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Study Chemistry of Medicinal Plants Using Laser and Infrared Spectroscopy

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Abstract

This research addresses the significant importance of medicinal herbs, highlighting their role as non-traditional crops. It explores the role of phytochemicals in various industries, including pharmaceuticals and food, as preservatives, flavorings, and more. Specifically, the research focuses on the use of ATR-FTIR and laser spectroscopy to analyze their active compounds, presenting a methodology with potential applications for ensuring the quality of medicinal plant products. In this study, three medicinal herbs (Calligonum comosum, Caper oleoresinus, and Purslane) were investigated using infrared and laser spectroscopy. The aim was to study these important species and determine their properties and composition. To achieve this, a semiconductor laser with a wavelength of 805 nm and a fast detector were used to measure the intensity and energy of the radiation. The spectral results showed clear intensity peaks in the 10,000–15,000 cm^{-1} range for the laser, and the infrared spectroscopy results showed strong absorption peaks indicating the active regions of the herbs. The importance of this research lies in the wide medical benefits of these herbs for improving the health of humans, as well as animals and other plants, as well as for preserving them and establishing reserves in their natural environment to benefit from scientific means, including lasers and spectral methods, in sustainable development.

Keywords: Medicinal herbs, FTIR spectroscopy, Laser, structure properties

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دراسة كيمياء النباتات الطبية بالليزر ومطيافية الاشعة تحت الحمراء

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خلاصة

يتناول هذا البحث الأهمية الكبيرة للأعشاب الطبيعية، مُسلّطًا الضوء على أهمية النباتات الطبية كمحاصيل غير تقليدية. ويستكشف دور المواد الكيميائية النباتية في مختلف الصناعات، بما في ذلك الصناعات الدوائية والغذائية، كمواد حافظة ومنكّهات وغيرها. ويركز البحث تحديدًا على استخدام مطيافية الأشعة تحت الحمراء بتحويل فورييه الكلي المخفف (ATR-FTIR) ومطيافية الليزر لتحليل مركباتها الفعالة، مقدمًا منهجية ذات تطبيقات محتملة لضمان جودة منتجات النباتات الطبية. في هذا البحث، دُرست ثلاثة أعشاب طبية طبيعية (الكلغان، والشفلح، والرجلة) باستخدام الأشعة تحت الحمراء والليزر. وكان الهدف من هذا البحث دراسة هذه الأنواع المهمة وتحديد خصائصها وتركيبها. ولتحقيق ذلك، استُخدم ليزر أشباه الموصلات بطول موجة 805 نانومتر، وكاشف سريع لقياس شدة وطاقة الأشعة. وأظهرت نتائج الأطياف قمم شدة واضحة لكل من نتائج الليزر في نطاق (10000-15000) سم$^{-1}$، وكذلك نتائج الأطياف تحت الحمراء، والتي أظهرت قمم امتصاص قوية تشير إلى المناطق النشطة للأعشاب. أهمية هذا البحث تكمن في الفوائد الطبية الواسعة لهذه الأعشاب لتحسين صحة الإنسان وكذلك الحيوانات والنباتات الأخرى، وكذلك للمحافظة عليها وإنشاء محميات في بيئتها الطبيعية للاستفادة من الوسائل العلمية منها الليزر والطرق الطيفية في التنمية المستدامة.

الكلمات المفتاحية: الأعشاب الطبية، مطيافية الأشعة تحت الحمراء، الليزر، خصائص البنية التركيبية

Introduction

Medicinal plants are considered non-traditional crops. Humans have used them throughout the ages as foods, medicines, and for a variety of purposes. Sometimes they were used as spices in cooking, to treat many human ailments, or to alleviate the symptoms of illness. Attenuated total reflection Fourier transform infrared (ATRI) spectroscopy was studied for the determination of croc in in commercial saffron samples. Calibration models were adopted based on the peaks in the 1700-900 cm^{-1} range, which were selected to determine the amount of croc in in the samples. Quantitative analysis of the samples was tested using ATRI using the reference UV–Vis spectroscopy method. [1-2]

Quality assurance (QA) is important in the field of pharmaceuticals to promote the standardization of products. In this study, the plant components of aqueous and methanolic extracts of the leaves of Portulaca oleracea L. and Portulaca quadrifida L. Fourier transform infrared chromatography showed the peaks of several functional groups (cm-1) of amines (-NH2), alcohols (-OH), carboxylic acids (-COOH), ketones (C=O), etc. The study represents a future platform for researchers that included drug and food safety assessments and weed management.[3]

Medicinal plant Portulaca oleracea L. and magnetite nanoparticles were used to develop a novel targeted transporter system to enhance the cytotoxic effect and overcome the limitations (permeability and localization) of plant components. Morpho-structural and magnetic properties of the new phytocarrier were investigated using a variety of methods, including XRD, FTIR, Raman, SEM, DLS), and magnetic determinations.[4] Three compounds have been identified as (3S)-5-hydroxy-3-(2-hydroxybenzyl)-7-methoxycroman-4-one, oleracone C (1), 5-hydroxy-3-(2-hydroxybenzyl)-7-methoxy-4H-croman-4-one, oleracone D (2), and 1-(2-hydroxy-

4,6-dimethoxyphenyl)-3-(2-hydroxyphenyl)propane-1-one, oleracone E (4), Their structures were elucidated using spectroscopic Various methods were used, including one-dimensional and two-dimensional nuclear magnetic resonance, high-resolution spray ionization mass spectrometry, and circular dichromatography. [5]

Adding herbal supplements to fish feed can be considered a growth promoter and immune system enhancer in preventing various fish infections. Therefore, this experiment was conducted to evaluate the effects of different levels of purslane (Portulaca oleracea) extract (POE) on growth performance., hematological indices and immune responses of rainbow trout fry.[6]

Silybum marianum (milk thistle) belongs to the Asteraceae family. Description of the Kalgan plant:2) meters, almost smooth, pale green. Stem simple, sparsely branched. - 1] Biennial plant, 1] (Asteraceae) Sheathed (containing grooves), with hairs giving it a cottony appearance.Up to this point, it contains toothed pockets, especially the thorn or leaf. [7]

Near-infrared (NIR) spectroscopy and a portable NIR spectrometer were used to detect Silybum marianum extracts. Eighty samples were collected. The silymarin content in all samples was determined using high-performance liquid chromatography. [8]

Iraqi lands are rich in medicinal plants, and its people have relied on herbs for treatment since ancient times. Among the most important of these is the milk thistle plant. It has a long history in Greek and Arabian medicine as a liver tonic which has been confirmed by scientific in vivo/ in vitro study and made the plant in the top of an effective drug for regenerating liver tissue and treating various liver diseases.[9] *Silybum marianum* is an annual herb with a wide range of therapeutic values due to its high nutritional content. The

compositional analysis of different parts of this plant, such as seeds and leaves, was performed using calibration-free laser-induced breakdown spectroscopy.[10]

This study highlights the efficacy of phospholipid-based phytosomes in enhancing the oral bioavailability of silymarin. The phytosomes were prepared using solvent evaporation and a complete optimization factor was employed. The final phytosome formulation was then developed for silymarin The improved plant-based silymarin formulation showed improved aqueous solubility (approximately 360 g/ml) compared to pure silymarin. [11]

Capparidaceae) found In Palestine, the chemical composition of plant parts was studied. This involved the chemical analysis of various extracts from the leaves, flowers, buds, fruits, and roots of the caper plant (Capparis spinosa L). [12]

Caper seeds are difficult to germinate, and while light is known to induce dormancy in some seeds, its effect on caper seed germination has not yet been thoroughly investigated. study analyzed the germination response of seeds to lighting with different wavelengths (white, red, blue, red + blue and darkness) and to A helium-neon laser beam was used, irradiating both dry and previously soaked caper seeds. [13]

The plant material was extracted using 85% methanol in a Soxhlet apparatus for 8 hours. fractionated it with ethyl acetate. Twenty adult male rats were used in this study Blood samples were collected via cardiac puncture to measure blood glucose, lipid profile, and renal function parameters. Blood cholesterol, triglyceride, and very low-density lipoprotein (VLDL) levels decreased significantly in all treated groups. High-density lipoprotein (HDL) levels increased significantly compared to the control group. Blood glucose levels decreased significantly in all treated groups compared to the control group. [14]

Kulgan or Camel Thistle

The milk thistle or or Mary's thistle (fig.1) is also called milk thistle, wild scale, ka'ib or in Iraqi "Aakul or Kulgan, which is considered a favorite camel meal. It is a plant species belonging to the genus of the artichoke family, Asteraceae. The leaves of this plant are large, leathery in texture, thick in size, with prominent veins, serrated, twisted edges, and strong, sharp thorns on their edges. The stem is erect, wingless, grooved, solid, grooved, and branched at the top. The leaves are alternate, lobed, and have thorny margins. The flowers are tubular, red, purple, and white. The fruit is poor, with hairs at the top that aid dispersal by the wind. It can be eaten after removing the thorns and leaves. It grows widely in the plains and mountains of Palestine and northern Jordan, [15-16]

Figure (1) Kulgan or Camel Thistle plant

Caper (Caparis spinose)

Caper is a desert plant (fig.2) that grows in mountainous regions and clings to the sides of valleys and high places. It is not a herb, but rather a thorny tree that spreads out in a circular shape on the ground. Caper is a deciduous plant that grows in the winter and grows in the Mediterranean environment, some parts of Asia, and South Africa. It is a staple ingredient in Mediterranean

cuisine. Capers are popular in Italy and add a delightful touch to popular Italian dishes. They are primarily used as a spice or garnish. Capers are sun-dried and used in pickles for their delicious flavor. Larger capers are known to have the strongest flavor, but if you want to enjoy the distinctive aroma of capers, smaller capers are best.

Capris spinosa is an herb with a long history of human use, both as a medicine and as a food. Mediterranean region and East Asia. The edible portion is the green leaves, which are characterized by their pungent taste. [17]

They are evergreen, and this is the portion suitable for human consumption. The fruits range in length from 2.5 to 5 cm and are dark green. When they ripen, the red flesh reveals a large number of seeds.[18]

Figure (2) Caper (Caparis spinose) plants

Purslane

Cress, literally or purslane or foolish purslane or purslane (scientific name: Portulaca oleracea) (fig.3) is an annual succulent plant belonging to the genus Purslane of the Purslane family. In Libya, it is called "Baqla" (baqla), and in some regions, including Tripoli, it is called "Blibasha." What is mentioned in one edition of the book "Al-Jami' li-Mufradat al-Adwiyah wa-l-Aghdhiyyah" by Ibn al-Baytar al-Maliki, that its name is also al-'Arfaj and al-'Arfajin, is a misprint (i.e., a distortion during the copying of

manuscripts) for the words "Farfah" and "Farfahin,"[19-20]

Figure (3) Purslane plants

Materials and Method

In this research, three Iraqi natural herbs (Kalgan, Shaflah, and Purslane) were selected for study using infrared spectroscopy and laser.

1-Testing and Measurement System

In this stage, a test experiment (figure 4) was built to measure the intensity and energy of the laser beam using the following devices:

•A low-power semiconductor laser with a wavelength of (805 nm)

•A fast, sensitive spectrometer with a sensitivity of (1 nm) (Ocean Optics)

• single-mode optical fiber

•computer with detector software

•Various holders and holders

•optical table

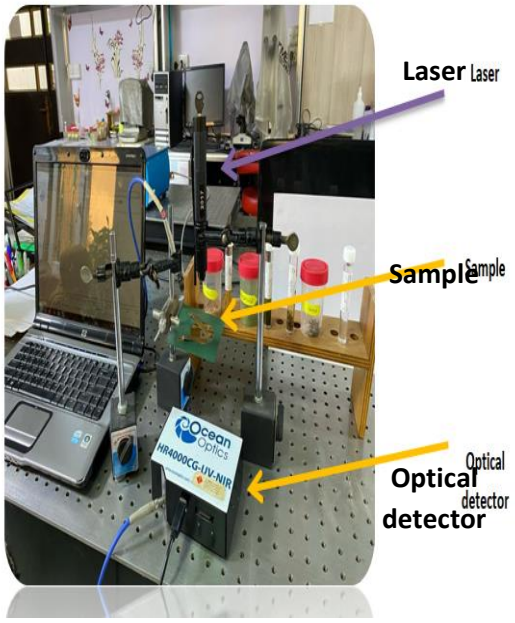

Figure (4) Testing and Measurement System

2- Infrared Spectrometer

This spectrometer was used to measure the vibrational spectra of the interaction of infrared radiation and the material to determine the energies of the active regions of each plant, as shown in Figure (5). The spectrometer specifications are

attached in Table (1). Special Opus spectrometer software was also used.

Table (1) Specifications for the Infrared Spectrometer

Properties	Values	Components
Spectral range	375 – 7,500 cm-1	IR laser sources
KBr beam splitter	500 – 6,000 cm-1	Detectors
measurement time	1 min,	Fourier transform
spectral resolution	4 cm-1	

Figure (5) ATR-FTIR spectrometer (BRUKER ALPHA)

3- Samples of plants

Three Iraqi natural herbs (Kalgan, Shaflah, and Purslane) were selected in their liquid and solid forms and placed in special laboratory containers, as shown in Figure (6).

Figure (6) Different sample models

Results and Discussion:

The search results are arranged and include the following steps:

1-Plant Materials

Three types of Iraqi medicinal plants were collected from different areas in Baghdad:

1- Kalgan (Alpinia galangal): The leaves of the Kalgan plant were collected.

2-Shaflah (Capparis spinosa): The fruits of the Shaflah plant were collected.

3-Purslane (Portulaca oleracea): The leaves of the Purslane plant were collected.

2-Plant Sample Preparation

•The plant samples were cleaned immediately after collection to remove dust and impurities.

•The samples were washed with distilled water to remove any remaining contaminants.

•The samples were divided into two parts:

o The first part: was shade-dried at room temperature for two weeks, then ground into a fine powder using an electric grinder.

o The second part: was used fresh without drying.

3-Sample Preparation for Spectroscopic Analysis

•The dry powder samples were prepared for infrared spectroscopy by placing them directly on an infrared spectrometer.

•For fresh samples, a small amount of the plant parts was placed directly on the spectrometer. For laser analysis, samples were prepared in the same manner as those for infrared spectroscopy.

4- (FTIR) Spectroscopy

•An FTIR spectrometer was used to analyze the plant samples.

•Infrared spectra were recorded for the samples in the wavenumber range of 400 to 4000 cm-1.

•The resulting spectra were analyzed to identify the functional groups present in the plant samples.

5- Laser Analysis

•A laser analyzer was used to analyze the plant samples.

•The laser spectra of the samples were recorded.

•The resulting spectra were analyzed to identify the chemical compounds present in the plant samples.

6-Data Analysis

•Specialized software was used to analyze the spectral data resulting from the two analyses.

•The resulting spectra for the different samples were compared to

identify differences in chemical composition.

•The results of the two analyses were compared with each other.

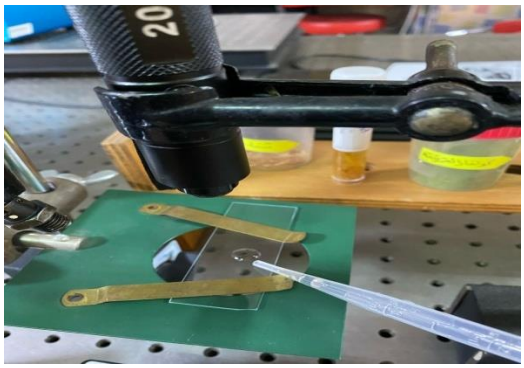

Figure (7) herbs sample on slide

The results were prepared and divided according to experiments as follows:

Experiment 1: In this experiment, the intensity and energy of the laser light directed at low power on samples of herbal extracts (Kalgan, Shaflah, and Purslane) with pure water were measured as follows:

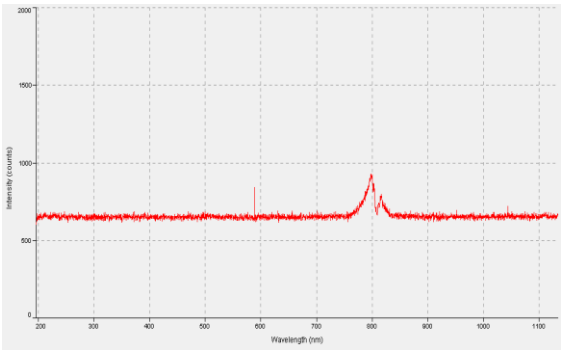

Figure (8)Laser intensity spectrum of purslane extract

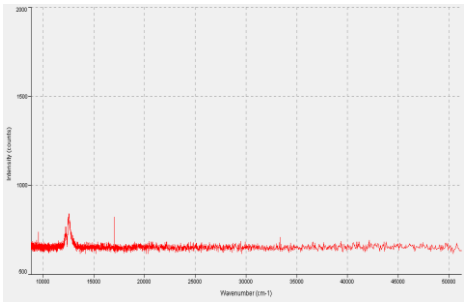

Figure (9) Laser intensity & wavenumber spectrum of purslane extract

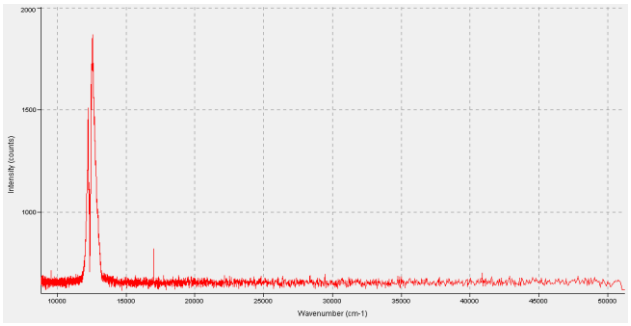

Figure (10)Laser intensity& wavenumber spectrum of Kalgan plant extract

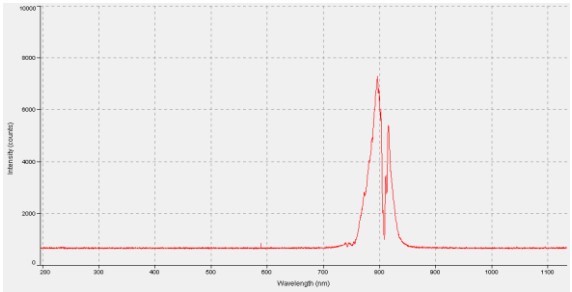

Figure (11)Laser intensity spectrum of Kalgan plant extract

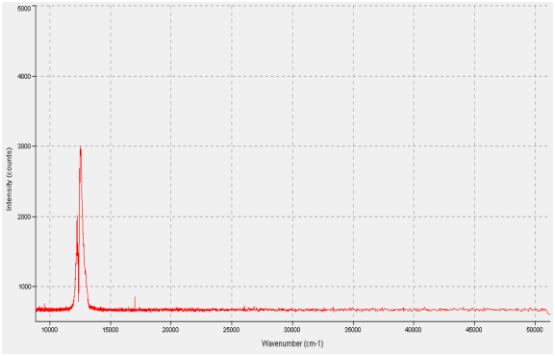

Figure (12)Laser intensity& wavenumber spectrum of the plant Shaflah plant extract

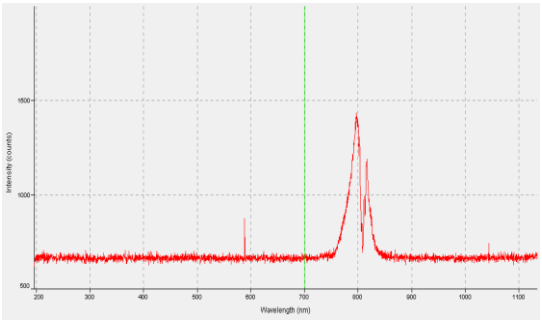

Figure (12)Laser intensity spectrum of the Shaflah plant extract

Experiment 2: In this experiment, the intensity and energy of the laser light directed at low power on samples of dry herbal (Kalgan, Shaflah, and Purslane) with pure water were measured as follows:

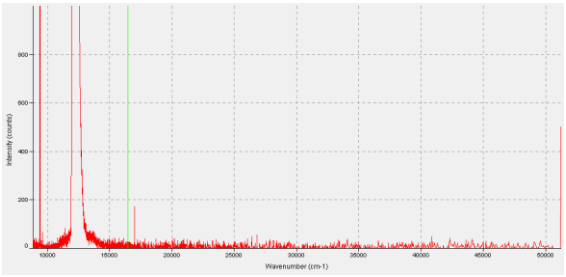

Figure (13) Laser intensity& wavenumber spectrum of Shaflah dry plant

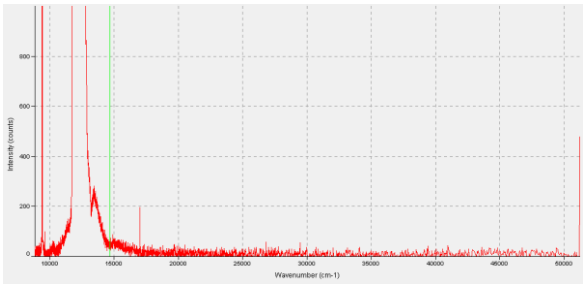

Figure (14) Laser intensity& wavenumber spectrum of purslane dry plant

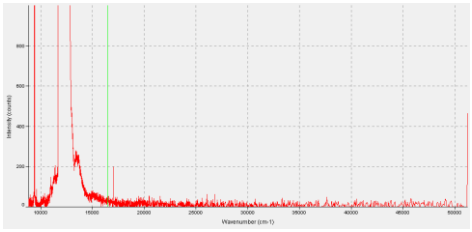

Figure (15) Laser intensity& wavenumber spectrum of Kalgan dry plant

Results and Discussion

The results of the study on three Iraqi medicinal herbs (purslane, caper, and saffron) are presented and discussed within the context of the known phytochemical composition of these species to strengthen the correlation between the theoretical background and the spectral results.

1. Near-Infrared (NIR) Laser Spectroscopy (Experiment 1 & 2)

The laser spectra of extracts and dry liquids of the three herbs (purslane, caper, and saffron) recorded using an 805 nm laser (≈12422 cm−1) showed distinct intensity peaks in the 10,000 to 15,000 cm−1 wavenumber range.

• Spectrochemical Interpretation: The strong absorption in this range, which falls within the near-infrared (NIR) spectroscopy region, indicates overtones and combinations of light-bonding vibrations, particularly the O-H and C-H groups. Identifying these interactions is a strong indicator of the presence of active phytochemicals in herbs:

• O-H vibration indicates the presence of phenolic compounds and flavonoids (present in all three species).

• C-H vibration indicates the presence of fatty acids (especially in purslane, known for its high omega-3 content) and terpenoids.

• Correlation and Discussion: The marked variation in peak intensity between extracts (Figures 9, 10, 12) and dried herbs (Figures 13, 14, 15) is attributed to differences in the relative concentration of these active compounds and water content among the plant species. These results are consistent with previous studies that used NIR spectroscopy for the non-destructive detection of chemical content in plants.

Experiment 3: In this experiment by using infrared radiation for dried herbs (figures 16,17,18) and their extracts (fig. 19), vibrational spectra were measured in the region (400-4000) cm^{-1}.

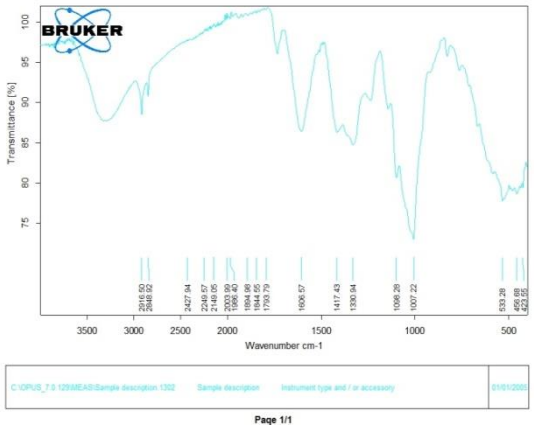

Figure (16) Infrared spectra of dried Kalgan leaves

• Based on the shape of the spectra, functional groups such as:

o Hydroxyl groups (OH) (possibly appearing in the 3300 cm-1 region).

o Carbonyl bonds (C=O) (possibly appearing in the 1700 cm-1 region).

o Carbon-hydrogen bonds (C-H) (possibly appearing in the 2900 cm-1 region).

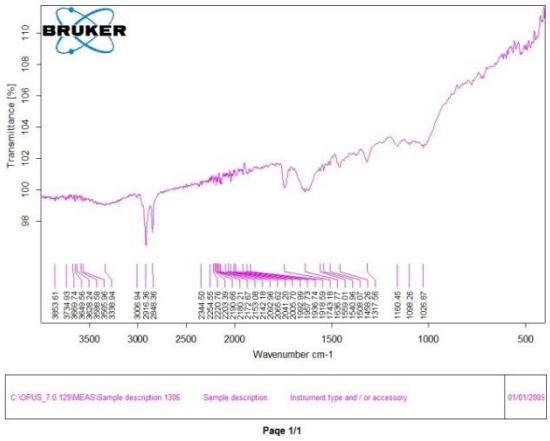

figure (17) Infrared spectra of dried purslane leaves

The spectra of dry purslane are expected to contain peaks and valleys indicating functional groups are:

• Hydroxyl groups (OH) (possibly occurring in the 3300 cm-1 region).

• Carbonyl bonds (C=O) (possibly occurring in the 1700 cm-1 region).

• Carbon-hydrogen bonds (C-H) (possibly occurring in the 2900 cm-1 region).

• Carbon-oxygen bonds (C-O) (possibly occurring in the 1000-1300 cm-1 region).

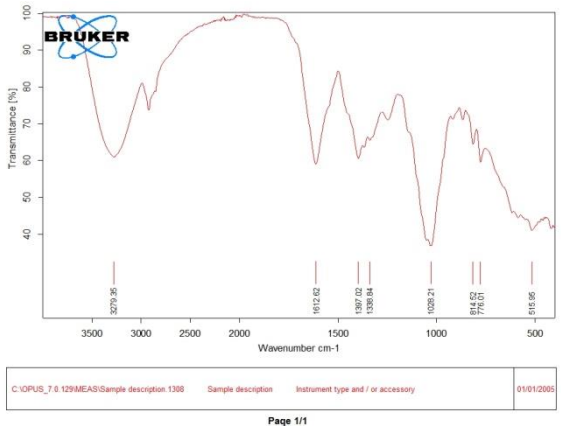

Figure (18) Infrared spectra of Shaflah dry plant

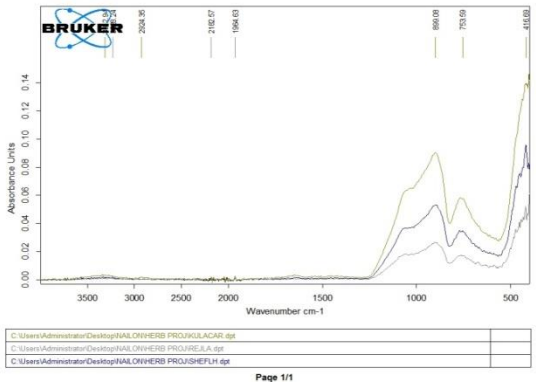

Figure (19) Infrared spectra of the three herbal extracts

2. ATR-FTIR Spectroscopy Analysis (Experiment 3)

ATR-FTIR spectroscopy, performed on dry and extracted samples in the 400–4000 cm−1 region, confirmed the presence of strong absorption peaks. These peaks were interpreted

to determine the chemical signature of each herb.

• Precise identification of functional groups:

• Peak at ~3300 cm−1 (Figure 18): The broad bands in this region are attributed to the stretching vibration of the hydroxyl group (O–H), confirming the presence of alcohols, phenolic acids, and flavonoids.

• Peak at 2924.35 cm−1 (Figure 19): This distinct peak indicates the asymmetric stretching vibration of aliphatic C–H bonds, confirming the presence of fatty acids and terpenoids, particularly in purslane. • Secondary peaks (~1700 cm−1): The expected presence of weak absorption in this region indicates the stretching vibration of the carbonyl group (C=O), an integral part of the structures of flavonoids and carboxylic acids.

• Footprint range (1000–1300 cm−1): Strong absorption in this range is associated with C-O vibrations, an indicator of the presence of sugars and phenolic acids.

• Comparison with databases: These interpretations of functional groups were confirmed by comparing the wavenumbers with standard spectral databases such as NIST and SDBS. The slight differences in the fingerprint shape between herbs (Figure 19) indicate variation in overall chemical composition, which explains the differences in their content of active compounds.

3. Chemical Discussion and Research Background

The spectral results from FTIR and laser methods confirm the phytochemical diversity of herbs.

• Confirmation of Results: The identification of the O-H and C=O groups by FTIR is consistent with previous studies that used FTIR to analyze purslane (Portulaca oleracea L.) extracts and demonstrated the presence of flavonoids. This methodology links rapid analytical tools to the intrinsic chemical

composition of plants, thus achieving the research objective.

• This study provides evidence for the effectiveness of ATR-FTIR spectroscopy and lasers as rapid, non-destructive analytical tools for quality assurance (QA) and botanical identification of medicinal herbal products. The ability to detect the spectral signatures of active compounds so quickly enhances the use of this technique as a primary screening tool in the pharmaceutical and food industries.

Conclusions

• In this research, laser (NIR) spectroscopy and ATR-FTIR spectroscopy were successfully used as rapid tools for detecting the spectral signatures of the active constituents in Iraqi medicinal herbs.

• ATR-FTIR analysis accurately identified the major functional groups (O-H, C-H, C=O), confirming the presence of flavonoids, fatty acids, and phenolic compounds. This analysis was performed by comparing the wavenumbers with standard spectral databases (NIST and SDBS).

• Differences in spectral peak intensity among the herbs indicate variations in the relative concentrations of the active chemical compounds, suggesting differences in their chemical composition.

• This study demonstrates the efficiency of FTIR and laser spectroscopy as non-destructive analytical methods that can be effectively used in quality control and chemical classification of medicinal plants.

• Other chemical analyses, such as high-performance liquid chromatography (HPLC) or mass spectrometry (MS), can be performed to confirm the results of the spectroscopic approach.

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