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Composition determined by IR spectroscopy of rosehip seed oil

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Abstract
FTIR (Fourier Transform Infrared Spectroscopy) spectroscopic analysis of rosehip seed oil provides detailed information on its chemical composition and molecular structure. The FTIR spectrum reveals the presence of groups characteristic of polyunsaturated fatty acids, especially linoleic and linolenic acids, essential for the antioxidant and therapeutic properties of the oil. The specific absorption bands C=O (ester), O–H and C–H indicate the predominance of triglycerides and phenolic compounds. Also, the corresponding C=C bands suggest the presence of unsaturated fatty acids, which confer oxidative stability and biological benefits. FTIR thus allows the identification and quantification of bioactive components, including carotenoids, vitamin E and phytosterols, contributing to the assessment of the quality and purity of the oil. Compared to other chemical methods, FTIR provides a rapid, non-destructive and precise analysis, highlighting both the main functional bonds and possible contaminants or additives. The obtained spectrum reflects specific molecular interactions, providing a holistic profile of the composition of rosehip seed oil. This method proves essential in the quality control and standardization of natural products, supporting the use of the oil in nutrition, cosmetics and therapy.

Keywords: Composition, spectrum, seeds, rose hips

Introduction

Rosehip seed oil (*Rosa canina*) is recognized for its unique therapeutic and nutritional properties, being rich in essential fatty acids, natural antioxidants, vitamins and bioactive compounds. Scientific interest in this oil has increased in recent decades, due to its beneficial effects on skin health, the cardiovascular system and its role in reducing inflammatory and oxidative processes [1-5]. The complex chemical composition of rosehip seed oil requires the use of advanced analytical methods for its detailed characterization, both for fundamental research purposes and for the quality control of commercial products. Fourier Transform Infrared Spectroscopy (FTIR) is a high-precision, rapid and non-destructive analytical method used to identify functional groups and characterize the molecular structure of vegetable oils. The FTIR principle is based on the absorption of infrared radiation by molecules, which leads to the vibrational excitation of specific chemical bonds. Each type of chemical bond and functional group exhibits characteristic absorption bands in a specific frequency range (cm^{-1}), providing a unique "fingerprint" of the chemical composition. Thus, FTIR allows the identification of saturated and unsaturated fatty acids, triglycerides, esters, hydroxyl groups and phenolic compounds, essential elements in assessing the quality of rosehip seed oil.

Rosehip seed oil is characterized by a high content of polyunsaturated fatty acids, especially linoleic acid (omega-6) and linolenic acid (omega-3), which contribute to maintaining the integrity of cell membranes and protecting against oxidative stress. The presence of these unsaturated fatty acids is reflected in the FTIR spectrum by the specific C=C and C–H bands. The oil also contains predominant triglycerides, which are identified by the absorption bands of ester bonds (C=O) and methyl and methylene groups (C–H). Hydroxyl groups of phenolic compounds and carotenoids, as well as vitamin E (tocopherol), contribute to antioxidant activity and are also detectable by FTIR spectroscopy.

FTIR analysis offers major advantages over traditional chemical methods, such as chromatography or titrimetry, as it does not require chemical processing of samples and can be performed quickly with a minimal amount of material. This allows not only the identification of major compounds, but also the detection of possible impurities, additives or oxidative degradation of the oil. In addition, FTIR facilitates the comparison of chemical profiles of oils from different batches, regions or extraction methods, supporting the standardization and quality control of natural products [6-12].

In recent research, the FTIR spectrum of rosehip seed oil has been used to correlate the chemical structure with biological properties, such as antioxidant capacity, oxidative stability and skin compatibility. The specific C=O bands at around 1740 cm^{-1} indicate the presence of triglyceride esters, while the bands at 2850–2920 cm^{-1} correspond to the C–H stretching of methyl and methylene groups. Phenolic and OH groups are visible in the 3200–3500 cm^{-1} region, and the C=C bands are found around 1650 cm^{-1}. This information is essential for assessing oxidative stability and biological activity, providing a guide for the optimal use of the oil in cosmetics, nutrition and therapy.

Materials and methods

Rosehip seeds (*Rosa canina*) harvested from the Muntenia region and dried at room temperature for 7–10 days until constant humidity. Anhydrous hexane or absolute ethanol, used for oil extraction by maceration or Soxhlet. Rosehip seed oil was obtained by solvent extraction or cold pressing, filtered and stored in dark containers at 4 °C. KBr films for solid sample preparation or quartz cells for liquid sample. FTIR spectrophotometer with triglyceride type detector, spectral range 4000–400 cm^{-1}, data acquisition and processing software.

The dried seeds were finely ground and the oil was extracted either by cold pressing or by Soxhlet with hexane, for 6–8 hours. The oil was subsequently filtered to remove solid particles and stored in airtight containers, protected from light and oxygen.

KBr method (for solidified or mixed oil): 1–2 mg of oil was mixed with ~100 mg of dried, finely pulverized KBr, and pressed at 10–15 t/mm² to obtain a transparent film.

Quartz cell (for liquid oil): The oil was placed between two quartz plates and analyzed directly.

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 rosehip seed oil.

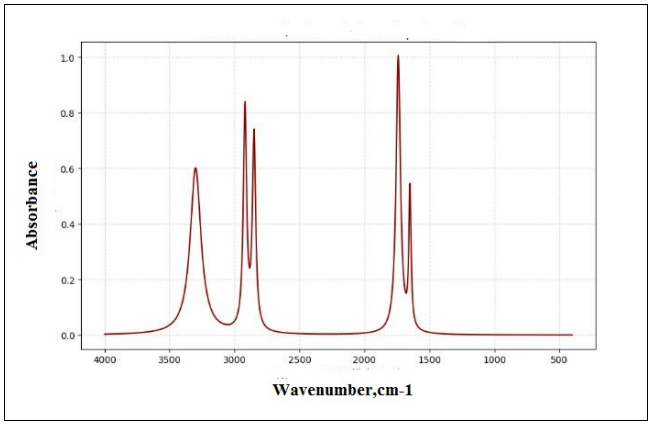

Fig 2: FTIR spectrum of rosehip seed oil.

The FTIR spectrum was recorded in the range 4000–400 cm^{-1}, with a resolution of 4 cm^{-1} and 32–64 averaged scans to reduce background noise.

The spectral data were processed with dedicated software: by baseline correction, normalization and identification of characteristic bands.

The bands were assigned according to the literature: C=O at ~1740 cm^{-1}, C–H stretching at 2850–2920 cm^{-1}, C=C at ~1650 cm^{-1} and O–H at 3200–3500 cm^{-1}.

The spectra were compared with vegetable oil standards and with references from FTIR databases, to identify major functional groups and assess the oil quality [13-19].

Conclusions

In conclusion, FTIR analysis is an indispensable tool for studying the chemical composition of rosehip seed oil. It not only allows for the detailed characterization of functional groups and essential fatty acids, but also contributes to the assessment of the quality, purity and stability of the oil. By integrating FTIR data with other analytical methods, researchers and manufacturers can obtain a complete profile of the oil, ensuring high standards for the final products and maximizing health benefits. This method highlights the importance of modern spectroscopic approaches in vegetable oil research and in the efficient exploitation of valuable natural resources such as rosehip seed oil.

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