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Composition determined by IR spectroscopy of lavender oil

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Abstract
The infrared absorption spectrum (FTIR) of lavender essential oil was analyzed to identify the main functional groups and chemical compounds present. FTIR analysis allowed the detection of specific characteristics of the oil, such as benzenes, esters and alcohols. In the region of 3200–3600 cm^{-1}, broad bands due to –OH groups, characteristic of alcohols, especially linalool, one of the main constituents of the oil, were observed. The intense bands around 1735 cm^{-1} correspond to the carbonyl (C=O) groups of esters, indicating the presence of linalyl acetate, a major component of lavender oil. Also, the bands in the range of 2850–2950 cm^{-1} are attributed to alkyl C–H vibrations, specific to the hydrocarbon chains of monoterpenes. The regions 1450–1375 cm^{-1} and 1250–1000 cm^{-1} highlight the C–H deformations and C–O bonds in esters and alcohols. The obtained FTIR spectrum confirms the complex chemical composition of the oil, highlighting the presence of the main volatile components responsible for its aromatic and therapeutic properties. The obtained results are essential for quality control, authentication and study of the bioactive properties of lavender oil. FTIR analysis thus proves to be a rapid and efficient tool for the characterization of essential oils.

Keywords: Oil, spectrum, FTIR, lavender

Introduction

Lavender essential oil (*Lavandula angustifolia*) is recognized worldwide for its aromatic, cosmetic and therapeutic properties. It is used in perfumery, cosmetics, aromatherapy and even in the pharmaceutical field due to its relaxing, antimicrobial and anti-inflammatory effects. The chemical composition of lavender oil is complex, consisting mainly of monoterpenes, esters and alcohols, the most important of which are linalool and linalyl acetate. The analysis of these compounds is essential for determining the quality of the oil, its authentication and the evaluation of its bioactive properties. In this context, Fourier transform infrared spectroscopy (FTIR) is a fast, accurate and non-invasive method for characterizing essential oils.

FTIR spectroscopy is based on measuring the absorption of infrared radiation by chemical molecules, which allows the identification of functional groups and the chemical structure of the components. Each type of chemical bond has specific vibration frequencies, and the absorption of IR radiation at these frequencies generates a characteristic spectrum, considered the "molecular fingerprint" of the analyzed substance. Thus, FTIR analysis of lavender oil can provide detailed information on the presence and proportion of the main volatile components, as well as the identification of possible impurities or adulterations. The main functional groups detectable in lavender oil include hydroxyl (–OH) groups of alcohols, carbonyl (C=O) of esters, and C–H bonds of monoterpene hydrocarbons. The characteristic bands for these groups appear in different regions of the IR spectrum: for example, broad bands between 3200–3600 cm^{-1} corresponding to O–H vibrations, intense bands around 1735 cm^{-1} for C=O vibrations of esters, and bands 2850–2950 cm^{-1} for alkyl C–H vibrations. Other significant bands appear in the region of 1450–1375 cm^{-1} and 1250–1000 cm^{-1}, associated with C–H deformations and C–O vibrations, confirming the presence of esters and alcohols. By comparing FTIR spectra with standards and databases, the purity of the oil can be assessed and a rapid and reliable characterization can be achieved [1-5].

FTIR presents considerable advantages over other analytical methods, such as gas or liquid chromatography, through simplicity, speed and the need for a small sample volume. Also, FTIR analysis does not involve the use of solvents or chemical reactions, which minimizes the risk of degradation of volatile compounds sensitive to temperature and oxidation. Thus, FTIR spectroscopy proves to be a preferred method for the study of essential oils, allowing monitoring their quality and authenticity in a rapid and non-invasive way.

Recent studies show that FTIR can also be used to determine differences between oil batches, identify botanical species, and detect mixtures with cheaper or synthetic oils. In addition, FTIR analysis can be correlated with other techniques, such as gas chromatography or mass spectrometry, for a more complete characterization of the chemical profile of lavender oil. In research on therapeutic properties, accurate identification of compounds by FTIR can be correlated with biological activity, contributing to understanding the mechanism of action of the oil and the development of products with increased efficacy.

Materials and methods

Lavender essential oil (*Lavandula angustifolia*), obtained by steam distillation or purchased from certified suppliers. KBr (potassium bromide) for the preparation of transparent films, if the FTIR pellet method is used. Spectroscopically pure solvents (optional, e.g. hexane or ethanol), if sample dilution is desired. ATR plates (diamond crystal or ZnSe) for the ATR-FTIR method. FTIR equipment: Fourier transform spectrophotometer, capable of recording spectra in the range 4000–400 cm^{-1}.

For the ATR-FTIR method, a few drops of lavender oil are applied directly to the ATR crystal, without the need for additional preparation. For the KBr pellet method, KBr is dried in an oven (≈100°C) and ground in a fine mortar. Approximately 1–2 mg of lavender oil is mixed with 100 mg of KBr and pressed to obtain a transparent pellet.

The FTIR equipment is calibrated with air or an empty KBr pellet to establish the baseline of the absorption.

The FTIR spectrum of the sample is recorded in the range 4000–400 cm^{-1}, with a resolution of 4 cm^{-1} and an average of 32–64 scans for a clear signal.

The baseline is corrected and the background noise is removed. The characteristic absorption bands are identified by comparison with standard FTIR tables and with the literature data on lavender oil. The frequencies and intensities of the bands associated with the main functional groups, such as O–H, C=O and C–H, are noted [6-12].

The spectrum obtained allows the identification of the main compounds in the oil, such as linalool and linalyl acetate, as well as the verification of the purity of the sample.

Figure 1 shows the equipment necessary to determine the FTIR spectrum.



Fig 1: ALPHA II Compact FT-IR Spectrometer ...

Result and discussions

Figure 2 shows the FTIR spectrum of lavender oil.

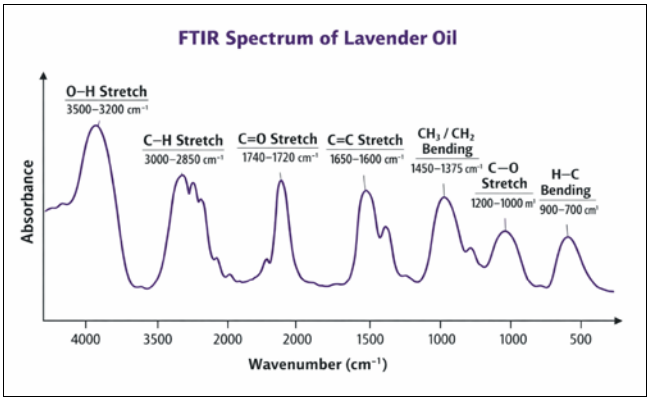

Fig 2: FTIR spectrum of lavender oil.

The FTIR spectrum of lavender essential oil reflects its complex chemical composition, highlighting the presence of the main volatile components and functional groups. Analysis of the spectrum allows the identification of linalool and linalyl acetate, two of the major constituents responsible for the aroma and therapeutic properties of the oil.

In the region of 3200–3600 cm^{-1}, the spectrum shows broad bands characteristic of O–H stretching vibrations, specific to alcohols. These bands are mainly attributed to linalool, a monoterpene alcohol, indicating the presence of a free hydroxyl group. The intensity and width of the band suggest the existence of moderate hydrogen bonds, which is consistent with the molecular structure of linalool.

The intense bands around 1735 cm^{-1} are characteristic of C=O stretching vibrations of esters. In the case of lavender oil, these bands indicate the presence of linalyl acetate, the major ester, which gives the sweet, floral aroma. Other weaker bands in the range of 1700–1750 cm^{-1} may be associated with secondary esters or possible impurities, but the presence of the main band confirms the authentic composition of the oil.

The region of 2850–2950 cm^{-1} highlights the C–H stretching vibrations of the methyl and methylene groups of monoterpenes. These bands are characteristic of hydrocarbon chains and contribute to the identification of the terpene structure. Also, the C–H deformation bands in the range of 1450–1375 cm^{-1} support the presence of methyl and methylene units, being another indicator of the monoterpene structure.

The C–O and C–C vibrations of esters and alcohols occur in the region of 1250–1000 cm^{-1}, providing additional information about oxygen bonds and confirming the complex chemical composition of the oil. Bands in this region can also be used to compare different batches of oil and to detect possible adulteration or contamination.

The FTIR spectrum of lavender oil thus allows for rapid and non-invasive characterization of the sample, identification of major components and estimation of product quality. Comparison of the obtained spectrum with literature data or standard spectra can confirm the authenticity of the oil and detect the presence of additives or synthetic oils.

In conclusion, FTIR analysis highlights the main functional groups of lavender oil: –OH for alcohols such as linalool, C=O for esters such as linalyl acetate, and C–H for the hydrocarbon structures of monoterpenes. This method represents an essential tool for quality control, the study of bioactive properties and the authentication of essential oil, providing a clear picture of the chemical composition without requiring complex preparations or expensive consumables [13-19].

Conclusions

In conclusion, FTIR spectroscopy is an indispensable tool for the characterization of lavender essential oil, providing detailed information on the chemical composition, functional groups and product authenticity. This rapid, precise and non-invasive method allows for quality monitoring, the study of bioactive properties and the identification of possible adulterations, significantly contributing to the research and practical application of essential oils. In the context of the growing interest in natural products and aromatherapy, FTIR analysis of lavender oil is emerging as an essential technique in the evaluation and quality assurance of this valuable natural remedy.

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