sample will absorb energy so that the result is an attenuated IR wave (Gredilla *et al.*, 2016).

ATR-FTIR spectroscopy involves directing the IR light at the interface between IR transparent materials with a high refractive index called the internal reflex element (IRE), for example, a prism of ZnSe, crystal, Ge, or silicon material, and the sample on the IRE. The angle of incidence of the IR beam is greater than the critical angle, which causes total internal reflection to occur. On the reflected surface, evanescent waves are formed, and these waves interact with the sample, attenuating the IR rays coming out of the IRE (Glassford *et al.*, 2013). Vibrational spectroscopy methods such as ATR-IR are fast, noninvasive, and sensitive methods for analyzing physical and chemical parameters in quality control (Bittner *et al.*, 2016). Besides, ATR-FTIR spectroscopy also offers high-quality characteristic information and is relatively inexpensive. The sample used does not require initial preparation, and it is also possible to carry out semiquantitative analysis, apart from qualitative analysis (Bunaciu and Aboul-enein, 2021; Kucharska-ambrożej and Karpinska, 2020; Peets *et al.*, 2017).

Chemometrics

Spectral overlap in the spectroscopic analysis becomes very likely to happen, so it is necessary to develop a method that involves recognizing a pattern as a filter to identify the part of the spectrum of the sample under study (Nikzad-langerodi *et al.*, 2017). The chemometric method is a practical qualitative and quantitative analysis (Mazivila and Olivieri, 2018). Chemometrics is a mathematical and statistical application in chemical data processing (Rohman, 2019). This method aims to produce valuable information from the data set using optimal sample measurement techniques and produce chemical information from the sample data (Kumar and Sharma, 2018).

The advantage of using chemometrics in the analysis is its ability to analyze multivariate data produced from measuring several variables in the same sample. This data is called multivariate data (Guillén and Cabo, 1997). Advances in chemometric methods can be used to analyze large amounts of complex sample data. In addition, this method also produces significant, accurate, and short-term data (Kumar and Sharma, 2018). Chemometric analysis methods are divided into supervised and unsupervised methods.

Supervised methods

The supervised pattern recognition method has been extensively used in analyzing data with different applications for purposes such as classification, discrimination (differentiating), individualization, and impurity detection (Kumar and Sharma, 2018). The analysis using this method uses prior knowledge-based machine reading (Li *et al.*, 2020). A model is formed based on a sample from a known class. This model can then predict the class of previously unknown samples (Kumar and Sharma, 2018). The objectives of the supervised method can be divided into two; classification and regression.

For classification purposes, sample fingerprint analysis is often performed for qualitative purposes such as differentiation, recognition, and traceability. This classification can be separated based on different approaches: the analysis of discrimination (differences) between classes and class modeling analysis (Oliveri, 2017). Discriminant/difference analysis ("hard modeling") focuses on problems in many classes (multiclass), which includes Partial Least Squares-Discriminant Analysis (PLS-DA), Linear DA, and k-nearest neighbor (Kumar and Sharma, 2018). For example, the problem includes differences in plant origin, geographic origin, and time of growth (Li *et al.*, 2020).

Class modeling analysis (soft modeling) focuses on one class's problems, and only that class is concerned. For example, in the problem of determining the authenticity and recognition of herbal medicine "A" (target sample), the data set containing fake herbal medicine "A" or samples other than herbal medicine "A" becomes a nontarget sample, preventing it from being analyzed on a regular and comprehensive basis. This condition causes the sample to fail in forming a class. Herbal medicine "A" is the target class in in-class modeling, and herbal medicine "A" that contains counterfeit ingredients or herbal medicine other than herbal medicine "A" is a separate heterogeneous group of the target class (Li *et al.*, 2020).

One example of a class modeling technique is the Soft Independent Modeling Class Analogy (SIMCA) (Kumar and Sharma, 2018). SIMCA combination or modification methods where the method approach is limited to those listed above because it is adjusted to the research needs (Kucharska-ambrożej and Karpinska, 2020).

For regression analysis purposes, it is generally carried out depending on the properties of the information obtained from the sample fingerprints. Regression techniques that are often used are Partial Least Square Regression, Support Vector Regression, and Artificial Neural Network. In vibrational spectroscopy, quantitative analysis cannot be carried out immediately. However, with multivariate calibration applications, data from vibrational spectroscopy can be indirectly used to measure certain substances (Li *et al.*, 2020). Hence, this regression analysis can be used for rapid screening and quantitative purposes (Ma *et al.*, 2018a, 2018b).

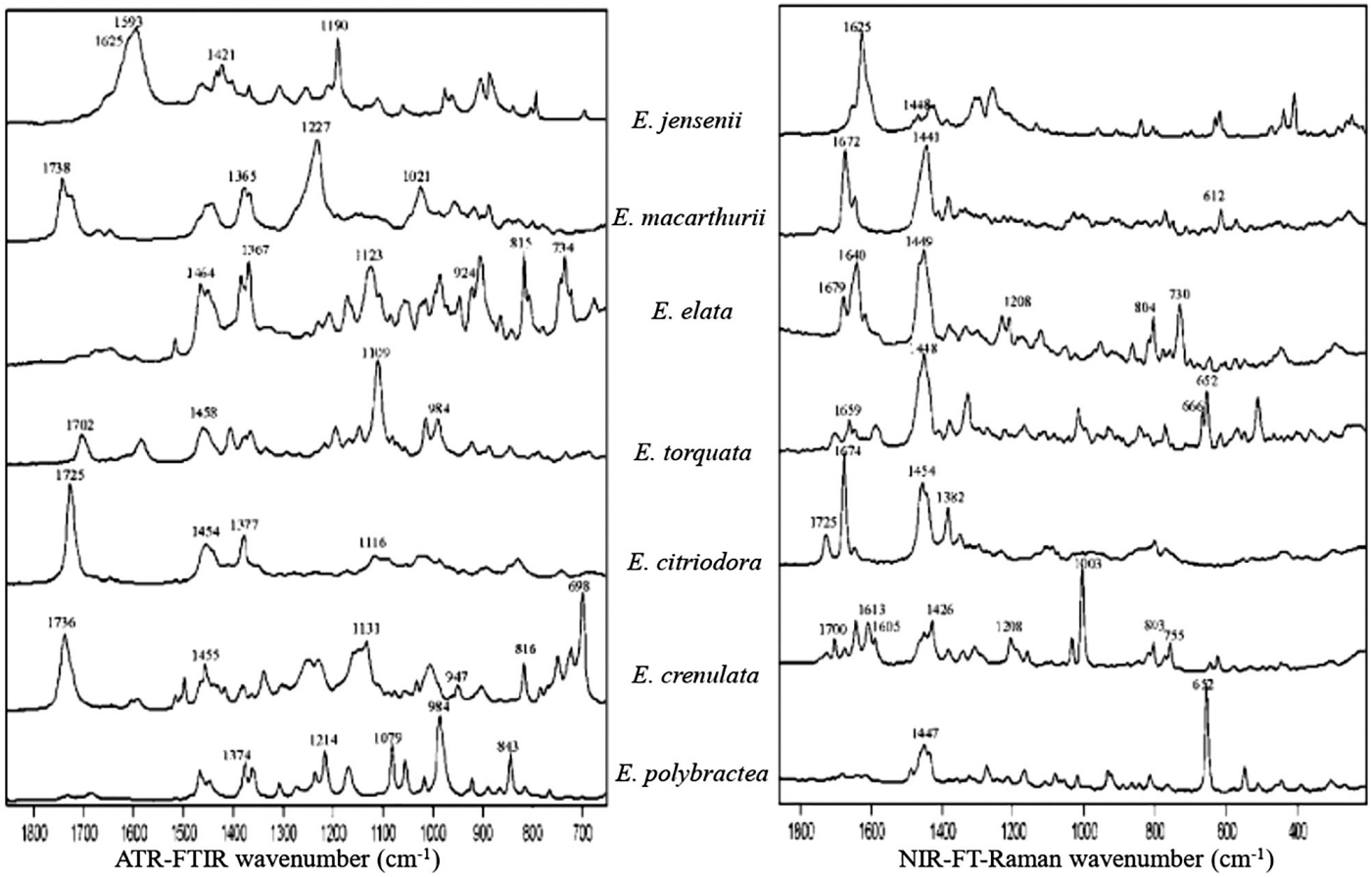

Figure 1. Essential oils spectra from the leaves of different *Eucalyptus* species using ATR-FTIR and NIR-FT-Raman spectroscopy (Baranska *et al.*, 2005).

Unsupervised methods

The unsupervised method is divided into exploratory analysis and similarity analysis (SA) methods (Kharbach *et al.*, 2020). Exploratory analysis extracts the main fingerprint characteristics and contributes to an unbiased view of the data set. This method can obtain information on cluster trends between groups, the relationship between variables, variables, and the sample (Callao and Ruisanchez, 2018; Yi *et al.*, 2016). The relationship between variables can explain which variables can complement or provide similar information and which variables are important in group differentiation (Callao and Ruisanchez, 2018).

In the exploratory analysis method, the principal component analysis (PCA) and hierarchical cluster analysis (HCA) methods are often used to analyze chemical fingerprints, and the combination of these two methods can complement each other (Kumar and Sharma, 2018; Li *et al.*, 2020). The HCA is an analysis method that produces a cluster hierarchy to classify samples based on the similarity of each fingerprint (Kumar and Sharma, 2018; Li *et al.*, 2018, 2020). The HCA method can be visualized as a dendrogram, a tree diagram showing the sequence of merging or splitting due to differences (Li *et al.*, 2020). The HCA method is used for exploration purposes, especially identifying similarities and differences in the samples under study, which reduces the data dimension and draws the dominant pattern in the complex matrix (Mazivila and Olivieri, 2018). This method is frequently used to investigate the similarity of fingerprints from different plants. Whereas in SA, the similarity parameters are statistically measured to see the similarity or dissimilarity of the various fingerprints obtained (Dai *et al.*, 2019; Kharbach *et al.*, 2020; Zhang *et al.*, 2019; Zhang and Sun, 2019).

Essential oils analysis

Essential oils, also known as aromatic plant essences, are volatile oils responsible for the flavor and aroma of organic materials (Amorati *et al.*, 2013). All plant organs, including buds, flowers, bark or wood, roots, fruits, leaves, twigs, stems, and seeds, synthesize them and store them in epidermic cells, secretory cells, cavities, canals, or glandular trichomes (Bakkali *et al.*, 2008).

Essential oils have a long history of use, which has resulted in a slew of quality control measures. The chromatographic method is frequently used to determine essential oils. Standard methods used to analyze and determine the components of essential oils from plants are GC-FID or GC-MS (d'Acampora Zellner *et al.*, 2010; Farag *et al.*, 2018). This method has the advantages of high accuracy, specificity, and sensitivity. However, unfortunately, it requires an extended analysis time (about 60–90 minutes) (Freitas *et al.*, 2018), a long sample preparation time, large amounts of organic solvents, and high temperatures that impact sample damage (Shi *et al.*, 2020). The addition of chemometric techniques to the analysis of the spectrum effectively displays specific differences between plant chemotypes (Baranska *et al.*, 2005; Schulz *et al.*, 2004; Schulz and Baranska, 2007). Some studies have successfully reported the analysis of essential oils

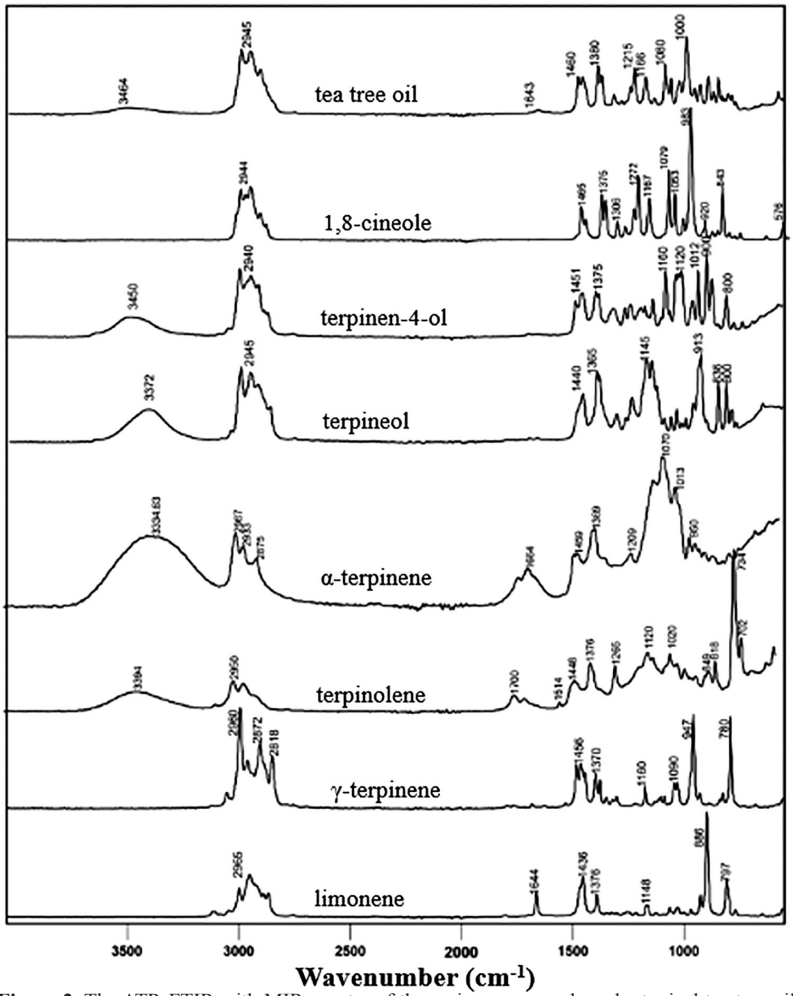

Figure 2. The ATR-FTIR with MIR spectra of the major compounds and a typical tea tree oil from *M. alternifolia* (Tankeu *et al.*, 2014).

using the GC-MS/GC-FID method with and without chemometric combination, as seen in Table 1.

Using the MCR-ALS chemometric technique, the chromatogram peaks of the highly overlapping *T. vulgaris* (A) and *T. serpyllum* (B) can be analyzed. The MCR-ALS algorithm can separate the coeluted peaks of groups A and B into pure chromatograms and mass spectra using the MCR-ALS algorithm. A quantitative analysis of the peaks eluted together is impossible without chemometric techniques. The PCA technique was used to identify intrinsic components that play a role in differentiating *T. vulgaris* and *T. serpyllum* after the MCR-ALS results were obtained (Asadollahi-Baboli *et al.*, 2015).

The spectrum data obtained from the *P. sordidum* plant was analyzed using a combination of PCA and CA. Both methods aid in reducing multivariate data and in the presentation of the results. The data for diagram formation is generated using the PCA technique, which plots both the oil sample (an object) and the oil content (variable). At the same time, the CA provides data for the classification tree from which the sample locations (objects) are gathered. By combining these two, researchers determined the relationship between the three *P. sordidum* populations studied and the essential oil composition that resulted (Brunnel *et al.*, 2016).

The HCA method is a technique that can be used to classify samples (variables) based on the distance between the relationships formed. Samples of *C. japonicum* and *C. setosum*, divided into 14 specimens, divided the two plants into four clusters, in which clusters four samples were grouped because they had a similar aroma (Zeng *et al.*, 2016).

The SA technique is a sample analysis technique based on the similarity between each sample and using the correlation coefficient. The SA results in analyzing *P. cablin* showed that samples taken from Hainan province differed from those from Guangdong and Guangxi provinces. Furthermore, the HCA technique in classifying *P. cablin* divides the sample into three main clusters based on 12 characteristic peaks from the GC-FID profiles (Yang *et al.*, 2016).

The combination of PCA and HCA is used to classify various Nigella clan species from several regions. The HCA technique shows two clusters, denoted as clusters 1a and 1b. Cluster 1a grouped all *N. sativa* from different regions into one group. Meanwhile, cluster 1b groups other *Nigella species* apart from *N. sativa*. The PCA technique is an additional multivariate tool to understand heterogeneity among different *Nigella* (different species and regions of origin). The OPLS-DA technique was used to determine whether *N. sativa* and *N. damascena* essential oils' profiles are uniquely identified as markers for each species (Farag *et al.*, 2018).

Table 1. Research on essential oil analysis from Myrtaceae plants using the GC-MS/GC-FID method and chemometric combination.

Plants	Analysis method	Chemometric method	References
Thymus vulgaris and *Thymus serpyllum*	GC-MS	Multivariate curve resolution-alternating least square (MCR-ALS) and PCA	Asadollahi-Baboli *et al.* (2015)
Phagnalon sordidum	GC-FID and GC-MS	PCA and canonical analysis (CA)	Brunnel *et al.* (2016)
Salvia hypoleuca	GC-FID and GC-MS	HCA	Sonboli *et al.* (2016)
Corymbia citriodora; Melaleuca bracteate; *Melaleuca linariifolia*; *Melaleuca ericifolia*; *Melaleuca lateritia*; *Melaleuca armillaris*; *Melaleuca globulus*; *Melaleuca styphelioides*; *Eucalpytus camaldulensis*; *Eucalpytus globulus*; *Eugenia supraaxillaris*; *Eugenia uniflora*; and *Syzygium samarangense*	GC-MS	HCA, PCA, and orthogonal projection to latent structures (OPLS)-DA	Farag *et al.* (2018)
Pogostemon cablin	GC-FID	SA and HCA	Yang *et al.* (2016)
Cirsium japonicum and *Cirsium setosum*	GC-MS	HCA	Zeng *et al.* (2016)
Baeckea frutescens; *Callistemon citrinus*; *Melaleuca leucadendra*; and *Syzygium nervosum*	GC-MS	Agglomerative HCA	Giang *et al.* (2020)
Eugenia florida DC.	GC-MS		Cascaes *et al.* (2021)
Myrcia eximia DC	GC-MS		Ferreira *et al.* (2020)
Myrcia lundiana	GC-FID and GC-MS		Melo *et al.* (2021)
Baeckea frutescens; and *Leptospemum javanicum*	GC-FID and GC-MS		Saad *et al.* (2021)
Psidium guajava	GC-FID and GC-MS		Fernandes *et al.* (2021)
Eugenia patrisii; Eugenia stipitate; Myrcia splendens; Myrcia sylvatica; P. guajava; Psidium guineense	GC-FID		Jerônimo *et al.* (2021)

Essential oils from Myrtaceae family

Myrtaceae is a plant family with a wide range of essential oils (Siddique *et al.*, 2020). The Myrtaceae family includes over 140 genera and about 3,500–5,800 species (Frauches *et al.*, 2016). The species from this family are aromatic plants with great agroindustrial potential (Sardi *et al.*, 2017) and are distributed in Australia, Africa, South America, India, Southeast Asia, and other Pacific islands (Thornhill *et al.*, 2015). The Myrtle family consists of various genera, including *Eucalyptus*, *Melaleuca*, *Eugenia*, and *Syzygium*.

The genus *Eucalyptus* consists of about 900 species and subspecies (Brooker and Kleining, 2004; Gilles *et al.*, 2010). *Eucalyptus* originates from Australia and Indonesia and has spread worldwide (Hamdy *et al.*, 2007; Payn *et al.*, 2008). This clan is one of three similar genera called "eucalypts," including *Corymbia* and *Angophora* (Farag *et al.*, 2018). *Eucalyptus* has been widely used for many purposes and has recently grown worldwide in warm temperatures (Tavares *et al.*, 2019). The essential oil extracted from this plant exhibits antifungal, antibacterial, antiseptic, antioxidant, expectorant, anticancer, and anti-inflammatory properties (Frauches *et al.*, 2016; Ghaffar *et al.*, 2015; Paosen *et al.*, 2017; Sebei *et al.*, 2015; Sharifi-Rad *et al.*, 2017b). In addition, this oil has been traditionally used for treating respiratory ailments, such as nasal congestion, influenza, and the common cold (Sebei *et al.*, 2015; Sharifi-Rad *et al.*, 2017b). The main constituent of *Eucalyptus* oil is 1,8-cineole (cineole or eucalyptol) (Mohamed *et al.*, 2015; Sebei *et al.*, 2015).

The genus *Eugenia* is the largest genus in the myrtle family, which includes more than 1,058 species distributed in tropical and subtropical areas (Farag *et al.*, 2018). Consumption of *Eugenia* fruit is highly recommended because it is rich in nutrients important for health (Seraglio *et al.*, 2018). The fruit is rich in minerals, vitamins, carotene, anthocyanins, phenolic compounds, sugar, and fiber (de Souza *et al.*, 2018; Santos *et al.*, 2015). The bioactive components have properties like antioxidants, antihypertensive, antidiarrheal, anti-inflammatory, antimicrobial, antifungal, antidiabetic, antigenotoxic, antihyperglycemic, antitumor, antimutagenic, antinociceptive, and gastroprotective (da Silva *et al.*, 2018; Dametto *et al.*, 2017; de Souza *et al.*, 2018; Han and Parker, 2017; Moura and Franzener, 2018; Ullah *et al.*, 2018). The main components of

Table 2. Research on essential oil analysis from Myrtaceae plants using the ATR-FTIR/FTIR-chemometric method.

Plants	Analysis method	Chemometric method	References
Eucalyptus jensenii; *Eucalyptus macarthuri*; *Eucalyptus elata; Eucalyptus torquate*; *Eucalyptus citriodora*; *Eucalyptus crenulate*; *Eucalyptus polybractea*	ATR-IR and NIR-FT-Raman	HCA	Baranska *et al.* (2005)
Eucalyptus citriodora; E. globulus	ATR-IR	PLS	Baranska *et al.* (2006)
Myristica fragnans; *Cinnamonium cassia*; *C. vulgaris*; *Pimoinella anisum*; *Eugenia caryophyllata*	ATR-FTIR	PLS	Wang and Sung (2011)
Melaleuca alternifolia	ATR-IR and NIR Spectroscopy	PCA and PLS	Tankeu *et al.* (2014)
Corymbia citriodora; *Melaleuca bracteate*; *M. linariifolia*; *M. ericifolia*; *M. lateritia*; *M. armillaris*; *M. globulus*; *M. styphelioides*; *E. camaldulensis*; *E. globulus*; *Eugenia supra axillaris*; *E. uniflora*; and *S. samarangense*	ATR-IR	HCA, PCA, and OPLS-DA	Farag *et al.* (2018)
Eugenia caryophyllus	ATR-FTIR spectroscopy	PLS	Tarhan (2021)

essential oils from this family are α-pinene and β-caryophyllene (Agredo, 2017; Mesquita *et al.*, 2017; Pereira *et al.*, 2017). In contrast to other species of this genus, *E. uniflora* contains selina-1,3,7(11)-trien-8-one and selina-1,3,7(11)-trien-8-one epoxide as the main components in its oil, which has antifungal activity (dos Santos *et al.*, 2018).

The genus *Melaleuca* consists of 260 species spread in Australia and Southeast Asia, the Caribbean, and the southern part of the United States (Tran *et al.*, 2013). The essential oil from this family exhibits anti-inflammatory, antibacterial, insecticidal, fungicidal, antiviral, and antioxidant properties (Baldissera *et al.*, 2016; Ebani *et al.*, 2018; Hammer, 2015; Louhibi *et al.*, 2015; Osunsanmi *et al.*, 2016; Padalia *et al.*, 2015; Sharifi-Rad *et al.*, 2017a; Siddique *et al.*, 2015). Research on the chemical composition of the essential oil of this genus has previously been reported, which is 1,8-cineole; eugenol methyl ether; α-pinene; terpinene-4-ol; α-terpinene; terpinolene; and caryophyllene oxide, which is the main component in most of the essential oils of various species in this family (Albouchi *et al.*, 2017; Fall *et al.*, 2017; Kong *et al.*, 2020; Siddique *et al.*, 2017, 2020).

The genus *Syzygium* includes approximately 1,139 species scattered in tropical and subtropical areas, many of which are medicinal plants in Southeast Asia (Li *et al.*, 2015). This clan belonged to the *Eugenia* clan until 1972. It was proven that the *Syzygium* and *Eugenia* clans were two different genera, seen from the analysis of anatomical data and confirmed by their molecular research (Byng *et al.*, 2015). The extract obtained from this clan has antibacterial, antiviral, antiprotozoal, antifungal, anti-inflammatory, antioxidant, anticancer, and antidiabetic activity (Byng *et al.*, 2015; Ranghoo-Sanmukhiya *et al.*, 2019; Rocchetti *et al.*, 2019; Syama *et al.*, 2018). This genus contains α-pinene, γ-terpinene, caryophyllene oxide, and β-caryophyllene as the main components (Gao *et al.*, 2012; Lee *et al.*, 2016).

Application of ATR-FTIR and chemometric in essential oil from Myrtaceae plants

The ATR-FTIR spectra can be used to identify the functional groups of the molecules in the samples. The basis for the analysis of essential oils lies in the main components contained in the Myrtaceae plants. The spectrum of terpenoid compounds is the main constituent component of essential oils. The spectrum analysis of terpenoid compounds is based on their vibrational spectrum. IR spectra of samples of commercially available terpenoids present in larger quantities of essential oils were recorded in the IR fingerprint region between 1,800 and 400 cm^{-1}. In the IR region, unique and reproducible spectral information is available for compound identification. Some studies have successfully reported the analysis of essential oils using the ATR-FTIR/FTIR-chemometric method, as shown in Table 2.

Baranska *et al.* (2005) successfully analyzed essential oils of the Myrtaceae family from the *Eucalyptus* using ATR-FTIR and NIR-FT-Raman spectroscopy and HCA chemometric methods. The combination of the two provided rapid results in chemotaxonomic characterization. Mid-IR is used for wavenumbers between 650 and 4,000 cm^{-1}, while HCA is used for wavenumbers 1,400–1,750 cm^{-1} (Baranska *et al.*, 2005). The main components of essential oils are recognizable by both vibrational spectroscopy techniques based on the spectral information of pure terpenoids. The spectroscopic analysis is based on straps of individual volatiles, so it is possible to distinguish between different essential oil profiles of several *Eucalyptus* species, as shown in Figure 1. The presented spectroscopic data has been shown to correlate with the data obtained by GC analysis (Baranska *et al.*, 2005).

Baranska *et al.* (2006) also analyzed commercially available terpenoid compounds present in *Eucalyptus* essential oil in larger quantities. Citronellal, β-citronellol, and 1,8-cineole were the main components found in *Eucalyptus* oil. Citronellal

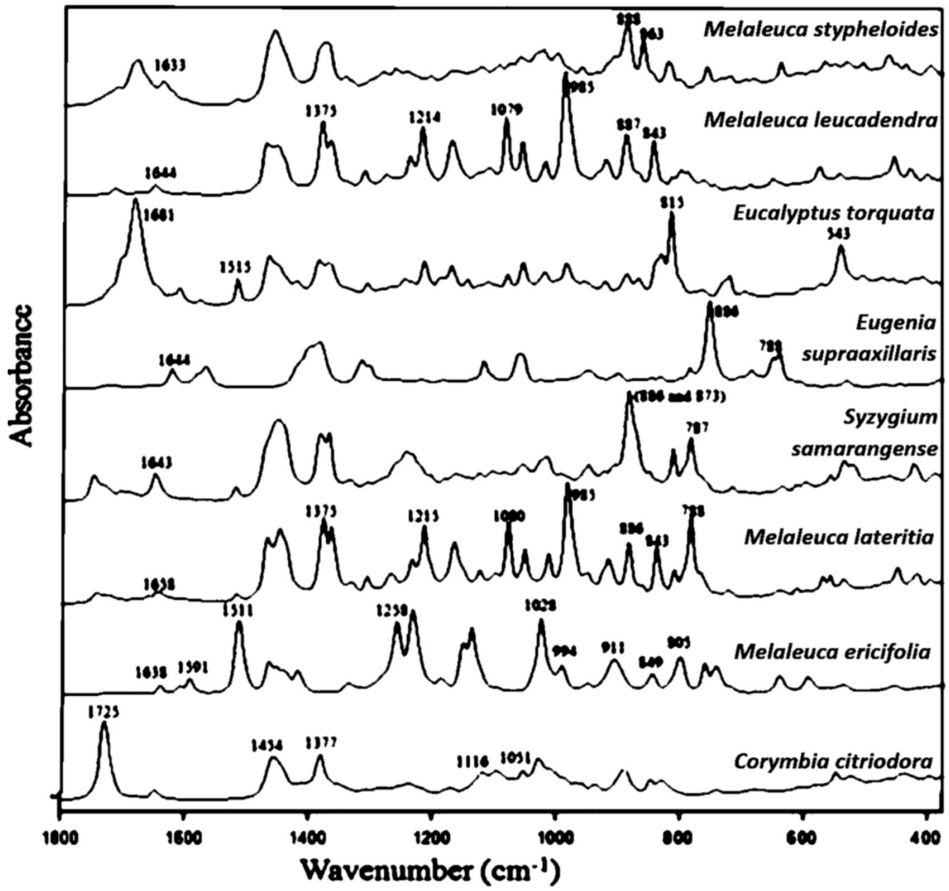

Figure 3. ATR-FTIR spectra of essential oils from the Myrtaceae family (Farag *et al.*, 2018).

and citronellol dominated the IR spectrum of *E. citriodora* oil, while 1,8-Cineole dominated the IR spectrum of *E. globulus* oil. The difference between *E. globulus* oil obtained from China and Australia can only be seen through a visual spectrum examination due to the slight difference in the two compositions. The HCA chemometric method was used to find specific spectral variations between *E. globulus* oil obtained from China and Australia. The spectra collection of *E. citriodora* oil was classified because it contained a large amount of 1.8 cineole (Baranska *et al.*, 2006).

Tankeu *et al.* (2014) successfully analyzed tea tree oil from *M. alternifolia* using ATR-FTIR spectroscopy in the mid-IR area with a wave number of 4,000–550 cm^{-1} and in the near-IR area with a wave number of 10,000–4,000 cm^{-1}. This study used samples of tea tree oil products from various cultivation sites in South Africa. The main components of *M. alternifolia* oil were 1,8-cineole; α-terpineol; terpinene-4-ol; α-terpinene; γ-terpinene; terpinolene; and limonene. The IR spectrum of the tea tree oil (product sample) indicated a slight deviation in the absorbance of the product sample component and the pure sample component, as shown in Figure 2. This was most likely due to the presence of other components in the sample.

Analysis using the PCA and PLS chemometric methods was also carried out. A PCA was performed on centralized spectral data to identify clusters and trends in the data. A PLS regression analysis was carried out on mid-IR and near-IR spectra data to develop a calibration model based on GC quantitative reference values for selected essential oil content. The GC-MS/FID analysis method was also compared. This regression model successfully predicted the contents of an unknown tea tree oil sample's seven main components. Mid-IR data provided better results when compared to near-IR in terms of sample prediction. The mid-IR data results in the calibration model were more similar to the GC reference values than the near-IR data results (Tankeu *et al.*, 2014).

Farag *et al.* (2018) has also successfully analyzed essential oils from the Myrtaceae family using ATR-FTIR spectroscopy and chemometric methods. The initial step was to isolate the essential oils contained in the leaves of 14 species of the Myrtaceae family (*Melaleuca, Eucalyptus, Syzygium, and Eugenia*) using the hydrodistillation method. The isolated essential oils were then measured using ATR-FTIR spectroscopy in the mid-IR region between 375 and 4,000 cm^{-1}. The results of the IR spectrum obtained were then further processed using HCA, which was carried out in the range of wave numbers 3,651–2,645 and 1,800–375 cm^{-1}. The ATR-FTIR spectroscopy analysis obtained various spectra of essential oils from the Myrtaceae family (w) (Farag *et al.*, 2018).

Another study conducted by Tarhan (2021) succeeded in analyzing eugenol, eugenyl acetate, and caryophyllene inside clove essential oil (*E. caryophyllus*) using ATR-FTIR and quantifying it using PLS. The main components of essential oils were recognized by both vibrational spectroscopy techniques based on the spectral information of pure terpenoids. The spectroscopic analysis was based on straps of individual volatiles, so it was possible to distinguish between different essential oil profiles of several *Eucalyptus* species. The presented spectroscopic data has been shown to correlate with the data obtained by GC analysis.

Table 3. The different main components of essential oils from some plants of the Myrtaceae family (Farag *et al.*, 2018).

No.	Plants	Different main component
1.	*Corymbia citriodora*	Citronellal
2.	*Melaleuca lateritia* and *E. globulus*	α-Pinene and 1,8-cineol
3.	*Syzygium samarangense*	α-Pinene, limonene, β-pinene, and p-cymene
4.	*Eugenia supraaxillaris*	α-Pinene and limonene
5.	*Eucalyptus torquate* and *E. camaldulensis*	1,8-Cineol, p-cymene, and cryptone
6.	*Melaleuca armillaris* and *M. linariifolia*	1,8-Cineol and limonene
7.	*Melaleuca leucadendra*	α-Pinene, limonene, and 1,8-cineol
8.	*Melaleuca bracteata* and *M. ericifolia*	Methyl eugenol
9.	*Melaleuca styphelioides*	Caryophyllene oxide and spathulenol
10.	*Eugenia uniflora*	Selina-1,3,7(11)-trien-8-one and selina-1,3,7(11)-trien-8-one epoxide

The detailed spectral analysis of the examined oils was based on their vibrational spectra. The functional group of eugenol contains a double bond and a strong band, as shown in the 1,640–1,500 cm^{-1}. Other characteristic peaks of eugenol at 1,637 and 1,610 cm^{-1} were due to the C = C expansion and contraction of the aromatic moiety. Peaks were seen at 1,430, 1,264, 1,233, 1,204, 1,119, 912, 816, and 794 cm^{-1}. This condition might be due to CH_2 deformation vibration, expansion, and contraction vibration of the CO bond of the hydroxyl-bonded carbon. Ether and alcohol group C–O vibration, C–C stretching vibration, N–CH_2–OCH_3, C–H vibration, CH_2 and C–H ring deformation, and coupling vibration-caryophyllene exhibited high intensity in the spectral range of 3,000–2,800 cm^{-1} due to the aliphatic peak (Tarhan, 2021).

This obtained spectrum showed several wavenumber spectra that can be used to differentiate between citronellol (1,454, 1,377, and 1,051 cm^{-1}); citronellal (1,725, 1,454, 1,377, and 1,116 cm^{-1}); methyl eugenol (1,638, 1,606, 1,591, 1,511, 1,258, 1,028, 994, 911, 849, and 805 cm^{-1}); *α*-pinene (1,658, 886, and 788 cm^{-1}); *β*-pinene (1,641 and 873 cm^{-1}); limonene (1,644 and 886 cm^{-1}); 1,8-cineole (1,375, 1,214,1,079, 983, and 843 cm^{-1}); *p*-cymene (1,515, 813, and 541cm^{-1}); and caryophyllene oxide (1,626, 1,457, 1,365, 888, and 866 cm^{-1}) (Farag *et al.*, 2018). These wavenumber spectra indicated conformity with those reported in previous publications regarding the interpretation of essential oils' vibrational spectrum isolated from Myrtaceae (Baranska *et al.*, 2005; Wang and Sung, 2011). Comparing the wavenumber spectrum between the essential oils studied and their main components showed that the different main components in each of the essential oils studied dominate the vibration spectrum produced by each essential oil (as shown in Table 3). Some components of essential oil, in small amounts, do not significantly affect the ATR-FTIR spectrum (Farag *et al.*, 2018).

Analysis of a sample will always be associated with its application in product quality control. Due to the content of biosynthetic conditions and the complexity of essential oils, quality control has become highly challenging. Classification based on plant chemical content does not always correspond to taxonomic classification, but this is not a problem because essential oil quality control is based on the main components of the oil, whether bioactive or industrial. Vibrational spectroscopy is nondestructive, fast, with minimal sample preparation and a minimum number of analytes. In this study, the ATR-FTIR spectrum produced fingerprints for each essential oil, showing the characteristic profile of the main chemical component. The chemometric method analysis has also succeeded in quickly classifying essential oils based on their chemical composition. This concluded that ATR-FTIR is a fast, efficient, and nondestructive method that can be applied to control essential oils' quality based on their chemical composition (Farag *et al.*, 2018).

Perspective and future direction

This review discussed the spectroscopic potential of ATR-FTIR in research on analyzing essential oil samples from the Myrtaceae family, including the genera *Eucalyptus*, *Eugenia*, *Melaleuca*, and *Syzygium*. Although GC-MS and GC-FID are essential oil analysis methods that are very commonly used, these methods have disadvantages in need for sample preparation, a long analysis time, large amounts of organic solvents, and high temperatures that cause the possibility of sample defects.

The ATR-FTIR spectroscopy method is an alternative method that is faster, easier, more efficient, and nondestructive and does not even require sample preparation because this method can be used on solid or liquid samples. As the overlapping ATR-FTIR spectrum can be a constraint in the analysis, another method is needed to assist the analysis process, namely, chemometrics. The chemometric method is an analytical method that applies mathematical and statistical techniques to analyze samples.

Chemometric methods are divided into many types, such as PCA, HCA, PLS-DA, SA, and others, where the use of this method is tailored to the needs of the analysis to be carried out and the data presented. HCA has been shown to classify the types of essential oils of the Myrtaceae family based on their chemical composition. Even though they have the same species, essential oils from different areas can be differentiated using this HCA method. Multivariate calibration applications such as PLS can indirectly assist in measuring certain substances.

From the above discussion, it can be seen that the use of a combination of ATR-FTIR spectroscopic methods and chemometric methods has the potential to enhance efficiency in obtaining basic sample information that can also be applied in the field of quality control. Due to the content of biosynthetic conditions and the complexity of essential oils, quality control has become highly challenging. For this reason, the use of this method is appropriate when viewed in terms of the benefits that have been previously described.

In addition to obtaining basic information from pure samples for quality control, ATR-FTIR spectroscopy can also be

used to control finished essential oils on the market without the need for sample preparation or analyte separation due to the advantages of this method, which can analyze samples in solid or liquid form. Hence, the combination of ATR-FTIR and chemometric methods provides a reliable method for adulteration detection, analysis of changes in compound structure, analysis of patterns and degradation products, estimate expiration date, and measurement substance.

Its application can also extend to various fields, such as the health sector and the forensic field. Further development will increase the application of more reliable and efficient analysis tools in the sample analysis process to obtain more sample information. This combination of ATR-FTIR spectroscopy and chemometric methods will remain a robust, nondestructive, efficient, simple, sensitive, and fast technique for analyzing various substances in various fields until the present and possibly beyond.

CONCLUSION

The Total reflectance total attenuation IR Fourier transform (ATR-FTIR) spectroscopy method is an alternative that is faster, simpler, more efficient, nondestructive, and even requires no sample preparation as it can be used on solid or liquid samples. Chemometric methods are divided into several categories, such as principal components analysis, HCA, PLS analysis, SA, and others, where the use of this method is tailored to the needs of the analysis performed and the data presented. The ATR-FTIR and chemometrics are recommended in future research in the analysis of essential oil samples from the Myrtaceae family. The combination of ATR-FTIR spectroscopy and chemical measurement provides a powerful, nondestructive, efficient, simple, and fast analysis method for a small sample. In addition to obtaining basic information from purified samples for quality control, the ATR-FTIR spectrometer can also be used to monitor finished essential oils on the market without the need for sample preparation or separation of analytes because of this method's ability to analyze samples in both solid and liquid states.

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AUTHOR CONTRIBUTIONS

All authors made substantial contributions to conception and design, acquisition of data, or analysis and interpretation of data; took part in drafting the article or revising it critically for important intellectual content; agreed to submit to the current journal; gave final approval of the version to be published; and agree to be accountable for all aspects of the work. All the authors are eligible to be an author as per the international committee of medical journal editors (ICMJE) requirements/guidelines.

CONFLICTS OF INTEREST

The authors report no financial or any other conflicts of interest in this work.

ETHICAL APPROVALS

This study does not involve experiments on animals or human subjects.

DATA AVAILABILITY

All data generated and analyzed are included within this research article.

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