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Exploring Leucas aspera: Phytochemical Composition, Pharmacological Potential, and Drug Discovery Prospects

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ABSTRACT

Leucas aspera, the common name for which is Thumbai, is a medicinal plant found widely distributed in seas under the tropics and subtropics, with special reference to South and Southeast Asia. From ancient times, it has been employed in Ayurvedic and folk medical systems in the management of various conditions such as fever, skin ailments, and respiratory disorders. The current review addresses the phytochemistry, pharmacological activities, and therapeutic implications of Leucas aspera. It is bioactive with multiple classes of compounds: flavonoids, alkaloids, terpenes, and essential oils, that give the plant antimicrobial, antioxidant, anti-inflammatory, analgesic, and antipyretic properties. Recent studies demonstrated the effectiveness of Leucas aspera against all types of bacteria and fungi, thus substantiating its traditional applications in medicine. There has also been some research into the cytotoxicity and anticancer effects of Leucas aspera from a pharmaceutical viewpoint. However, with its potential for medicinal applications, more studies are needed to establish dosage standardization, mechanism of actions, and clinical efficacy. This review will try to provide scientific backing for the traditional uses of Leucas aspera and approach the prospects of its applications in modern medicine.

Keywords: *Leucas aspera, medicinal plants, phytochemistry, pharmacological activities, antimicrobial properties, antioxidants, anti-inflammatory agents, ethnomedicine, traditional medicine, essential oils, cytotoxic agents, Ayurveda, bioactive compounds.*

1. INTRODUCTION

Leucas aspera is the name given to the species in Latin, while the Tamil name is Thumbai, English calls it White Dead Nettle, and the other names are Thumbe, Dronapushpi, and Chitrapatrika in Sanskrit. These herbaceous plants grow in tropical and subtropical areas of India, Southeast Asia, and some parts of Africa. These plants are often found in disturbed habitats like roadsides, forests, and fields[1]. The plant has a long history of utilization in traditional medicine systems due to various healing properties. The stimulant, expectorant, asperient, and diaphoretic properties of the flowers are more concrete. However, they are used in insecticides and given to children for the treatment of colds when mixed with honey [2]. The leaves are used as insecticides and mosquito repellants; leaf juice is used to treat chronic skin ailments such as psoriasis and rheumatism. An alcoholic extract of these plants has been traditionally used with honey in folk medicine for relieving stomach pain and indigestion. The first scientific description of Leucas aspera took place in 1753 by Carl Linnaeus [4]. The genus name Leucas stems from the Greek word leucos, meaning white, referring to the plants' white flowers; species name aspera emanates from Latin meaning rough, referring to the feel of dully green leaves and stems [4]. It has, throughout

history, formed the synergy relating ecosystem balance and erosion prevention acting as a soil binder. The capacity to survive well in a degraded area and importance in folk medicine have contributed to the widespread occurrence of this plant in tropical regions[3].

Taxonomical Classification[4]

Kingdom : Plantae

Sub-kingdom : Tracheobionta (Vascular plant)

Super division: Spermatophyta (Seed plant)

Division : Angiosperma

Class : Dicotyledonae

Sub-class : Gamopetalae

Series : Bicarpellatae

Order : Tubiflorae

Family : Labiatae

Genus : Leucas

Species : aspera

Synonyms: Leucas zeylanica (Linnaeus), Leucas albiflora, Leucas paniculata, Leucas ciliata (William Roxburgh)

Distribution

The herb has a pleasant aroma and is distributed in countries like India, the Philippines, the plains of Mauritius and Java, and also within the boundaries of Tropical Asia and Africa [5]. It has competitive weeds, with an annual herb found in the crop fields of the highlands, the fallow lands, cultivated fields, sandy soils, wastelands, and roadsides, 15-60 cm height, quadrangular stem and branches[5].

Species of Leucas (Family - Lamiaceae)

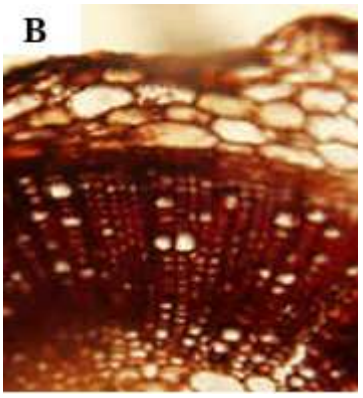
Leucas aspera, Leucas cephalotes, Leucas indica, Leucas lanata, Leucas lavandulaefolia, Leucas martinicensis ,Leucas mollissima, Leucas plukenetii, Leucas stelligera, Leucas urticaefolia, Leucas zeylanica [6]

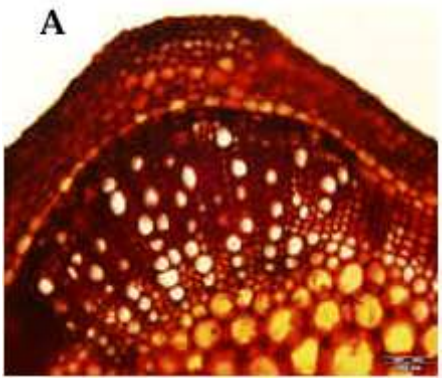
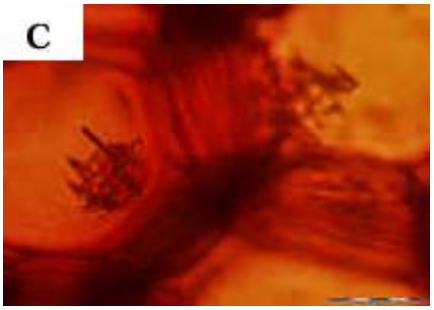
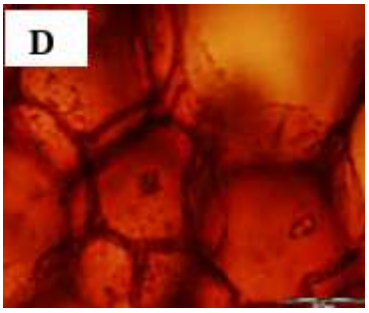
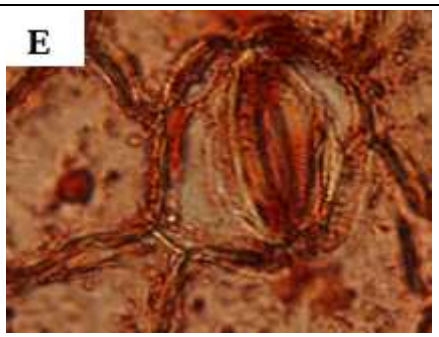
Table:1 Illustrates Morphological Description of Leucas aspera

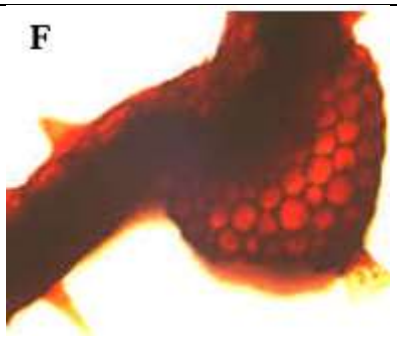
Sl no.	Plant Part	Morphological Observation	Reference
1	Habit	Leucas aspera is an annual herb, 15-60 cm tall, with a stout, hispid and very sharply quadrangular stem and branches.	[7]
2	Stem	This stem is light greenish-yellow in color, rough, hairy, quadrangular in shape with four prominent furrows, approximately 4 mm thick, has prominent nodes and internodes, and a slightly bitter taste.	[7]
3	Leaves	The leaves are usually yellowish green in color and ovate or lanceolate in shape with a size varying from 3 to 9 cm in length and 1 to 2.5 cm in width. The leaves are glabrous and with entire or crenate edges. The leaf blades are scattered in opposite direction, vary from acute to acuminate, and are either sessile or attached to short petioles. The leaves occur in very dense globose clumps of 2-3.5 cm in diameter.	[8]
4	Calyx	The flowers are tubular and they may be anywhere between 8-13 mm long with a slight curve above where nutlets grow; they are ribbed and hirsute in the upper half with an equal number of nerves up to ten with 6-10 unequal pubscent or hirsute teeth.	[8]
5	Flowers	The flowers are white, sessile, small, and are borne in dense terminal or mostly axillary whorls. Bracts linear, ~6 mm	[9]

		long, acute, bristle-tipped with slender ciliated hairs. Inflorescence widely spaced.	
6	Corolla	Measures 1 cm long; upper lip densely white-woolly and concave. Tube 5 mm long and pubescent above; lower lip longer by twice, 3-fid; mid-lobe, larger than others, obovate, rounded; lateral lobes small and sub-acute. Stamens 4, didynamous; anthers connivent, disc entire or lobed; nutlets ovoid, triquetrous.	[10]
7	Root	This is a plant with woody hardness marking and shardy roundness, split open or sometimes appearing as stretch-marked cubes, yet semi-rigid in the main.	[1]
8	Fruit	The nutlets are oblong, 2.5 mm long, with a brown color, smooth, straight inner face, and angular to the outer face and rounded. The fruit is a schizocarp cincinnule.	[2]
9	Seed	The seed of about 0.3 cm long, 0.1 cm wide, oblong, trigonous, and smooth, is dark brown.	[11]

Table: 2 Describes Microscopic Observation of leucas aspera

Sl no.	Plant plant	Microscopic observation	Images	references
1	Root	The outer structure is an epidermis of a single layer of rectangular and thin-walled cells. The secondary cortex is made up of parenchymatous cells that are thin-walled and tangentially elongated. Secondary phloem comprises sieve-tube elements and phloem parenchyma, while secondary xylem consists of vessels, tracheids, fibres, and xylem parenchyma. The vessels are long and have short projections; vessels and tracheids have simple pits. The xylem fibres are long, have pointed ends, and possess moderately thick walls, with some having simple pits. Medullary rays are 1-2 cells wide and can be as much as 8 cells high.	 Portion of root T.S	[12]

2	Stem	It has a squarish outline with bearing two ridges and two furrows. The epidermis is single-layered composed of oval to rectangular thin-walled cells attached to only unimolecular to trigonal trichomes. Secondary cortex, ridges and 5-9 layers of collenchymatous cells of 2-4 tangentially elongated parenchymatous cells. Endodermis single-layered with barrel-shaped thin-walled cells. Pericycle is single-layered with small thin-walled cells where some convert into pericyclic fibre. Narrow phloem comprises vessels, tracheids, fibres, and abundant xylem parenchyma. Cylindrical vessels with simple pits and spiral wall thickening. Pith consists of circular to oval, thin-walled parenchymatous cells.	 Portion of stem T.S.  Crystals in pith cells of stem(Needle shaped & cuboid)  Crystals in pith cells of stem (Rhombohedral)	[7]
3	Leaf	Petiole consists of single-layered epidermis with unicellular to trigonal pointed trichomes. The cortex is made of single-layered, round-to-angular collenchyma cells. Parenchyma consists of thin-walled cells with prismatic calcium oxalate crystals. Vascular bundles are smaller	 Stomata on leaf	[2]

		towards corners and larger toward the center. Midrib has epidermis on both sides and bears unicellular to tricellular trichomes. There are 1-2 layers of collenchyma on the lower surface and 3-4 layers on the upper surface, followed by 4-7 layers of round to oval parenchyma cells. Centrally present are arc-shaped vascular bundles. Lamina: Epidermis on both sides with sparse trichomes on the upper surface. Single-layered palisade, with 3-5 layers of irregular spongy parenchyma. Stomatal index ranged from 16.6-40.5 on the lower surface and 16.6-30.7 on the upper surface.	 Leaf T.S	

Bioactive Compounds

Glycerin, 1- (3-methyl-butyryl) pyrrolidine, Benzene acetaldehyde, Propane, 1,3-triethoxy-, Thymine, 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl, 4H-Pyran-4-on, 3,5-dihydro-2-methyl, 2-Furan carboxaldehyde, 5-(hydroxymethyl), Caryophyllene, A-Caryophyllene (Humulene), Azulene, dodecanolic acid, Nerolidol-2, Delthyl phthalate, Caryophyllene oxide, 4-Hydroxy-2-methoxy-cinnamaldehyde, Tetradecanoic acid, Phytol, etc. [16](Anandan et al. 2012). Flavonoids, alkaloids, phenolic acids, stilbenes, lignans, lignin, and tannins are phenolic compounds that are well known in plants as scavengers of free radicals with multiple biological effects, including antioxidant activity[13].

Among the diterpenes, lignans and flavonoids isolated from the plant are prostaglandins that induce contraction, inhibition and antioxidant activity [13]. Diterpene alcohol, particularly, has been found as the predominant chemical class in Leucas aspera plant [14], whereas low concentration of catechin compound has been exhibited to possess larvicidal activities [2].

Table:3 Illustrates Pharmacological Activities of Leucas aspera

Sl no.	Pharmacological activity	Extract/ Part used	Findings	References
1	Antibacterial	Whole plant	It appeares that the hubs are very effective against S. aureffus, E. coli, P. aeruginosa, Salmonella spp., Shigella spp., Klebsiella pneumoniae, and B. subtilis.	[15][16]
2		Root	The course of study lasted for three years allowing the human being to learn in stages and develop his	[17]

			reasoning at different phases of learning.	
3		Leaves	Hexane and chloroform extracts also exhibited activity on Gram-positive and Gram-negative bacterial species.	[16][18]
		Flowers	Methanolic extracts and alkaloidal residues have been shown to be active against S. aureus, B. subtilis, E. coli, and P. aeruginosa-	[19]
	Antifungal	Whole plant	Fungicidal activity was evaluated against Trichophyton, Epidermophyton, Candida and Aspergillus.	[20] [21]
		Flowers	An alkaloidal residue acting against C. albicans, C. neoformans, A. niger, and T. mentagrophytes.	[17]
	Anticancer	Whole plant	The cytotoxicity of hydroalcoholic extracts verified through a brine shrimp test confirmed instant cytotoxicity (LC50 = 52.8 µg/mL).	[23]
		leaves	Methanolic extract has cytotoxicity (LC50=30µg/ml).	[23]
	Antioxidant	Whole plant	Higher rate of antioxidants, give DPPH IC50=99.58±1.22 µg/ml	[16]
		Root	Improved free radical scavenging capability (IC50=6.55 µg/ml)	[17]
		Leaves	The ethanolic extract eliminated nitric oxide and shielded against DNA damage.	[24]
	Hepatoprotective	Whole plant	Liver injury can be prevented by methanolic and petroleum ether extracts.	[25]
	Anti inflammatory	Whole plant	The anti-inflammatory properties observed in the mast cell degranulation can be	[26]

			elaborated upon with the help of the various extracts.	
	Antidiabetic	Leaves and stem	When using methanolic extracts in Swiss albino mice, there was a decrease in blood glucose.	[27] [28]
	Cytotoxic	Root	The ethanolic phase (80% ethanolic extract) of the roots shows significant cytotoxicity with an LC_50 of 52.8 µg/ml.	[29]
	Angiosuppressive	Leaves and stem	CAM assay and high on tumor cells suppression in angiogenesis	[30]
	Anti malarial	Leaves	Actively kills the P. falciparum parasite (3D7 strain)	[31]
		flowers	The ethyl acetate extract proved active against P. falciparum.	[31]
	Larvicidal	Whole plant	Was effective against Aedes aegypti and Culex quinquefasciatus.	[32]
	Wound healing activity	Whole plant	Enhanced the healing of rats by Baicalein-7-O-β-D-glucuronide.	[33]
	Antivenom	Whole plant	The triterpenoid extract directly counteracted the venom-induced oxidative stress.	[34]

Essential Oil

The essential oils of Leucas aspera possess notable antimicrobial potency against Pseudomonas aeruginosa, Haemophilus influenzae, and Staphylococcus aureus, and Candida albicans, whereas this essential oil showed no activity against Bacillus subtilis, Proteus vulgaris, Neisseria gonorrhoeae, and Tricoderma viride. In addition, the essential oils inhibited Staphylococcus aureus, Vibrio cholerae, Salmonella typhi, Escherichia coli, Proteus vulgaris, Pseudomonas pyocyanea, and Shigella flexneri [35].

Table:4 Phytochemical classification of leucas aspera

Sl No.	Phytochemical compound	Secondary metabolites	References
1	Terpenes and Terpenoid compounds	Oleanolic acid, Ursolic acid, Squalene, β-caryophyllene, αhumulene, α-pinene, epia-α-bisabolol, Limonene, x-thujene, Menthol, Leucasperone A, Leucasperone B, Leucasperone C	[1][19][38]
2	Sterols and Fatty compound	3-Sitosterol, 9,12,15-Octadecatrienoic acid methyl ester, nHexadecanoic acid, Linoleic	[37] [36]

		acid, Oleic acid, Stearic acid, Ceryl alcohol, Dotriacontanol	
3	Glycoside compounds	Glucoside, Linifolioside, Leucasperosides A, Leucasperosides B, Leucasperosides C,	[19],[48]
4	Long chain compounds	(4-(24-Hydroxyl-1-oxo-5-n-propyltetracosanyl)-phenol), 28-Hydroxypentatriacontan-7-one, 7-Hydroxydotriacontan-2- one, 1-Hydroxytetratriacontan-4-one, 32-Methyltetratriacontan-8-ol, Nonatriacontane, 5- Acetoxytriacontane	[1][37]
5	Flavonoid compounds	Catechin, Acacetin, Apigenin, Chrysoeriol	[1][38]
6	Lignane compound	Nectandrin B, meso-Dihydroguaiaretic acid, Macelignan, (-)- Chicanine, Licarin A, erythro-2-(4-allyl-2,6-dihydroguaiaretic1-(4-hydroxy-3-methoxyphenyl)propan-1-ol	[1][19]
7	Miscellaneous compound	Nicotine alkaloids, Galactose sugar, 1,2 Benzenedicarboxylic acid bis(2-methylpropyl) ester, 1-Octen-3-ol, Amyl propionate, Isoamyl propionate, Asperphenamate	[1] [39]

Table 5: Extraction of leucas aspera

S.No	Extract Type	Parts Used	Pharmacological Activities	Refernces
1	Aqueous Extract	Leaves, Stem	Anti-inflammatory, Antioxidant, Analgesic, Antipyretic	[40]
2	Ethanolic Extract	Leaves, Flowers	Antimicrobial, Antidiabetic, Anticancer (preliminary evidence)	[1]
3	Methanolic Extract	Leaves, Flowers	Antioxidant, Antispasmodic, Hepatoprotective	[41]
4	Hydroalcoholic Extract	Leaves, Stem	Wound healing, Antiallergic, Diuretic	[42]
5	Powder Extract	Leaves, Flowers	Anti-inflammatory, Analgesic, Antimicrobial	[43]

2. ETHNOMEDICINAL USES

Since ancient times, L. aspera has been employed in curing ailments of various types. Several studies conducted on this plant extract have concluded that this extract is non-toxic to the patient who obtains treatment through it. One of the significant ethnomedicinal functions recorded for parts of such plants would be protection against snake venom and scorpion bites. Moreover, the smoke of the leaves of this plant has indicated a potential role in the protection against filarial vector mosquitoes. Diverse populations both rural and urban employ L. aspera for innumerable purposes in their day-to-day life within the world. Its extracts are capable of reducing fever, coughs, and colds, while it serves as a spice to savour dishes. The juice extracted from flowers has shown efficacy in folklore medicine as a cure for intestine worm infections in children. The leaves are used in preparations consumed to cure psoriasis and skin diseases, to cure headaches, and to alleviate painful

inflammation. Traditionally, young vegetative shoots along with flowers of L. aspera and equal amount of fruits of some medicinal plants are orally taken to treat dysmenorrheic disorders. [44]

3. TOXICITY STUDY

The toxicity levels of L. aspera were assessed through an investigation in an animal model using Swiss albino mice. The acute toxicity study was carried out on the females only, while both male fellow and female Wister rats were subjected to sub-acute toxicity study. Experimental protocols were approved by committee for purpose of control and supervision of experiments on animal ethics[25]. Animals were caged, and the changes were then observed for the first 4 hours, followed by a 24 hour observation for the mortality test. The results did not show any behavioural changes or mortality incidents throughout the period of study; administration of L. aspera extracts was safe up to 2000 mg/kg body weight. So, this can be mentioned cut-off dose for the animals in that study[45]. Kripa Tambe OECD 1995

Molecular Docking and In-Silico Studies

Computational Insights into Bioactivity

The latest developments in computational biology are evaluating the bioactive compounds in Leucas aspera through molecular docking and in-silico studies. It predicts the binding affinity and interaction mechanisms of phytochemicals with target proteins involved in various diseases through these computational approaches.

Docking Studies on Anticancer Activity

Molecular docking studies have confirmed that certain flavonoids from Leucas aspera, for example, quercetin and luteolin, bind strongly to the EGFR and HER2 receptors which are very important in cancer progression [Mahaboob Begum Sm et al F2024]. Therefore, the compound may be targeted for cancer therapy developed from the natural products of the plant [46]**.**

Antimicrobial and Antiviral Potential

Structural computational study shows that both of these are claimed to be associated with essential oils and alkaloids from Leucas aspera that interact with bacterial DNA gyrase and viral proteases and inhibit the growth of microbes and the replication of viruses[47]. Several docking studies featured strong binding scores for caryophyllene and humulene against SARS-CoV-2 Mpro protease. These studies really underscore the possibility of this plant becoming a basis for antiviral drug manufacture [48]**.**

In-Silico Toxicity & ADME Profiling Studies

In-Silico Toxicity & ADME Profiling Studies in bioavailability and prediction about Absorption, Distribution, Metabolism, and Excretion indicated that the bioactive compounds of Leucas aspera are probably well absorbed by the oral route and have low toxicity with appreciable pharmacokinetics. Therefore they provide good grounds and excellent candidates for drug development. Their experimental validation is still needed for confirmation of these computational predictions [40]**.**

Drug Development Constraints

Partially very hopeful and therapeutic, but many are the challenges involved in bringing Leucas aspera into clinically approved drugs:

- Standardization of Extracts – Variability in extraction and formulation due to environment and genetic conditions necessitates protocols for standardization.[16]
- Mechanistic Studies – Molecular mechanisms of bioactive compounds in disease pathways require further evaluation.
- Clinical Validation – Promising preclinical data is not, however, enough without stringent clinical trials for safety and efficacy assessments in humans[49].
- Enhanced Bioavailability-Such novel drug delivery systems as nanoparticles and liposomal formulations can certainly improve bioavailability of active constituents [**5]**
- Regulatory Compliance- The commercial use of herbal medicine must comply with appropriate regulations for approval.

Potential for Combination or Synergistic Therapy

Improving Therapeutic Potency

The therapeutic efficacy of Leucas aspera is enhanced in combination with standard medicines. Its antimicrobial, anticancer and anti-inflammatory activities can be synergized with synthetic drugs that would lead to improved bioavailability and efficiency while reducing adverse effects **[50].**

Antimicrobial Synergy

Extracts of Leucas aspera potentiated the antibacterial activities of the standard antibiotics ampicillin and ciprofloxacin against bacterial strains resistant to these antibiotics, such as Staphylococcus aureus and Pseudomonas aeruginosa. This indicates that it might help mitigate antibiotic resistance by means of combination therapy **[49].**

Combination Therapy in Cancer

In vitro studies reveal that Leucas aspera flavonoids, when administered in combination with chemotherapeutic agents like doxorubicin, enhance cancer cell apoptosis and reduce the toxicity induced by chemotherapy. This indicates the potential of these flavonoids for integrative therapy in cancer [50].

Anti-Inflammatory and Pain Management

A combination of extracts from Leucas aspera with NSAIDs such as ibuprofen may greatly augment the anti-inflammatory and analgesic efficacy and decrease gastric irritability, thereby rendering them good alternatives for the management of chronic pain [49] .

Future Directions of Research:

Future research on Leucas aspera should focus on:

• Isolate and characterize novel bioactive compounds with targeted pharmacological effects.

• Development of standardized herbal formulations for large-scale clinical use.

• Combination therapies in which compounds derived from Leucas aspera are used along with conventional drugs.

• Research for biotechnological approaches such as genetic engineering to enhance secondary metabolite production.

Leucas aspera has a good promise as a multifunctional medicinal plant, and continued studies on it might reach the breakthrough level in herbal medicine and modern pharmaceuticals. Future research could be aimed at pharmacokinetic and pharmacodynamic studies assessing the interactions with synthetic drugs; clinical studies on polyherbal formulations containing Leucas aspera; and Explore nanoformulation approaches to improving drug delivery and efficacy. Future research must focus on following areas:

Future Perspectives:

1. Future research should include exploring the pharmacokinetics and pharmacodynamics of interaction with synthetic drugs.

2. It should have clinical trial data about Leucas aspera inclusion in polyherbal formulations.

3. Future studies should focus on possible nanoformulation approaches that could improve drug delivery and efficacy.

4. CONCLUSION

Leucas aspera is a medicinal plant with significant ethnobotanical and pharmacological importance. Its rich phytochemical profile, including flavonoids, alkaloids, terpenoids, and essential oils, contributes to its diverse biological activities such as antimicrobial, antioxidant, anti-inflammatory, and analgesic effects. Traditional medicinal practices have long utilized *Leucas aspera* for treating various ailments, and scientific research continues to validate its therapeutic potential.

Studies have demonstrated the plant's antibacterial, antifungal, and cytotoxic properties, supporting its use in traditional medicine. The antioxidant activity of *Leucas aspera* further strengthens its potential in preventing oxidative stress-related disorders. However, despite its promising pharmacological properties, further in-depth studies, including clinical trials and toxicity assessments, are required to establish its safety, efficacy, and mechanisms of action.

Standardization of bioactive compounds and formulation development could pave the way for its integration into modern medicine. Future research should focus on identifying the molecular pathways through which *Leucas aspera* exerts its pharmacological effects. The findings in this review support the continued exploration of *Leucas aspera* as a valuable medicinal plant for future pharmaceutical and therapeutic applications.

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