Miniaturized mid-infrared gas sensors combined with chemometrics for the discrimination of commercial Lavender Essential oils

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ABSTRACT - Essential oils (EOs) are increasingly valued across multiple industries due to their natural and bioactive properties, yet issues such as adulteration and mislabeling pose significant challenges to quality assurance. This study investigates the use of mid-infrared (MIR) spectroscopy combined with a hollow waveguide (HWG) for rapid, non-destructive analysis of the volatile fraction of five commercial *Lavandula angustifolia* essential oils. Spectral data, collected over 400–4000 cm^{-1}, revealed characteristic absorption bands related to key EO constituents. Principal component analysis (PCA) demonstrated clear discrimination among brands, reflecting compositional differences likely influenced by botanical origin, extraction processes, and storage conditions. The results highlight MIR-HWG spectroscopy coupled with chemometrics as a promising, cost-effective alternative for quality control and authentication of essential oils in commercial settings.

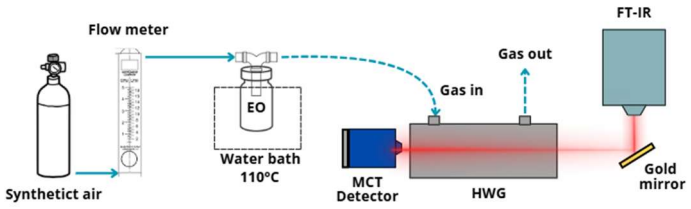
Keywords: Essential oils, Lavandula angustifolia, Mid-infrared spectroscopy.

Introduction

Essential oils (EOs) are widely used across various industries, including food, cosmetics, perfumery, pharmaceuticals, and aromatherapy, due to the growing demand for natural and bioactive products (1). However, the high market value of EOs often leads to issues such as adulteration, dilution, or mislabeling, which compromise product quality, efficacy, and consumer safety. Among these, *Lavandula angustifolia* EO is particularly valued for its pleasant aroma and therapeutic properties. Traditionally, gas chromatography coupled with mass spectrometry (GC–MS) is the standard method for analyzing EO composition and detecting adulteration. While GC–MS offers high sensitivity and resolution, it is also costly, time-consuming, and requires specialized training (2). As an alternative, vibrational spectroscopy techniques such as mid-infrared (MIR) spectroscopy have gained attention for rapid, non-destructive, and cost-effective EO analysis (3). When combined with multivariate statistical tools like principal component analysis (PCA), MIR enables the identification of chemical differences and authentication of EO samples.

In this study, we evaluated the potential of MIR spectroscopy using a hollow waveguide (HWG) to analyze the volatile fraction of five commercial *L. angustifolia* EOs. The methodology involved sample heating to enhance volatilization and synthetic air to transport volatile compounds through the HWG for spectral acquisition.

Experimental



Scheme 1. Schematic of the optical setup.

Five commercial samples of lavender essential oil (EO) were obtained from different national brands. Mid-infrared (MIR) spectra of lavender EO samples were acquired using an Alpha Bruker spectrometer (Bruker OPTIK GmbH, Ettlingen, Germany) equipped with a hollow waveguide (HWG). Prior to analysis, each sample was heated in a water bath at 110 °C for 15 minutes to enhance volatilization. A synthetic air flow of 50 mL/min was then applied to carry the volatile compounds through the HWG, where spectral measurements were recorded. OPUS software was used to collect the spectra in absorbance mode over the range of 400–4000 cm^{-1}, with 16 scans per sample acquired in quintuplicate at a spectral resolution of 4 cm^{-1}. Chemometrics technique was performed using MetaboAnalyst 6.0.

Results and discussion

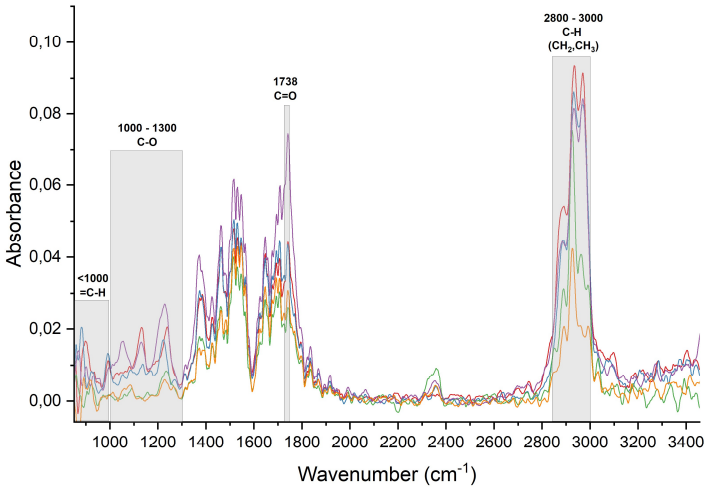
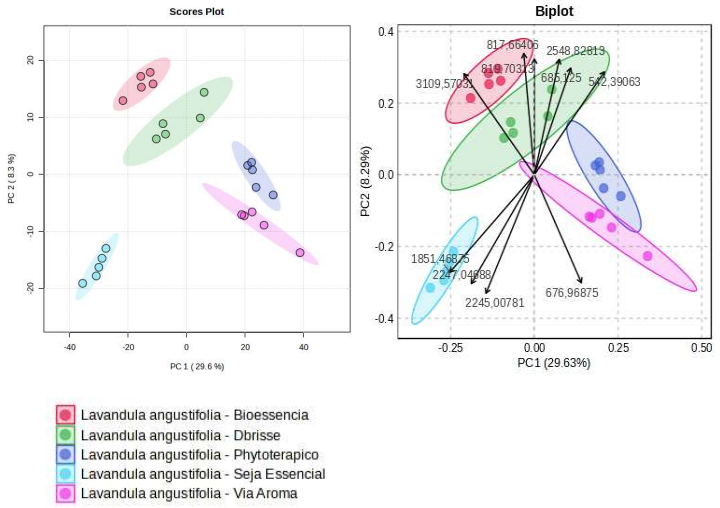


Figure 1. FT-IR spectra of lavender essencial oil in the regions 400 – 3500 cm^{-1}.

The infrared spectra of the *Lavandula angustifolia* EO samples revealed characteristic absorption bands corresponding to key functional groups and volatile constituents. The region between 2800–3000 cm^{-1} showed C–H stretching vibrations of CH_2 and CH_3 groups, with peaks around 2877 cm^{-1}, typically attributed to linalool, linalyl acetate, ocimene, and caryophyllene (2,5). A distinct absorption at 1738 cm^{-1} indicated C=O stretching, consistent with ester functionalities found in linalyl acetate and camphor (1,2). Finally, bands between 1000–1300 cm^{-1} were attributed to C–O stretching, supporting the presence of oxygenated monoterpenes (1). These spectral features align with the typical chemical profile of lavender essential oil.



Principal Component Analysis (PCA) was applied to explore and discriminate the chemical profiles of five commercial *Lavandula angustifolia* essential oil samples from different brands. The score plot revealed a clear separation among the samples, with distinct clusters and no overlap between brands, indicating specific chemical profiles for each product. The first two principal components (PC1 and PC2) jointly explained 37.9% of the total data variance, with PC1 accounting for 29.6% of the variability. The biplot highlighted the influence of spectral variables on sample distribution, suggesting that different chemical constituents—likely volatile compounds characteristic of lavender—were key to the observed discrimination. Specifically, samples from the Bioessência brand were associated with variables contributing positively to PC2, while those from the Via Aroma brand were influenced by variables with negative loadings on both principal components. These findings indicate compositional differences among the evaluated essential oils, which may be attributed to factors such as the botanical origin of the raw material, extraction methods, storage conditions, or even potential adulteration.

Conclusions

This study demonstrated that mid-infrared (MIR) spectroscopy, using a hollow waveguide (HWG) as a gas cell for direct analysis of the volatile phase of compounds, combined with multivariate analysis by PCA, is an effective tool for the characterization and differentiation of commercial *Lavandula angustifolia* essential oils. The chemical differences detected among the samples indicate variations in the volatile composition, possibly resulting from botanical origin, extraction methods, storage conditions, and even potential adulterations.

The proposed methodology offers a rapid, non-destructive, and cost-effective alternative to conventional techniques such as GC–MS, facilitating quality control and authenticity verification of these products in the market.

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