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## GC-MS Profiling Of Petroleum Ether Root Extracts Of *Psidium guajava*.

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### ABSTRACT

*Psidium guajava* L. (Myrtaceae), referred to as guava, is extensively utilized in traditional medicine for gastrointestinal, metabolic, and inflammatory ailments. Although leaves and fruits have been thoroughly investigated, the roots are relatively underexamined. The objective of this work was to analyze the volatile and semi-volatile phytochemical components of the petroleum ether root extract of *P. guajava* utilizing Gas Chromatography–Mass Spectrometry. The dried and powdered roots of *P. guajava* were extracted using petroleum ether using a Soxhlet system. The concentrated extract underwent analysis via GC–MS, with chemicals identified according to retention time, mass spectrum fragmentation, and comparability with the NIST library. GC–MS analysis identified fifteen predominant chemicals accounting for 100% of the overall chromatogram area. The primary components comprised octacosane, 2-methyl- (17.91%), tetrapentacontane (17.20%), 2-methylheptacosane (16.28%), nonacosane (14.60%), tetracontane (11.33%), hexatriacontane (7.04%), and bis(2-ethylhexyl) phthalate (5.39%). The identified chemicals included long-chain hydrocarbons, fatty acids, and sterol derivatives, indicating a highly lipophilic chemical profile. The existence of these bioactive chemicals indicates possible antioxidant, anti-inflammatory, antibacterial, and cytoprotective properties of guava roots. This study presents the inaugural GC–MS dataset of petroleum ether root extract from *P. guajava*, enhancing pharmacognostic understanding and prospective nutraceutical applications of its root system.

**Keywords:** *Psidium guajava* L., Gas Chromatography–Mass Spectrometry, petroleum ether root extract

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## INTRODUCTION

*Psidium guajava* L. (Myrtaceae), known as guava, is a medicinal plant with extensive distribution and a longstanding history of application in traditional medicine [1]. Although the leaves and fruits are extensively documented for its antibacterial, antidiarrheal, anti-inflammatory, and antioxidant qualities [2,3,4], there is a relative paucity of scientific research on the roots, despite their significant importance in local ethnomedicinal traditions [5]. In numerous traditional medicine systems throughout West Africa, the Philippines, Fiji, and South Africa, guava roots are utilized for internal and external therapeutic applications [6,7].

Ethnobotanical studies reveal that guava roots are commonly utilized to treat gastrointestinal ailments, including diarrhoea, dysentery, abdominal pain, indigestion, and constipation, usually prepared as potent teas or decoctions [8]. Their astringent properties, historically linked to tannin-rich components, endorse their conventional application in acute gastrointestinal disorders. Moreover, root decoctions are utilized for respiratory disorders such as coughs, pharyngitis, and pulmonary inflammation, highlighting their significance in the treatment of mucosal infections [1, 6].

Topical applications of guava roots are significant. Crushed roots, prepared as poultices or aqueous washes, are conventionally utilized on wounds, ulcers, bedsores, and other dermal diseases to facilitate healing and avert microbiological contamination [2,8]. Additional documented use encompasses alleviation of dental pain, abdominal discomfort, fever, and excessive menstrual flow, demonstrating the plant's adaptability within various indigenous medicine traditions [6,8].

Conventional methods mostly depend on basic extraction techniques. Decoctions made by boiling roots in water are the predominant method for oral or external treatment, whereas poultices consist of the direct application of freshly crushed root material to the afflicted areas [8,9]. These enduring medicinal applications indicate the existence of physiologically active phytochemicals with potential antibacterial, astringent, anti-inflammatory, and analgesic properties [10]. Notwithstanding the extensive conventional application of *P. guajava* roots, its phytochemical characterisation is comparatively underexplored in relation to investigations of the leaves and bark [11,12]. To rectify this deficiency, phytochemical studies employing contemporary analytical methods are essential for the systematic identification of chemical ingredients that may substantiate traditional assertions [5,13,14].

This study examines the petroleum ether extract of *P. guajava* roots, with Gas Chromatography–Mass Spectrometry (GC–MS) analysis conducted to clarify its volatile and semi-volatile phytochemical composition. This profiling may yield significant insights into the bioactive chemicals that underlie the plant's traditional therapeutic properties and may additionally facilitate future pharmacological and drug development research [11,13].

## MATERIALS AND METHODS

Fresh roots of *Psidium guajava* L. were harvested from the Roorkee district of Uttarakhand, India, in December 2025. The botanical specimen was verified by morphological traits by Dr. Avadhesh Kumar Koshal (Botanist, Faculty of Science, Motherhood University, Roorkee), and representative voucher specimens were documented for archival purposes (Voucher No.: MU/BOT/UG/2025/023). Subsequent to collection, the roots were meticulously washed under running tap water and subsequently rinsed with distilled water to eliminate soil and residual debris. The purified samples were sectioned into small fragments and shade-dried at room temperature for roughly 10–14 days until a stable weight was attained. The desiccated substance was further ground with a mechanical grinder to yield coarse root powder. The powdered sample was sieved for uniform particle size, sealed in airtight containers, and maintained in a cool, dry environment until subsequent extraction operations were conducted.

### Extraction Protocol

Petroleum ether (boiling range 60–80 °C) served as the extraction solvent because of its efficacy in isolating non-polar and semi-volatile compounds. Approximately 100 g of the desiccated root powder was placed into a Soxhlet extraction equipment and thoroughly extracted with petroleum ether for a duration of 6 hours. Uninterrupted hot percolation guaranteed thorough solvent circulation until the siphon tube yielded clear solvent, signifying comprehensive extraction of non-polar chemicals [13,15].



**Table 1: GC-MS Identified Compounds of Petroleum Ether Extract of *P. guajava* Roots**

Peak #	Compound Name	R. Time	Base m/z	Area	Area %	Height	Height %
1	n-hexadecanoic acid	36.962	73.05	25,703,799	1.95	4,115,247	1.48
2	9,12-octadecadienoic acid (Z,Z)	40.988	67.10	4,075,543	0.31	1,046,642	0.38
3	9-octadecenoic acid (E)	41.159	55.10	4,905,348	0.37	1,301,001	0.47
4	octadecanoic acid	41.798	73.10	19,212,293	1.45	3,576,865	1.29
5	Heneicosane	44.845	57.10	2,625,341	0.20	858,536	0.31
6	Eicosane	46.989	57.10	15,387,713	1.16	4,901,916	1.77
7	Dotriacontane	49.069	57.10	46,537,796	3.52	13,759,881	4.96
8	bis(2-ethylhexyl) phthalate	49.616	149.05	71,195,438	5.39	19,865,249	7.15
9	hexatriacontane	51.069	57.10	92,971,952	7.04	25,854,122	9.31
10	tetracontane	52.999	57.10	149,675,904	11.33	35,344,617	12.73
11	nonacosane	54.855	57.10	192,943,430	14.60	42,586,271	15.34
12	tetrapentacontane	56.647	57.10	227,293,490	17.20	46,676,680	16.81
13	2-methylheptacosane	58.471	57.10	215,107,298	16.28	40,007,297	14.41
14	$\beta$ -sitosterol acetate	60.028	147.15	16,976,790	1.28	3,519,830	1.27
15	octacosane, 2-methyl	60.609	57.10	236,622,143	17.91	34,228,685	12.33

The identified chemical classification of constituents reveals four principal chemical classes: Including long-chain aliphatic hydrocarbons (C<sub>20</sub>–C<sub>54</sub> range), fatty acids and esters, phthalate esters, and phytosterol derivatives. The long-chain hydrocarbons were the largest percentage of the extract, together representing roughly 80% of the overall peak area. These non-polar aliphatic compounds are typically acquired in substantial yields from petroleum ether extractions owing to their pronounced lipophilicity and elevated boiling temperatures. Minor amounts of fatty acids, including n-hexadecanoic acid, octadecanoic acid, and unsaturated C<sub>18</sub> fatty acid derivatives, were identified. The detection of  $\beta$ -sitosterol acetate signifies the existence of sterol-derived elements inside the root matrix, corroborating the presence of membrane-associated lipid constituents. Bis(2-ethylhexyl)phthalate, commonly detected in plant extracts and environmental matrices, was found in moderate quantities.

## DISCUSSION

The GC-MS study of the petroleum ether extract from *Psidium guajava* roots indicated a predominance of high molecular weight n-alkanes, such as tetrapentacontane, 2-methyl-octacosane, tetracontane, and nonacosane. Long-chain hydrocarbons are frequently identified as components of plant cuticular waxes, serving as hydrophobic barriers that safeguard plant tissues against desiccation, microbial invasion, and environmental stress. In addition to their structural function in plants, long-chain alkanes have been shown to possess antibacterial, antioxidant, and surface-active characteristics, potentially enhancing the traditional topical uses of guava roots in wound healing and ulcer treatment [28].

Alongside hydrocarbons, many fatty acids were identified in tiny quantities, including palmitic acid (n-hexadecanoic acid), stearic acid (octadecanoic acid), linoleic acid (9,12-octadecadienoic acid), and oleic acid (9-octadecenoic acid). Fatty acids are extensively recognized for their anti-inflammatory, antioxidant, and hypolipidemic properties, corroborating the traditional medical application of guava root decoctions in the treatment of gastrointestinal disorders, abdominal pain, and inflammatory illnesses. Their presence in petroleum ether extracts indicates that the lipophilic fraction of the root contains bioactive compounds that can modulate cellular oxidative stress and inflammation [29].

The detection of bis(2-ethylhexyl)phthalate in the extract aligns with reports of this compound in various plant matrices. While phthalates are often regarded as environmental pollutants, plant-derived phthalate esters have been linked to antibacterial and anti-inflammatory properties, hence supporting the traditional application of guava roots for treating infections and inflammatory conditions [30]. Furthermore, the finding of  $\beta$ -sitosterol acetate, a derivative of phytosterol, highlights the nutraceutical potential of the lipophilic root fraction. Phytosterols are widely recognized for their antioxidant, anti-

inflammatory, and anticancer activities, and  $\beta$ -sitosterol in particular has been studied for its immunomodulatory and wound-healing properties [31]. The existence of this sterol ester indicates that the petroleum ether extract of guava roots may play a role in the pharmacological effects associated with the plant in ethnomedicine [32].

The chemical composition of the root extract significantly contrasts with earlier investigations on guava leaves, which are abundant in flavonoids, phenolic acids, and tannins [33]. This observation highlights organ-specific metabolic variation, wherein roots preferentially accumulate long-chain alkanes, fatty acids, and sterol derivatives, whereas leaves are enriched with polyphenolic compounds. This tissue-specific metabolite distribution may indicate adaptive physiological capabilities of the plant and imply that certain plant portions could be selectively utilized for distinct medicinal purposes [34].

The GC-MS profiling of the petroleum ether extract offers an extensive overview of the root's lipophilic compounds, many of which demonstrate established bioactivities consistent with the plant's traditional usage for wound healing, gastrointestinal comfort, and anti-inflammatory purposes [35]. These findings not only corroborate certain ethnopharmacological assertions but also establish a chemical foundation for subsequent inquiries into the pharmacological and nutraceutical potential of guava roots.

### CONCLUSION

This study is the inaugural thorough GC-MS profile of the petroleum ether extract from *Psidium guajava* roots, offering significant insights into the lipophilic phytochemical makeup of this traditionally significant plant component. The examination disclosed a chemical composition predominantly characterized by long-chain alkanes, fatty acids, phthalate esters, and sterol derivatives, with high molecular weight hydrocarbons comprising the majority of the extract. The data indicate that roots preferentially accumulate non-polar metabolites, whereas leaf extracts are generally abundant in flavonoids and phenolic compounds, underscoring the organ-specific distribution of bioactive elements throughout the plant.

The discovered compounds exhibit various pharmacological actions, such as antibacterial, antioxidant, anti-inflammatory, hypolipidemic, and wound-healing characteristics. Long-chain hydrocarbons and fatty acids may play a role in the conventional application of guava roots for gastrointestinal ailments, dermal infections, and inflammatory diseases.  $\beta$ -Sitosterol acetate and other sterol derivatives suggest potential nutraceutical significance, underscoring the plant's role in health enhancement and illness prevention.

These findings offer a scientific basis for the conventional medical applications of guava roots and lay the groundwork for subsequent research. The lipophilic compounds found in this work necessitate additional pharmacological assessment, encompassing *in vitro* and *in vivo* investigations, to examine their antioxidant, anti-inflammatory, antibacterial, and other bioactive properties. Furthermore, the petroleum ether fraction may provide a significant source of bioactive chemicals for pharmaceutical research, nutraceutical formulations, and functional foods, highlighting the importance of roots as an underutilized plant component with considerable therapeutic potential.

This study enhances the chemical characterization of *P. guajava* roots and emphasizes the necessity of rigorous phytochemical profile of traditionally utilized plant materials. The data produced in this document can inform future bioactivity-guided fractionation research and assist in substantiating the ethnopharmacological assertions related to guava roots, facilitating innovative drug discovery and nutraceutical uses.

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