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GC-MS profiling of essential oil of Indian lavender- *Bursera penicillata* (Sesse & Moc. Ex DC.) Engl.

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Abstract

This study investigated the chemical composition of *Bursera penicillata* essential oil using gas chromatography-mass spectrometry (GC-MS) to assess its potential therapeutic applications. Essential oils have gained significant attention as natural alternatives for antimicrobial and wound-healing treatments because of their bioactive constituents. *B. penicillata*, a member of the Burseraceae family, is traditionally used in herbal medicine; however, its phytochemical profile remains underexplored. The essential oil was extracted from fresh bark resin through hydrodistillation and analyzed using a Shimadzu GCMS-TQ8050 NX system. The analysis identified 71 compounds, with isopulegol acetate being the dominant component, followed by acetyl betulinaldehyde, geranyl acetate, and caryophyllene. These constituents belong to various chemical classes including terpenes, fatty acids, steroids, and triterpenes. The essential oil contained a diverse range of bioactive compounds with potential antimicrobial and wound-healing properties. Terpenes such as isopulegol acetate and geranyl acetate are known for their antibacterial and anti-inflammatory activities, whereas fatty acids contribute to skin barrier integrity and hydration. Steroids and triterpenes, including urs-12-en-28-al and acetyl betulinaldehyde, are associated with collagen synthesis and fibroblast proliferation, which are crucial for tissue regeneration. The presence of hydrocarbon derivatives suggests additional protective effects against microbial colonization. This study highlights the complex phytochemical composition of *B. penicillata* essential oil and its potential therapeutic significance. Future studies should focus on validating its pharmacological properties through in vitro and in vivo experiments as well as exploring formulation strategies to enhance its stability and bioavailability for clinical applications.

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Introduction

Bursera penicillata, a versatile species within the Burseraceae family, is a deciduous tree renowned for its essential oil, which is abundant in monoterpenes, sesquiterpenes, and fatty acids, and contributes to its antioxidant, antimicrobial, and anti-inflammatory properties (Piña-Torres *et al.*, 2018). Originally native to Mexico and Central America, this species has demonstrated remarkable adaptability to semi-arid climates including Bangalore, India. It exhibits a rapid growth cycle, produces fruit within a few years, and attains optimal oil yield at maturity. Historically, it has been employed in traditional medicine for wound healing and treatment of respiratory and gastrointestinal disorders, underscoring its therapeutic significance (Prabhakar Tirumani *et al.*, 2016).

The essential oil of *B. penicillata* is particularly rich in bioactive constituents including α-pinene, limonene, and β-caryophyllene, which have been extensively studied for their broad-spectrum antimicrobial effects (Tirumani *et al.*, 2017). Research has shown its efficacy against gram-positive bacterial pathogens, such as *Staphylococcus aureus* and *Bacillus cereus*, as well as against opportunistic fungal species, such as *Candida albicans* and *Aspergillus niger*. Oil disrupts microbial membranes and biofilm formation, making it a promising alternative to natural antimicrobial therapies (Jayaveera *et al.*, 2008; Theagarajan Prabhu, 1983).

Beyond its medicinal value, *B. penicillata* plays a critical role in the ecosystem balance and biodiversity conservation. Its essential oil has applications in the cosmetic, fragrance, and pharmaceutical industries, positioning it as a sustainable botanical resource. The growing interest in plant-based antimicrobial solutions further highlights the need for comprehensive phytochemical and pharmacological investigations of this species, strengthening its potential as a therapeutic and commercial agent (Mittal *et al.*, 2019).

Essential oils have long been recognized for their medicinal and therapeutic potential, particularly for wound healing and infection control (Chandra *et al.*, 2017; Lahmar *et al.*, 2017). These volatile biologically active compounds are widely utilized in pharmaceuticals, cosmetics, and traditional medicine because of their diverse pharmacological properties, including antimicrobial, anti-inflammatory, and antioxidant effects (Iseppi *et al.*, 2021; Das *et al.*, 2022). The increasing burden of antibiotic resistance and chronic wounds has driven the need for natural alternatives, prompting extensive research on plant-derived essential oils as effective therapeutic agents. Among these, species belonging to the Burseraceae family have garnered attention because of their rich composition of bioactive secondary metabolites (Aswany *et al.*, 2023; Gnat *et al.*, 2021).

Despite its historical medicinal use, there is a lack of comprehensive phytochemical characterization of *B. penicillata* essential oils. Investigating its chemical profile through GC-MS analysis is crucial for understanding its therapeutic potential and validating its traditional applications (Gamal El-Din *et al.*, 2022). Gas Chromatography-Mass Spectrometry (GC-MS) is a highly sensitive and reliable analytical technique for identifying volatile organic compounds in essential oils. It provides qualitative and quantitative insights into chemical composition, enabling the identification of major bioactive constituents. Profiling the essential oil of *B. penicillata* using GC-MS allows for a deeper understanding of its phytochemical diversity, which may offer novel antimicrobial and wound-healing solutions (Poudel *et al.*, 2021).

The rationale for this study lies in the limited phytochemical characterization of *B. penicillata* essential oil despite its traditional medicinal use. The identified research gap is the lack of gas chromatography-mass spectrometry (GC-MS) profiling and pharmacological validation. This study aimed to analyze its chemical composition, identify its bioactive compounds, and explore its potential in antimicrobial and wound healing applications.

Materials and methods

Plant material and collection of essential oil

Burcera penicillata (Sesse & Moc. Ex DC.) Engl. tree was located in the landscape garden of Osmania University and authenticated by Dr. L. Rasingam, Scientist E& HoO, Botanical Survey of India, Deccan Regional Center, Hyderabad (BSI/DRC/2022-23/Identification/730, Dated 30.01.2023). The essential oil of *B. penicillata* (BPE) was obtained by hydrodistillation from fresh bark resin using a Clevenger-type apparatus for two hours. The essential oil obtained was separated, dried over anhydrous sodium sulfate, and stored in sterile amber glass vials at 4°C until further use.

GC-MS analysis

GC-MS analysis of the essential oil was conducted using a Shimadzu GCMS-TQ8050 NX instrument equipped with an AOC-20i+ autosampler. The sample was prepared by diluting the essential oil with a suitable solvent before injection into the system. Splitless injection mode was employed to maximize the transfer of volatile compounds into the column. The injection temperature was set at 280°C to ensure efficient vaporization of the sample components. The oven temperature program was designed to facilitate the separation of the volatile constituents.

Initially, the column oven was maintained at 70°C for 5 min, followed by a ramping rate of 5°C/min until it reached 310°C, which was held for 10 min. The total flow rate of the carrier gas, helium, was maintained at 14.1 mL/min, with a column flow of 1.00 mL/min. (Herrera-Calderon *et al.*, 2022).

The GC-MS system was operated in pressure-controlled mode with a linear velocity of 36.7 cm/sec. The ion source temperature was maintained at 200°C and the interface temperature was set to 280°C. A solvent cut time of 4.50 minutes was used to eliminate early solvent interference. Mass spectrometric detection was performed in Q3 scan mode, covering a mass range of 50–700 m/z. The scan speed was set at 3333 amu/s, with an acquisition time between 5.00 and 63.00 minutes. The system utilized a relative detector gain mode set at 1.09 kV with a threshold of zero (Shah *et al.*, 2023).

After acquisition, spectral data were processed using the NIST20 library for compound identification based on mass fragmentation patterns and retention indices. The chromatogram showed distinct peaks corresponding to the individual volatile compounds present in the sample. Each identified compound was assigned a retention time and relative peak area percentage, allowing for quantification of major and minor constituents. Qualitative and quantitative analyses of the identified components were further validated by comparison with standard spectra from the library database (El-Kased and El-Kersh, 2022).

Results and discussion

The analysis detected 71 compounds that were identified based on their retention times and mass spectral fragmentation patterns using the NIST20 library (Fig. 1, Table 1). The major compounds identified were isopulegol acetate (66.76%), uvaol (7.46%), and geranyl acetate (3.33%). These dominant constituents belong to terpene, fatty acid, steroid, and saponin classes. The peak area percentages indicated their relative abundance in the essential oil.

The TIC (Total Ion Chromatogram) profile showed multiple well-resolved peaks with varying intensities, indicating the presence of a diverse range of phytochemicals. Identification relied on the matching of retention times, molecular ion peaks, and characteristic fragment ions to reference spectra from the library database. High-resolution mass spectra provided structural insights into the detected compounds, ensuring reliable qualitative analysis.

GC-MS analysis of the *B. penicillata* essential oil revealed a diverse range of phytochemicals, including terpenes, fatty acids, triterpenes, steroids, and other organic compounds. The presence of these constituents highlights the complexity of the oil and its potential for various biological applications as well as a multifaceted approach to promote skin regeneration and antimicrobial activity.

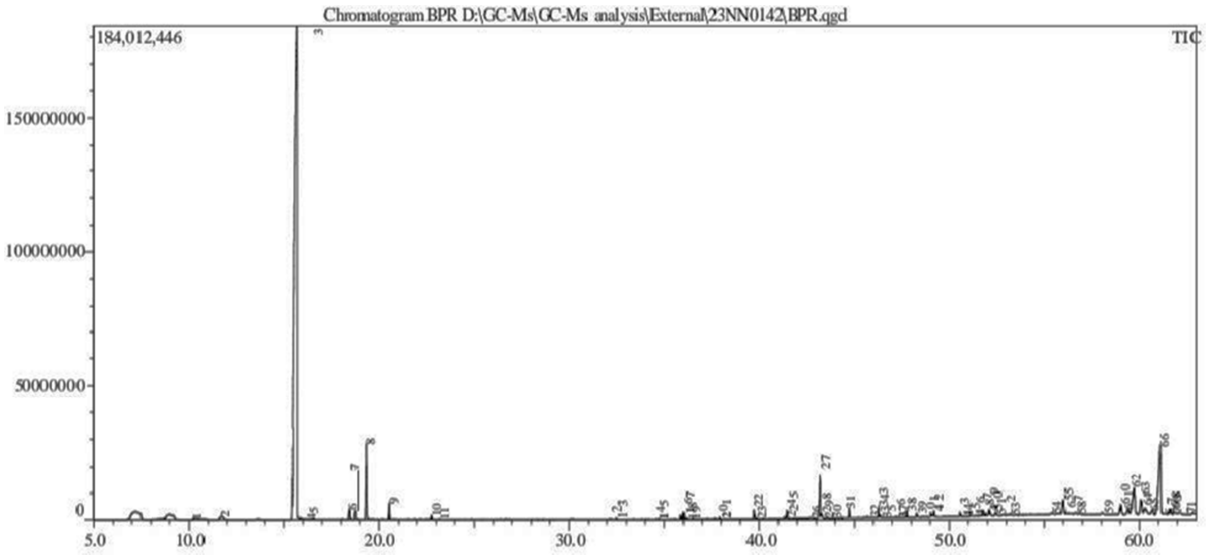

Fig. 1. GC-MS chromatogram of *B. penicillata* essential oil

Table 1. GC-MS analysis of the *B. penicillata* essential oil

Peak	Area%	Category	Name
26	2.31	Fatty acid	13-Docosenoic acid, methyl ester, (Z)-
17	0.32		11-Octadecenoic acid, methyl ester
27	0.23		13-Docosenoic acid, methyl ester, (Z)-
16	0.2		9,12-Octadecadienoic acid(Z,Z)-, meth
19	0.09		11,14-Octadecadienoic acid, methyl est
33	0.09		15-Tetracosenoic acid, methyl ester, (Z)
18	0.08		6-Octadecenoic acid, methyl ester, (Z)-
13	0.07		Hexadecanoic acid, methyl ester
25	0.06		9-Octadecenoic acid (Z)-, oxiranylmeth
34	0.04		Tetracosanoic acid, methyl ester
64	7.46	Triterpene	Acetyl betulinaldehyde
61	1.32	Steroid	Urs-12-en-28-al, 3-(acetyloxy)-, (3β-)
58	0.82		28-Norolean-17-en-3-one
59	0.48		Methyl 2Î±,3Î²-dihydroxyolean
66	0.45		Urs-12-en-28-al, 3-(acetyloxy)-, (3β-)
67	0.27		Methyl 2Î±,3Î²-dihydroxyolean
55	0.19		Urs-12-ene
54	0.1		28-Norolean-17-en-3-one
56	0.09		28-Norolean-17-en-3-ol
3	66.76	Terpene	Isopulegol acetate (monoterpene ester)
8	3.33		Geranyl acetate (monoterpene ester)
9	0.75		Caryophyllene (bicyclic sesquiterpen)
6	0.61		α ±-Terpinyl acetate (monoterpene ester)
10	0.16		α±-Farnesene (acyclic sesquiterpene)
69	0.13		3β-9,19-Cyclolanostan-3-ol-acetate, (triterpene ester)
60	3.14		Humulane-1,6-dien-3-ol
62	0.85		
7	2.26		2,6-Octadien-1-ol, 3,7-dimethyl-, acetat
68	0.21		Ursolic aldehyde
46	0.16		α - Amyrone
65	0.11		Uvaol
50	0.05		
57	0.15		24-Norursa-3,12-diene
53	1.07	Others	(3S,6aR,6bR,8aS,12S,14bR)-4,4,6a,6b,
2	0.56		2,4,6-Octatriene, 2,6-dimethyl-, (E,Z)-
48	0.43		7-[(6-Hydroxy-2,5,5,8a-tetramethyl-1,4]
63	0.43		Methyl 3Î²-acetoxylup-20(29)-en-28-
21	0.4		2-Methyltetracosane

30	0.38	Tetratetracontane
32	0.35	Pentacosane
24	0.31	Tetracosane
41	0.29	Nonacosane
37	0.27	Octacosane
49	0.25	7-[(6-Hydroxy-2,5,5,8a-tetramethyl-1,4]
40	0.19	Glycidyl (Z)-9-nonadecenoate
38	0.18	cis-13-Docosenoyl chloride
42	0.17	Tetratetracontane
23	0.1	Tetradecanamide
47	0.1	Tetratetracontane
5	0.08	Cyclopentane, 1-acetoxymethyl-3-isopr
20	0.08	Heneicosane
51	0.08	Pentatriacontane
44	0.07	Octacosanal
22	0.06	cis-Methyl 11-eicosenoate
28	0.06	Methyl 20-methyl-heneicosanoate
1	0.05	1-Undecene
15	0.05	1,6,10,14-Hexadecatetraen-3-ol, 3,7,11
35	0.05	Pentacosane
39	0.05	3-Methyloctacosane
45	0.05	3,11-Dioxa-2,12-disilatridecane, 2,2,4,4
12	0.04	7,9-Di-tert-butyl-1-oxaspiro (4,5)deca-6
14	0.04	1,6,10,14-Hexadecatetraen-3-ol, 3,7,11,
29	0.04	2-Methylpentacosane
36	0.04	3-Methylheptacosane
52	0.04	(5-Methyl-1-(4-methylpent-3-en-1-yl)-2
11	0.03	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,
43	0.03	Cyclohexane, hexadecyl-
4	0.02	Cyclohexanol, 1-methyl-4-(1-methyleth)
31	0.02	3-Methylhexacosane

Terpenes are well known for their antimicrobial, anti-inflammatory, and wound-healing properties. Isopulegol acetate (66.76%), a monoterpene ester, has been reported to exhibit antibacterial and antifungal properties, making it a key component for preventing infections in open wounds. Similarly, geranyl acetate (3.33%) and caryophyllene (0.75%), both of which belong to the monoterpene and sesquiterpene classes, respectively, have shown significant anti-inflammatory and skin-repairing effects by modulating oxidative stress and promoting collagen synthesis.

The presence of humulane-1,6-dien-3-ol (3.14%) and α-farnesene (0.16%) suggests additional antioxidant and antimicrobial effects, which can enhance tissue recovery and protect against opportunistic microbial colonization. These terpenes disrupt bacterial membranes, leading to reduced microbial viability in wounds and preventing secondary infections.

Fatty acids are essential for maintaining the integrity of the skin barrier and for antimicrobial defense. 13-docosenoic acid, methyl ester (2.31%), 11-octadecenoic acid, methyl ester (0.32%), and 9,12-octadecadienoic acid (0.20%) are long-chain fatty acid derivatives that affect cell membrane stability, hydration, and antimicrobial activity. These compounds create an unfavorable environment for bacterial and fungal growth, thereby reducing the risk of biofilm formation in infected wounds.

Fatty acid methyl esters, including hexadecanoic acid and methyl ester (0.07%), exhibit anti-inflammatory effects crucial for modulating immune responses in wounds. The reduction in local inflammation leads to faster tissue regeneration and reduced scarring.

Steroidal and triterpenoid compounds, such as urs-12-en-28-al, 3-(acetyloxy)- (1.32%), 28-norolean-17-en-3-one (0.82%), and methyl 2α,3β-dihydroxyolean (0.48%), contribute significantly to wound healing and skin repair. These compounds possess potent anti-inflammatory and fibroblast-stimulating properties, which accelerate tissue regeneration and

re-epithelialization in the injured skin. They also help in angiogenesis, the process of new blood vessel formation, which is crucial for wound healing.

Acetyl betulinaldehyde (7.46%), a triterpenoid, enhances collagen synthesis and fibroblast proliferation, which are key processes in wound closure. It also exerts antimicrobial activity against gram-positive bacteria, which are commonly associated with wound infections.

Hydrocarbons such as tetratetracontane (0.38%), pentacosane (0.35%), and tetracosane (0.31%) function as emollients and skin protectants. These compounds help to form a protective barrier against wounds, reduce moisture loss, and prevent external microbial contamination. Additionally, these hydrocarbons aid in reducing oxidative stress, which is vital in limiting excessive inflammation and tissue damage.

Compounds such as glycidyl (Z)-9-nonadecenoate (0.19%), cis-13-docosenoyl chloride (0.18%), cyclohexane, and hexadecyl- (0.03%) exhibited broad-spectrum antimicrobial activity. They enhance the penetration of other bioactive molecules into the skin, thereby improving the bioavailability of the therapeutic agents.

Conclusion

GC-MS analysis of *B. penicillata* essential oil highlights its rich composition of terpenes, fatty acids, steroids, and triterpenes, supporting its wound healing and antimicrobial potential. Its dominant compounds contribute to infection control, reduction of inflammation, and skin regeneration. Future research should focus on mechanistic studies, clinical trials, and nanoformulation strategies to enhance the stability and therapeutic efficacy. Investigating its synergistic potential with existing treatments could pave the way for novel natural therapeutics in medicine and skincare.

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