# The Influence of Extraction Method on the Composition of Essential Oils from Lemon Peels Analysed with FTIR

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## ABSTRACT

The extraction method selected for extracting essential oils from lemon peels has a marked impact on both the yield and the chemical composition of the resulting product. In this study, the chemical profiles of the oils extracted with solvent extraction using hexane and steam distillation were analysed via Fourier Transform Infrared Spectroscopy (FTIR). The findings demonstrate that hexane extraction preferentially recovers non-polar constituents, such as alcohols, phenols, and aromatic compounds. In contrast, steam distillation is more effective at isolating volatile and aliphatic hydrocarbons, particularly limonene and related terpenes, which are significant for their characteristic citrus aroma. The FTIR spectra showed the characteristic existence of certain functional groups such as alkanes, alkenes, carbonyls, and aromatics that enabled distinction between the compositions of the essential oils from the two extraction processes. The results emphasise the importance of selecting the extraction process, particularly when designing essential oil compositions for targeted purposes in the food, pharmaceutical, or cosmetic industries. In general, these results provide useful information regarding how methods for extraction could potentially be modified to more closely match the intended results.

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## 1.0 Introduction

Essential oils are complex, naturally synthesised, volatile aromatic fluids found in plants. They are greatly prized for their odour, potential therapeutic action, and ability to function as preservatives (Durczyńska & Żukowska, 2024). Essential oils contain a mixture of compounds, predominantly terpenoids and phenolic compounds, responsible for their diverse array of biological activities (de Sousa *et al.,* 2023; Rashidinejad & Jafari, 2020). Lemon essential oil, principally gotten from the lemon fruit peel, contains principally volatile chemicals, of which the most prevalent is D-limonene and typically contributes between 60% and over 80% of the oil (El Aboubi *et al*., 2022). The other main constituents include citral, which accounts for the lemon smell, and monoterpenes like γ-terpinene, β-pinene, and linalool (Ahmed & Mariod, 2022). The extraction method has significant influence on the yield and chemical composition of the essential oil (Souiy, 2024). A variety of methods, including subcritical fluid extraction, solvent extraction, Soxhlet extraction, hydrodistillation, cold pressing, and microwave-assisted hydrodistillation, can be employed to extract essential oil from lemon peels (Ibrahim *et al.,* 2024).

For example, steam distillation, a well-established technique for extracting essential oils, involves volatilising oil components using steam, condensing the vapour, and collecting the resulting liquid (Nour *et al*., 2024). The loss of some heat-sensitive or less volatile chemicals or thermal degradation are potential consequences of this method (Shrivastava, 2023). Solvent extraction entails soaking plant material in a usually non-polar solvent such as hexane to extract volatile and some non-volatile compounds (Cravotto *et al*., 2022). Upon evaporation of the solvent, a "concrete" residue remains, which can be subjected to further processing for the isolation of the essential oils (Cao *et al.,* 2025). This method is effective in the recovery of a wider range of compounds, such as waxes and pigments, and is therefore suitable for fragile or resinous plant material (Gaikwad *et al.,* 2025; Lee *et al.,* 2024). The method of extraction can have a considerable influence on the chemical composition of lemon essential oil and thus its quality and applicability for different uses (Stratakos & Koidis, 2016). Though steam distillation is still the industrial standard, solvent extraction can yield oils with altered or improved chemical composition (Brah *et al.,* 2024).

Lemon oil has applications across different industries, such as food and beverages, pharmaceuticals, cosmetics, and perfumery, due to its distinctive aroma and bioactive properties, such as antimicrobial, antioxidant, and anti-inflammatory activities (Lin *et al.,* 2024; Santana *et al*., 2020). It is a natural flavouring ingredient for baked goods, candies, and beverages because of its antioxidant properties.Essential oils not only enhance flavour but also aid in food preservation (Kačániová *et al*., 2024). Lemon oil is used in cosmetics as an ingredient in face washes, moisturisers, and toners because it aids in the prevention of acne, oil management, skin whitening, and anti-ageing (Guzmán & Lucia, 2021). This is due to its distinctive smell and a range of bioactive traits such as antimicrobial, antioxidant, and anti-inflammatory activities (Ahmed & Mariod, 2022; Klimek-Szczykutowicz *et al.,* 2020). The pharmaceutical sector incorporates lemon oil due to its diverse biological functions, like antibacterial, antifungal, antiviral, antioxidant, and anti-inflammatory properties (Cimino *et al.,* 2021; Das *et al.,* 2021). They can be utilised as active ingredients in medications or as flavouring and perfuming agents in pharmaceutical formulations (Nazir & Ahmad Gangoo, 2022).

Different methods, including Fourier Transform Infrared Spectroscopy (FTIR), can be used to analyse and compare the chemical profiles of essential oils obtained by different extraction methods (El Orche *et al*., 2024). FTIR is a non-destructive analytical technique that provides a molecular fingerprint by measuring the absorption of infrared radiation at specific wavelengths (Kalra *et al*., 2023). These absorptions relate to the vibrational energies of chemical bonds in the molecules (Guerrero-Pérez & Patience, 2020). FTIR is widely utilised for qualitative and semi-quantitative analysis of essential oils, facilitating the identification of functional groups, the detection of adulteration, and the assurance of quality control (Fréda Zamanileha *et al*., 2024). Using FTIR analysis makes it easy and quick to compare these compositional differences in detail, which helps us understand how different extraction methods change the properties of essential oils (Cubas Pereira *et al.*, 2024).

This study investigates how the chemical composition of essential oils from lemon peels is influenced by the extraction technique, such as steam distillation or hexane solvent extraction. The existence of significant functional groups in the oils generated by each method was investigated using FTIR analysis. The aim of the study is to determine which extraction technique produces the best oil qualities by comprehending these variations. It is expected that the results will aid in determining which extraction method is best suited for particular uses of lemon peel essential oils.

## 2.0 Materials and Methods

### *2.1 Materials*

The lemon fruits (Fig. 1) were purchased from Majengo market in Dodoma City and taken to the chemistry research laboratory at the College of Natural and Mathematical Sciences of the University of Dodoma (UDOM) and used as the primary raw material for this study. Fresh peels were carefully removed, cut into small pieces (approx. 1 cm²) to increase surface area and kept at 4°C. Hexane of analytical grade was used as an extraction solvent.Hexane is particularly effective for extracting non-polar compounds like terpenes, which are often found in essential oils. Its ability to selectively extract specific components is advantageous when focusing on particular substances within a complex mixture. After solvent extraction, the low boiling point of hexane (69°C) makes it simple to drain away from an extract, allowing a high-purity essential oil.

Figure 1
*Lemon Fruits (a) Lemon Pills (b) and Grinded Lemon Leels (c)*


The steam distillation method was used in the extraction of volatile compounds like lemon peel essential oils with low-pressure steam and distilled water, differentiating the essential oils from non-volatile compounds. The method is widely used to extract essential oils from plant material, for example, lemon peel. A round-bottom flask, basket heater, Soxhlet extractor with a syphon arm, condenser, measuring cylinder, beaker, funnel, specific gravity bottle, and digital weighing balance were some of the apparatus and glassware used.

### *2.2 Extraction Methods*

Samples were divided into two equal portions for parallel extraction by the two methods. For solvent extraction, a Soxhlet extractor was utilised to extract the essential oil from ground lemon peel using hexane as a solvent. A cellulose thimble was first filled with 100 g of ground lemon peel and then set inside the Soxhlet extraction chamber.

A round-bottom flask beneath the Soxhlet extractor was then filled with 500 mL of hexane. The flask was heated to 60°C, which caused the hexane to evaporate. After rising in the condenser, the vapour cooled and turned back into a liquid. The essential oils were extracted when the liquid hexane dripped onto the lemon peel in the thimble. Following completion, the hexane extract was concentrated using a rotary evaporator at 40°C under reduced pressure to remove the solvent and leave behind the essential oil (Redfern *et al.*, 2014). For steam distillation, 100 grams of ground lemon peel were placed in a flask. Steam was generated and then allowed to flow through the sample continuously for three hours. This procedure vaporised the volatile compounds in the lemon peel and then condensed them to form a distillate with both water and essential oils. After the distillation, the distillate was collected and poured into a separating funnel. The immiscibility between water and oil allowed the separation of the oil layer from the aqueous phase with ease. To remove any traces of water, the separated oil was dried over anhydrous sodium sulphate (Machado *et al*., 2024).

*2.3 FTIR Analysis*

The PerkinElmer FTIR instrument with Spectrum IR ES Version 10.7.2 software, found at UDOM, was used to scan the extracted essential oils.Each essential oil sample was placed directly on the diamond ATR crystal in the form of a drop, allowing immediate measurement and minimal sample preparation. The spectra, recorded at a resolution of 4 $cm^{-1}$ and covering the mid-infrared from 4000 to 400 $cm^{-1}$, exhibited strong molecular vibrations characteristic of the functional groups in the oils. The obtained spectra were scanned for absorption bands that corresponded to particular functional groups, and such bands were precisely assigned using literature values obtained from published works.

It provides a quick, non-destructive fingerprint of the oils that can be used for determining their authenticity, purity, and quality (Njuguna *et al*., 2022).

*2.4 Data analysis*

FTIR spectra were compared for peak positions (wavenumbers) and intensities (% (transmittance). Major functional groups and characteristic compounds were identified. Differences between the two extraction methods were analysed and interpreted.

## 3.0 Results

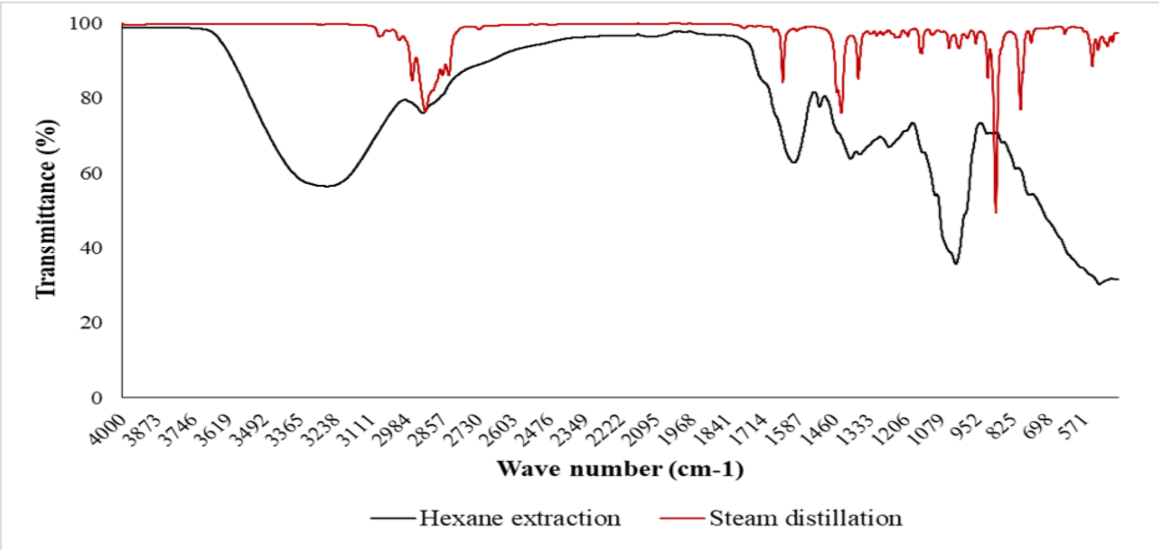
The FTIR peak values of lemon essential oils obtained by solvent extraction using hexane and by steam distillation are presented in Table 1, and the spectra are presented in Fig. 2.

Table 1

*FTIR Spectra for both Hexane Extraction and Steam Distillation, Including the Wave Number, % Transmittance, and Interpretation/Assignment*

| Extraction Method | Wave Number ($cm^{-1}$) | % Transmittance | Interpretation / Assignment |
|---|---|---|---|
| Hexane Extraction | 3272 | 56.39 | O–H stretching (alcohols, phenols) |
| | 2928 | 76.00 | C–H stretching (alkanes) |
| | 2857 | 77.00 | C–H stretching (alkanes, possibly) |
| | 1603 | 62.67 | Aromatic C=C stretching |
| | 1514 | 77.59 | Aromatic ring skeletal stretching |
| | 1404 | 63.77 | $CH_3$ bending vibrations |
| | 1028 | 35.69 | C–O stretching (alcohols, ethers) |
| Steam Distillation | 2965 | 84.59 | C–H stretching (alkanes) |
| | 2928 | 76.51 | C–H stretching (alkanes) |
| | 1644 | 84.17 | C=C stretching (alkenes) |
| | 1436 | 75.91 | Aliphatic hydrocarbon bending |
| | 1376 | 84.95 | Aliphatic hydrocarbon bending |
| | 1241 | 96.08 | C–O stretching (esters, ethers) |
| | 1147 | 91.93 | C–O stretching (esters, ethers) |
| | 886 | 49.41 | Aromatic C–H out-of-plane bending |
| | 797 | 76.87 | Aromatic C–H out-of-plane bending |
| | 542 | 88.54 | C–X stretching (likely artifact or impurity) |

Figure 2
*FTIR Spectrum of Essential*




The FTIR spectra of lemon peels essential oil (Fig. 2) shows significant variations in the number and intensity of absorption peaks, reflecting variations in chemical composition and efficiency of extraction. For oil extracted with hexane, intense peaks are found at 3272 cm$^{-1}$ (56.39% transmittance), which correspond to O–H stretching vibrations typical of alcohols and phenols, reflecting the presence of polar compounds. Sharp C–H stretching bands at 2928 cm$^{-1}$ (76.00%) and 1603 cm$^{-1}$ (62.67%), the latter of which is characteristic of aromatic C=C stretching, suggest that aromatic functionalities predominate. Other peaks at 1514 cm$^{-1}$ (77.59%) and 1404 cm$^{-1}$ (63.77%) are due to aromatic ring stretching and $CH_3$ bending, respectively, while the strong absorption at 1028 cm$^{-1}$ (35.69%) results from C–O stretching in alcohols and ethers. The reduced transmittance at these wavenumbers indicates higher absorbance, corresponding to a greater content of these functional groups in the hexane-extracted oil.

In contrast, the steam-distilled oil spectrum displays fewer but sharper peaks with prominent absorptions at 2928 cm$^{-1}$ (76.51%) and 2965 cm$^{-1}$ (84.59%) for the C–H stretching of alkanes, and at 1644 cm$^{-1}$ (84.17%) for alkenes' C=C stretching, indicative of prevalence of non-polar volatile components. Presence of peaks at 1436 cm$^{-1}$ (75.91%) and 1376 cm$^{-1}$ (84.95%) indicates presence of aliphatic hydrocarbons. C-O stretching bands at 1241 cm$^{-1}$ (96.08%) and 1147 cm$^{-1}$ (91.93%) indicate the presence of esters and ethers, which are commonly present in essential oils. Bands corresponding to 797 cm$^{-1}$ (76.87%) and 886 cm$^{-1}$ (49.41%) result from C–H out-of-plane bending in aromatics, and the band at 542 cm$^{-1}$ (88.54%) is likely a result of C–X stretching, an artifact. The generally higher transmittance values across most of the bands in the steam-distilled spectrum are reflective of a lower concentration of absorbing species, as one would be expected in the selective extraction of less polar and more volatile species. In general, the FTIR analysis indicates that hexane extraction leads to a broader range of functional groups comprising more polar and aromatic compounds and that steam distillation separates predominantly non-polar volatile constituents.

## 4.0 Discussion

The results of this study show clear variations in their chemical compositions, indicating the influence of the extraction method on the components of essential oils. The essential oil extracted with hexane is composed of alcohols or phenols, which is indicated by the presence of an O–H stretching band at 3272 cm$^{-1}$ (Mihrin *et al.*, 2020). Aromatic and alkene peaks at 1604 and 1515 cm$^{-1}$ indicate the existence of aromatic rings and unsaturated groups in complex crude oil mixes (Valderrama & Rojas De, 2017). In general, hexane-extracted oil has lower transmittance values (%T), which suggests a more complex combination with overlapping contaminants or functional groups (Asemani & Rabbani, 2020).

In contrast, the steam-distilled essential oil shows higher C–H stretching transmittance bands at 2928 and 2965 $cm^{-1}$, reflecting a higher concentration of aliphatic hydrocarbons, which are characteristic of more purified oils (de Smidt *et al.,* 2025). The presence of strong $CH_2/CH_3$ bending and C–O stretching bands in a compound is virtually certain evidence for the presence of aliphatic chains, ethers, and esters. Such compounds often get separated and concentrated from one another by steam distillation since they are volatile and can be separated from non-volatile compounds by steam distillation (Shin *et al*., 2015). The characteristic out-of-plane C–H bending vibrations of substituted aromatic rings, observed as peaks at 797 and 886 $cm^{-1}$, serve to identify specific aromatic or alkenic compounds such as limonene and α-pinene (Agatonovic-Kustrin *et al*., 2020). Steam-distilled oil's higher %T readings indicate fewer contaminants and a simpler chemical profile (Jacob *et al.,* 2024).

The results for steam-distilled essential oil show unique alkenic and aromatic characteristics that correspond closely to the molecular structure of limonene, the main monoterpene hydrocarbon found in lemon essential oils (Uwidia *et al.,* 2020). Limonene, with the molecular formula $C_{10}H_{16}$, is characterised by a cyclohexene ring with an isopropenyl substituent, giving rise to its typical unsaturated and aromatic functional groups observed in the FTIR spectrum (Obermeier & Strube, 2025). The steam-distilled oil's distinct aromatic peaks at 797 and 886 $cm^{-1}$ are corresponding with the structure of limonene and correspond to out-of-plane C–H bending vibrations of substituted cyclic alkenes (Boughendjioua, 2017). These peaks are indicative of the presence of specific substituted aromatic rings or alkenes, which are concentrated during steam distillation due to the selective volatility of limonene and related terpenes (Nandiyanto *et al.,* 2022).

## 5.0 Conclusion and Recommendations

This study compared the influence of steam distillation and solvent extraction with hexane on the chemical composition of essential oils extracted from lemon peels.The extracts were analysed and compared using FTIR spectroscopy.The results show that the extraction method selection has a major effect on the functional group composition and overall chemical complexity of the resulting oils. The essential oil extracted with hexane was rich in aromatic and non-polar compounds, indicated by the presence of O–H, aromatic C=C, and alkene peaks.Solvent extraction with hexane yields a more complex and less refined oil mixture because the method extracts a wider range of compounds, including some polar compounds. On the other hand, the steam distillation method appears to yield essential oil containing more aliphatic hydrocarbons, containing monoterpenes like limonene. The out-of-plane aromatic absorption peak and the C-H stretch of the essential oil spectrum also validate the presence of such aliphatic compounds. Increased transmittance content in FTIR spectra of steam-distilled oils indicates a purer, less complicated product with a lower impurity and a chemistry profile more in tune with industry and pharmaceutical applications.

These findings confirm that the suggested use of the lemon essential oil should direct the choice of oil extraction method. Because steam distillation gives oils of higher purity and better-defined chemistry, it is best utilised in those industries, including the food, pharmaceutical, and aromatherapy sectors, where purity and content of limonene are of paramount importance. Solvent extraction, in contrast, can be used more if the bioactive and aroma chemicals are needed from the extract, like in perfume products.To further optimise extraction parameters and investigate the bioactivity and sensory characteristics of the oils from both processes, additional work is proposed. In addition, use of the new method of analysis with the assistance of FTIR is likely to be able to provide quality in essential oil production and provide more information regarding trace constituents.

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### 8.0 Declaration of Conflicting Interests

The authors declare no conflict of interest.

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