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GC-MS Analysis of Phytochemical Compounds Present in the Leaf Extracts of Plant *Maytenus emarginata*

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Abstract

The evergreen tree *Maytenus emarginata* also referred to as the thorny staff tree, can withstand a variety of desert stressors. This work serves as a foundation for identifying the active ingredients in leaves and further isolating the chemical because their therapeutic potential has not yet been investigated. The purpose of this study is to screen for phytochemicals in *Maytenus emarginata* leaves and use GC-MS analysis to further analyze the components found in the leaves. Based on their polarity—petroleum ether, distilled water, and methanol—the leaves were extracted one after the other. The methanol extracts, petroleum ether, and distilled water all contained the phyto-constituents that were investigated. Different chemicals were found in the petroleum ether and methanol extract according to the GC-MS analysis. The biological activity and significance of the chemicals found are based on GC-MS analysis.

Keywords: *Maytenus emarginata* , Phytochemical screening, Petroleum Ether, Distilled Water, Methanol, GC-MS analysis.

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Introduction

Maytenus emarginata (Wild) is a member of the Celastraceae family. Known locally as "Kankero," "Baikal" in Hindi, and "Thorny staff tree" in English, this evergreen shrub can withstand any kind of desert hardship. India is known as the botanical garden of the globe and is the world's greatest producer of herbal medicine (Ahmedull, 1999). A vast array of organic substances known as secondary metabolites, which are typically complex and distinctive structures, can be biosynthesised by plants. Numerous secondary metabolites have been discovered to have intriguing medicinal properties and to be used in products such as pesticides, medicines, dyes, colors, sweeteners, tastes, and scents. Numerous chemical components found in plants used in traditional medicine can be used to treat infectious, chronic, and acute illnesses (Duraipandiyan, 2006). Natural antioxidants like as flavonoids, tannins, and other phenolic compounds are plentiful in phytochemicals. Other bioactive substances with beneficial health effects include steroids, alkaloids, volatile oils, tri-terpenoids, and alkaloids. The study of phytochemicals—naturally occurring molecules with potential disease-prevention properties—involves identifying chemically active compounds and evaluating antioxidant activity in plant secondary metabolites (Akinmoladun, 2007).

Plants have helped researchers find and create new medications that can be used to treat a variety of illnesses. Pharmaceuticals derived from plants are readily accessible, less costly, safe, effective, and less likely to cause adverse effects (Yadav, 2011). To standardize herbal treatments and their formulations, several modern approaches can be used to identify, characterize, and quantify active chemical components in plant material. It is common practice to use gas chromatography in conjunction with mass spectrometry to analyze the active components in traditional medicines, herbal treatments, and medicinal plants. More and more hyphenated tools, like GC-MS studies, are being used to analyze the active components in medicinal plants. This is because this technique has been useful for analyzing volatile essential oils, lipids, alkaloids, fatty acids, and non-polar components (Mythili, 2013). The preservation of the healthcare system relies heavily on herbal plant medicine, which has been practiced for generations. Many different types of medicinal therapies, including those that fight inflammation, germs, fungi, and viruses, are based on Akin-Osanaiye (2011) notes that there has a long history of using active components extracted from medicinal plants. More than three quarters of the global population relies on plants that are part of traditional medicine for their main health care. When it comes to people's health, these traditional medicines made from plants play a significant role all around the globe. According to Rasika (2011), there are several main types of plant-based products. These include cosmetics, herbal remedies, natural health aids, personal care items, and phytopharmaceuticals. These days, GC-MS research is used to examine medicinal plants since it is a useful tool for analyzing volatile oils, fatty acids, lipids, alkaloids, and non-polar components as well as polar, semi-polar, and non-polar components. For a long time, people all over the globe have turned to *Maytenus* plants for relief from a variety of gastrointestinal problems, rheumatism, inflammation, fever, ulcers, and asthama.

Children are fed powdered *Maytenus emarginata* leaves together with milk as an anthelmentic. The leaves' decoction is used as a mouthwash to treat toothaches. Heal wounds are treated with the leaves (Pullaiah, 2006). To treat hepatitis and liver inflammation, the delicate leaves are chewed uncooked. *Maytenus emarginata* shows significant anti-tumor properties that support to use in the treatment of cancer (Sagwan, 2011).

Materials and Methods

Plant Collection- We collected fresh leaves of *Maytenus emarginata* from the region of Ajmer, Rajasthan, India. The plant was identified and confirmed by the University of Rajasthan herbarium library and given voucher specimen number. A grinding machine was used to grind the plant's leaves into a powder after they had been sun-dried.

Preparation of Plant Extract- The dried and powdered plant material was divided into three portions each designated for extraction with one of the selected solvents: water, methanol, and petroleum ether. The use of different solvents allows for the selective extraction of compounds based on their polarity.

GC-MS (Gas Chromatography-Mass Spectrometry) **Analysis**- A potent analytical method for identifying and measuring volatile and semi-volatile substances in complicated mixtures, such plant extracts, is GC-MS. GC-MS analysis was used in this investigation to clarify the chemical makeup of the *Maytenus emarginata* plant extracts. The sophisticated Instrumentation Research institution (AIRF), a state-of-the-art institution renowned for its state-of-the-art instrumentation and proficiency in sophisticated analytical techniques, was the site of the analysis.

Sample Preparation: The plant extracts, which were previously obtained using solvents of varying polarities (water, methanol, and petroleum ether), were carefully prepared for GC-MS analysis. A small aliquot of each extract was taken, and further purification was performed if necessary to remove any non-volatile impurities that could interfere with the analysis. The samples were then concentrated under reduced pressure using a rotary evaporator to ensure that the volatile components were adequately concentrated. The final extracts were dissolved in an appropriate solvent (usually hexane or methanol) to make them compatible with the GC-MS system.

Instrumentation and Conditions: The GC-MS analysis was performed using a high- resolution GC-MS system available at AIRF. The system is equipped with a capillary column, which provides excellent separation of complex mixtures, and a mass spectrometer, which allows for precise identification of the separated compounds based on their mass-to-charge ratio (m/z).

•**Gas Chromatography**: The GC component of the system was operated with a capillary column, typically a fused silica column coated with a non-polar stationary phase. The column was selected based on its ability to effectively separate the range of compounds expected in the plant extracts.

The temperature program was optimized to gradually increase the oven temperature, facilitating the elution of compounds based on their volatility. Helium was used as the carrier gas, ensuring efficient and consistent transport of the sample through the column.

•**Mass Spectrometry:** The mass spectrometer was operated in electron ionization (EI) mode, a standard technique that ionizes the compounds as they elute from the GC column, breaking them into characteristic fragments. The mass spectrometer scanned the ionized fragments over a range of m/z values, typically from 50 to 600 m/z, allowing for the detection and identification of a wide variety of compounds.

Data Acquisition and Analysis: As the compounds in the plant extracts eluted from the GC column, they were detected by the mass spectrometer, which generated a chromatogram—a graphical representation of the compounds based on their retention times and intensity. Each peak in the chromatogram corresponds to a different compound in the extract.

•**Identification of Compounds**: The mass spectra obtained for each peak were compared against reference spectra in established mass spectral libraries, such as the National Institute of Standards and Technology (NIST) library, to identify the compounds present. The matching process involved comparing the fragmentation pattern of each compound in the sample with those in the library, allowing for precise identification.

•**Quantification**: The relative abundance of each identified compound was determined by integrating the area under the corresponding peak in the chromatogram. While GC- MS provides qualitative identification, it can also be used semi-quantitatively to estimate the concentration of compounds based on the peak areas.

Fourier Transform Infrared (FTIR) Spectroscopy- An effective analytical method for determining the functional groups and bonding structures found in both organic and inorganic materials is Fourier Transform Infrared (FTIR) spectroscopy. Through the detection of certain vibrations of chemical bonds inside the molecules, FTIR offers vital information on the molecular makeup of plant extracts. The functional groups and general molecular structure of the bioactive chemicals found in the dried extracts of *Maytenus emarginata* were described in this study using this technique.

Sample Preparation: The dried plant extracts were carefully prepared for **FTIR analysis.** A small amount of the dried extract (about 2-5 mg) was mixed with potassium bromide (KBr) powder in a ratio of approximately 1:100. The mixture was finely ground to ensure homogeneity, and then pressed into a thin, transparent pellet using a hydraulic press. This KBr pellet preparation method is standard in FTIR analysis as it provides an optically clear medium that does not interfere with the infrared light passing through it.

Instrumentation and Analysis: The FTIR analysis was conducted using an advanced FTIR spectrometer, which operates by passing a beam of infrared light through the sample. The spectrometer detects the frequencies at which the sample absorbs the infrared light, corresponding to the vibrational energies of the chemical bonds within the molecules.

•**Infrared Spectra Collection:** The FTIR spectrometer was set to scan the sample across a broad range of wavenumbers, typically from 4000 cm^-1 to 400 cm^-1. This range covers the most common vibrational modes of organic molecules, including stretching and bending vibrations of bonds like O-H, N-H, C-H, C=O, C=C, and others.

•**Data Acquisition:** As the infrared light interacts with the sample, it is absorbed at specific wavenumbers corresponding to the vibrational frequencies of the bonds in the molecules. The FTIR spectrometer collects this data and generates an infrared absorption spectrum, which is a plot of absorbance (or transmittance) versus wavenumber.

Interpretation of FTIR Spectra: The FTIR spectra obtained from the plant extracts were analyzed to identify the characteristic peaks corresponding to various functional groups. Each peak in the spectrum represents a specific vibrational mode of a chemical bond within the molecules present in the extract.

•**Identification of Functional Groups:** The position (wavenumber) and intensity of the peaks were compared against known reference data to identify the functional groups present in the extracts. For example:

O-H Stretching: A broad peak around 3200-3600 cm^-1 indicates the presence of hydroxyl groups (O-H), commonly found in alcohols, phenols, and carboxylic acids.

C=O Stretching: A strong peak around 1700 cm^-1 is characteristic of carbonyl groups (C=O), which are present in aldehydes, ketones, carboxylic acids, and esters.

C-H Stretching: Peaks around 2800-3000 cm^-1 correspond to C-H stretching vibrations, indicative of alkyl groups.

N-H Bending: Peaks around 1500-1600 cm^-1 suggest the presence of amine groups (N-H).

C-O Stretching: Peaks around 1000-1300 cm^-1 can indicate the presence of ethers, esters, or alcohols.

Bonding Structures:

The general pattern of peaks, including their width and shape, gives details on the environment and molecular structure of the functional groups. For example, a large O-H peak, which is common in phenolic compounds, indicates hydrogen bonding.

GC-MS and FTIR ANALYSIS

To further characterize the chemical composition of the extracts, Gas Chromatography-Mass Spectrometry (GC-MS) and Fourier Transform Infrared (FTIR) spectroscopy analyses were conducted. These techniques provide a more in-depth understanding of the molecular structure and composition of the bioactive compounds present in the methanolic extracts of *Maytenus emarginata* .

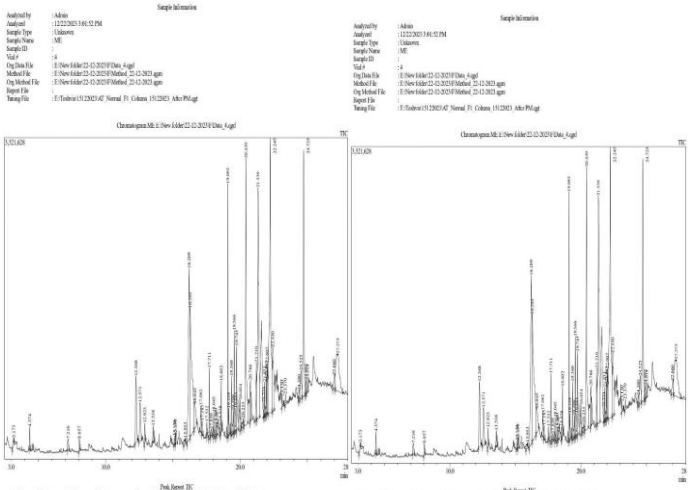
GC-MS analysis is particularly valuable for identifying and quantifying volatile and semi- volatile compounds within the extracts. The chromatograms obtained from the GC-MS analysis revealed the presence of various bioactive constituents, including flavonoids, phenolic acids, alkaloids, and phytosterols. Each peak in the chromatogram corresponds to a different compound, and the mass spectrum provides information on the molecular weight and structure of these compounds. This analysis is crucial for identifying specific compounds that might be responsible for the observed bioactivities, such as antioxidant and anticancer effects.

FTIR spectroscopy was employed to identify the characteristic functional groups present in the extracts. The FTIR spectra provided a molecular fingerprint of the extracts, revealing the presence of hydroxyl groups (–OH), carbonyl groups (C=O), and aromatic rings, which are indicative of phenolic compounds, flavonoids, and other polyphenols. The identification of these functional groups corroborates the results of the qualitative and quantitative analyses, confirming the presence of these bioactive compounds in the extracts. Together, the GC-MS and FTIR analyses provide a comprehensive understanding of the chemical composition of *Maytenus emarginata* , laying the groundwork for further bioactivity studies.

These sections provide a thorough examination of the extraction process, the qualitative and quantitative analysis of bioactive compounds, and the advanced chemical characterization of the plant extracts, offering a solid foundation for understanding their potential therapeutic benefits. Each step is crucial in building a complete profile of these medicinal plants, from basic extraction and identification to in-depth chemical analysis, ultimately supporting their traditional use and potential for modern therapeutic applications.

Results and Discussion

GC-MS of *Maytenus emarginata*

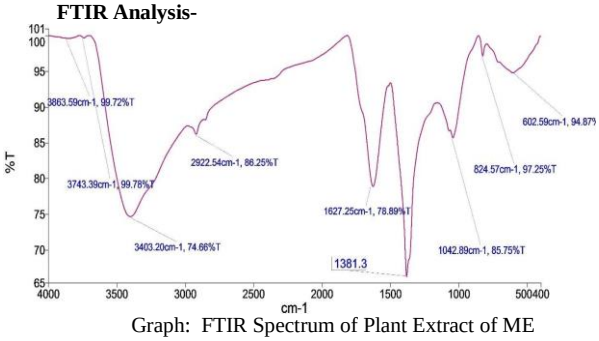


* List of Compound name found after analysis of GC in *Maytenus emarginata* plant Extract-

1. Acetic acid
2. Glycerin
3. Furfural
4. Undecane
5. 5-Undecanone
6. 2-(4-Chlorophenyl)-1,3,2-dioxaborolane
7. Chlordimeform
8. Phenol, 2,6-dimethoxy-

9. n-Tridecan-1-ol
10. 2,4-Di-tert-butylphenol
11. 1H-Inden-1-one, 2,3-dihydro-3,3,5,6-tetramethyl-
12. 1-Decanol, 2-hexyl-
13. Heptadecane
14. 6,6-Diethylhexadecane
15. 3-Chlorocatechol, cyclic phenylboronate
16. 8-Pentadecanone
17. Triacontane, 1-iodo-
18. Pentadecanal-
19. 2-Isopropyl-5-methyl-1-heptanol
20. Dotriacontane
21. 1-Decanol, 2-hexyl-
22. Tetrapentacontane
23. 3,7,11,15-Tetramethylhexadec-2-ene
24. 1-Nonadecene
25. Neophytadiene
26. 3,7,11,15-Tetramethylhexadec-2-ene
27. 8-Octadecanone
28. Neophytadiene
29. 9,17-Octadecadienal, (Z)-
30. 9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
31. Hexadecanoic acid, methyl ester
32. Carbonic acid, octadecyl vinyl ester
33. n-Hexadecanoic acid
34. Eicosyl heptafluorobutyrate
35. Supraene
36. Squalene
37. 9,12-Octadecadienoic acid (Z,Z)-, methyl ester
38. 9,12,15-Octadecatrienoic acid, methyl ester, (Z,
39. 1,2-Octadecanediol
40. Phytol
41. 9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
42. Octadecanoic acid
43. Tetrapentacontane, 1,54-dibromo-
44. 1-Decanol, 2-hexyl-
45. Tetrapentacontane
46. 1,6,10,14,18,22-Tetracosahexaen-3-ol, 2,6,10,15
47. Oxirane, 2,2-dimethyl-3-(3,7,12,16,20-pentame
48. Heptacosyl heptafluorobutyrate
49. threo-7,8-Bromochlorodisparlure
50. erythro-7,8-Bromochlorodisparlure

FTIR Analysis-



Graph: FTIR Spectrum of Plant Extract of ME

The FTIR spectrum of Plant Extract, identified as *Maytenus emarginata* (ME), reveals a complex mixture of functional groups, indicative of the diverse phytochemical composition of the extract. The broad absorption band of indicate that ME may have significant antioxidant properties due to the presence of phenolic compounds. The spectrum also shows a distinct peak near 2920 cm^{-1}, corresponding to C-H stretching vibrations, indicative of aliphatic compounds. The sharp peak around 1700 cm^{-1} is particularly noteworthy, as it represents carbonyl (C=O) stretching, suggesting the presence of ketones, aldehydes, or acids, which are often associated with bioactive properties. Additionally, the presence of peaks in the range of 1600-1500 cm^{-1} indicates aromatic C=C stretching, which is typical of flavonoids and other polyphenolic compounds. The FTIR spectrum of ME highlights the complex nature of this plant extract, showcasing the presence of multiple functional groups that could contribute to its medicinal properties, particularly in the context of antioxidant and anticancer activities.

Conclusion

The connection between phytochemical compounds and their biological effects is the main focus of creative thought these days. For many years, the plant *Maytenus emarginata* has been used to treat a wide range of conditions, such as fever, asthama, ulcers, rheumatism, toothaches, digestive problems, cooling effects, and blood purification. The chromatographic study of the plant's methanolic extract, petroleum ether, and chloroform, however, is currently lacking in publications. The existence of a few noteworthy chemicals found in the plant Maytenus *emarginata* using GC-MS analysis is presented below. Plant extracts subjected to GC-MS analysis may provide insight into the types of active ingredients found in medicinal plants. It is believed that these phytoconstituents are what cause the plant Maytenus ematginata to exhibit its traditional action.

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