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Research Article

PROFILING RARE BOTANICAL COMPOUNDS THROUGH GAS CHROMATOGRAPHY–MASS SPECTROMETRY: UNLOCKING NEW POTENTIAL IN NATURAL COSMETICS

LAKSHMI SHREE N*, SUCHI MODI

Department of Life Sciences, Rabindranath Tagore University, Bhopal, Madhya Pradesh, India.
***Corresponding author: Lakshmi Shree N; Email: lakshmishree171998@gmail.com**

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ABSTRACT

Objectives: This study explores the chemical composition and cosmetic potential of four aromatic plants-Clove (*Syzygium aromaticum*), Patchouli (*Pogostemon cablin*), Bay Leaf (*Cinnamomum tamala*), and Galangal (*Alpinia galanga*)-using Gas chromatography–mass spectrometry (GC-MS) analysis and *in vitro* biological assays.

Methods: Ethanol extracts of authenticated, herbarium-archived plant materials were prepared through Soxhlet extraction. GC-MS was used to identify phytochemicals in each extract. Antimicrobial activity was assessed against *Klebsiella pneumoniae*, *Streptococcus mutans*, and *Candida albicans* using the agar well diffusion method. Antioxidant activity was measured using the 2,2-diphenyl-1-picrylhydrazyl assay, while anti-inflammatory potential was evaluated by inhibiting protein denaturation. Results were analyzed statistically using one-way analysis of variance, with $p<0.05$ considered statistically significant.

Results: Patchouli showed strong antimicrobial action with a 22.3±0.7 mm inhibition zone against *S. mutans*, while Clove inhibited *K. pneumoniae* with a zone of 19.8±1.2 mm. Galangal demonstrated notable anti-inflammatory activity with 74.6%±2.1% inhibition in the albumin denaturation test. Bay leaf extract had strong antioxidant activity with an IC_{50} of 43.2 µg/mL. GC-MS analysis revealed bioactive and rare compounds such as azulene, 1′-acetoxychavicol acetate, and elemicin, each with potential cosmetic value.

Conclusion: The presence of multifunctional phytochemicals across these botanicals highlights their value in natural skincare development. With proven antioxidant, antimicrobial, and anti-inflammatory properties, these authenticated extracts offer promising clean-label ingredients for innovative, plant-based cosmetic formulations.

Keywords: Aromatic plants, Gas chromatography–mass spectrometry profiling, Bioactive compounds, Cosmeceuticals, Antioxidant activity, Anti-inflammatory effects, Herbal skincare, Clean-label formulations.

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INTRODUCTION

The growing consumer demand for natural and plant-based skincare solutions has intensified interest in botanical sources known for their therapeutic properties. Among these, aromatic plants are particularly valued for their rich essential oil content and bioactive compounds, which exhibit a variety of dermatologically relevant effects, including antimicrobial, anti-inflammatory, and antioxidant activities [6,8-10]. Despite their established roles in traditional medicine, several of these botanicals remain insufficiently characterized from a scientific and molecular standpoint. Species such as *Pogostemon cablin* (Patchouli), *Syzygium aromaticum* (Clove), *Cinnamomum tamala (*Bay leaf), and *Alpinia galangal* (Galangal) are widely used in ethnomedicine, yet they lack detailed phytochemical profiling and experimental validation of their cosmeceutical potential [14,17,18,20,21,29,30].

Gas chromatography–mass spectrometry (GC-MS) provides a robust analytical technique for identifying complex mixtures of plant-derived compounds, offering insights into their chemical signatures [5,13]. When coupled with targeted *in vitro* assays, such profiling can help elucidate the biological activities of these phytochemicals, enabling their potential application in skincare [1,4,15,28]. This study aims to bridge the gap between traditional usage and modern scientific validation by investigating the phytochemical profiles of these four aromatic species through GC-MS and evaluating their antioxidant, antimicrobial, and anti-inflammatory properties for potential cosmetic integration [16].

METHODS

Collection and authentication of plant material

All plant specimens used in the study - *P. cablin*, *S. aromaticum*, *C. tamala*, and *A. galanga*-were authenticated by a subject expert from the Department of Botany, Rabindranath Tagore University, Bhopal, based on morphological features and regional flora. Voucher specimens were prepared and archived under reference numbers: RNTU-HERB/PC-01, RNTU-HERB/CT-02, RNTU-HERB/SA-03, and RNTU-HERB/AG-04 for documentation purposes.

Inclusion and exclusion criteria

Only healthy, mature plant parts, free from visible fungal growth, discoloration, or pest infestation, were selected for the study. Inclusion was restricted to plant material collected during peak harvesting season to ensure maximal phytochemical yield.

Any plant samples that showed signs of physical damage, contamination, or improper drying were excluded. No previously stored or commercially processed materials were used.

Extraction protocol

Each plant sample was shade-dried, powdered, and subjected to ethanol-based Soxhlet extraction for 6 h. The resultant extracts were then concentrated using rotary evaporation under vacuum [5]. Final extracts were stored at 4°C until subsequent analysis, and extraction yields were duly recorded.

GC-MS profiling

Chemical analysis of the extracts was conducted using a Shimadzu GC-MS-QP2020 NX instrument. Helium was used as the carrier gas (Table 1). Identification of compounds was performed by comparing acquired mass spectra with entries from the NIST 11 database [13].

Antimicrobial activity assessment

The antimicrobial effects of the extracts were evaluated using the agar well diffusion method. In this approach, each botanical extract was introduced into agar wells inoculated with *Streptococcus mutans*, *Klebsiella pneumoniae*, and *Candida albicans*. After 24 h of incubation at 37°C, the inhibition zones were measured to assess microbial suppression [1,31,34].

Evaluation of antioxidant capacity

To assess the antioxidant capabilities, the 2,2-diphenyl-1-picrylhydrazyl radical scavenging method was utilized. The degree of radical inhibition was quantified by observing the absorbance reduction at 517 nm. This decrease is indicative of the extract's potential to neutralize free radicals and oxidative stress [11,33].

Anti-inflammatory assay

The anti-inflammatory properties were analyzed through the inhibition of protein denaturation in egg albumin. Diclofenac sodium served as the standard for comparison. The results reflected the ability of the plant extracts to stabilize proteins under heat-induced stress conditions, simulating an anti-inflammatory response (Fig. 1) [4,24,26,31,33].

Phytochemical relevance and cosmetic potential mapping

Following bioassay results, identified compounds were evaluated for potential skincare applications through a review of current literature and database analysis. Attention was focused on phytochemicals exhibiting dual action, primarily antioxidant and anti-inflammatory. These findings were mapped to appropriate product types such as sunscreens, acne treatments, and serums (Fig. 2 and Table 2) [16,32].

Statistical analysis

All experimental assays were performed in triplicate. Data were expressed as mean±standard deviation (SD). Statistical significance between samples was analyzed using one-way analysis of variance. A ($p<0.05$) was considered statistically significant. Analysis was performed using GraphPad Prism 9.0.

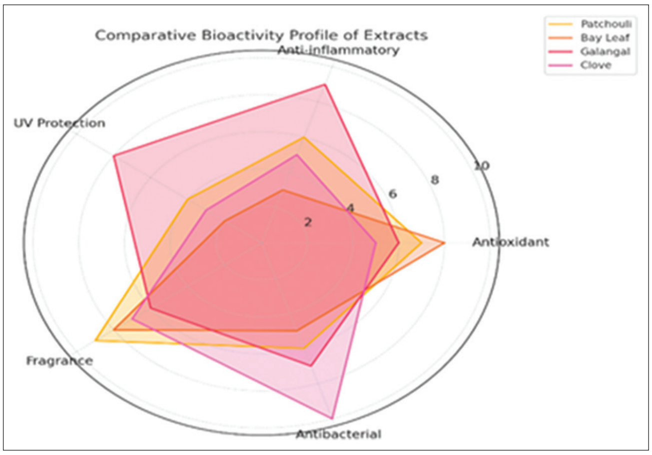

Fig. 1: Bioactivity radar plot comparing the four botanical extracts across five functional categories of cosmetic interest: antioxidant potential, anti-inflammatory response, ultraviolet protective effect, fragrance profile, and antibacterial properties. Each metric was assigned a value on a uniform 0–10 scale, integrating experimental data with published findings

RESULTS

Patchouli (*P. cablin*)

GC-MS profiling of the Patchouli extract identified azulene as a prominent constituent (Fig. 3). Recognized for its distinctive deep-blue color and calming effects, this compound is typically associated with anti-inflammatory applications in skincare. Another compound, spathulenol, was also detected; it is known for its potential to soothe the skin and reduce allergic reactions, indicating dermatological relevance.

Bay leaf (*C. tamala*)

Analysis of bay leaf extract revealed the presence of elemicin, a rare phenylpropanoid with antioxidant activity. This was complemented by the detection of methyl eugenol, a compound valued both for its

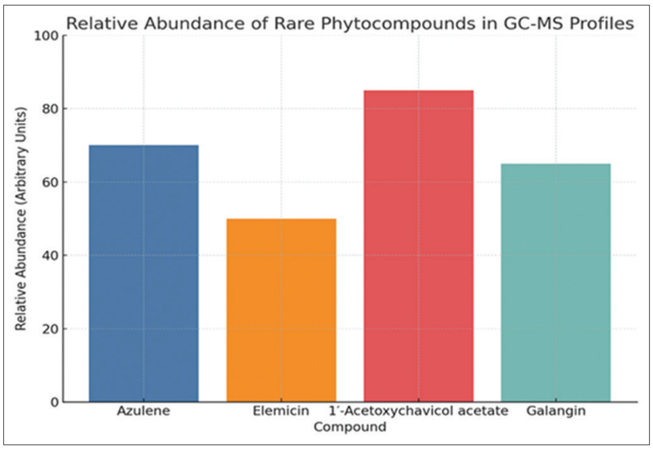

Fig. 2: Comparative peak area analysis of select rare compounds detected in the gas chromatography–mass spectrometry profiles of patchouli, bay leaf, galangal, and clove extracts. Notable molecules such as azulene, elemicin, 1′-acetoxychavicol acetate, and galangin were dominant in their respective plants, highlighting their uniqueness and relevance for innovative cosmetic applications

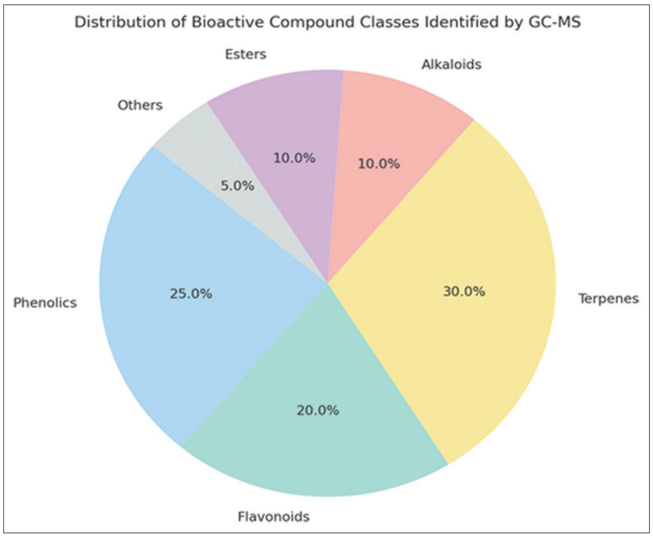

Fig. 3: Distribution of phytochemical classes identified by gas chromatography–mass spectrometry in ethanol extracts of Clove, Patchouli, Bay Leaf, and Galangal. Terpenes and phenolic compounds were the most prominent chemical groups detected. Flavonoids, esters, and alkaloids appeared in smaller quantities, while infrequent constituents were grouped under the category "Others" to account for low-abundance compounds with potential bioactivity

Table 1: Summary of rare compounds and their cosmetic functions

Compound	Plant source	Skincare function	Additional notes
Azulene	Patchouli	Soothes skin, reduces inflammation	Commonly incorporated in high-end soothing products
Elemicin	Bay Leaf	Antioxidant activity, aromatic properties	Not widely adopted; requires further safety profiling
1′-Acetoxychavicol acetate	Galangal	Potent anti-inflammatory agent	Shows promise in acne treatment formulations
Galangin	Galangal	UV shielding and antioxidant support	Belongs to flavonoids; ideal for anti-aging solutions
Caryophyllene oxide	Clove	Anti-inflammatory and enhances skin absorption	Functions as a fragrance stabilizer as well

These distinctive plant-derived actives present valuable opportunities for formulating effective, clean-label, and multifunctional skincare products. UV: Ultraviolet

Table 2: Functional overview of selected rare phytocompounds for skincare applications

Compound	Plant origin	Key bioactivity	Proposed skincare application
Azulene	Patchouli	Reduces inflammation, provides antioxidant defense	Ideal for calming serums and products for sensitive skin
Elemicin	Bay Leaf	Exhibits mild antioxidant action, aromatic traits	Suitable for botanical fragrances and pre-serum treatments
Acetoxychavicol acetate	Galangal	Anti-inflammatory and antimicrobial effects	Recommended for acne-care gels and soothing balms
Galangin	Galangal	Offers UV shielding and oxidative stress reduction	Applicable in anti-aging creams and sun-protective bleaches

Table 3: Bioassay results with statistical values

Bioassay type	Plant extract	Test organism/method	Result (mean±SD)	Significance (P-value)
Antioxidant activity (IC_{50})	*Cinnamomum tamala* (Bay leaf)	DPPH Radical Scavenging	43.2±1.8 μg/mL	<0.05
Anti-inflammatory activity (%)	*Alpinia galanga* (Galangal)	Protein denaturation assay	74.6±2.1%	<0.05
Antibacterial Activity (zone of inhibition)	*Pogostemon cablin* (Patchouli)	*Streptococcus mutans*	22.3±0.7 mm	<0.05
Antibacterial activity (zone of inhibition)	*Syzygium aromaticum* (Clove)	*Klebsiella pneumoniae*	19.8±1.2 mm	<0.05

SD: Standard deviation

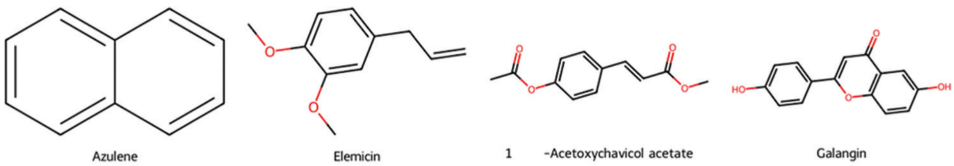

Fig. 4: Molecular structures of bioactive compounds identified through gas chromatography–mass spectrometry: azulene (Patchouli), elemicin (Bay Leaf), 1′-acetoxychavicol acetate, and galangin (Galangal). These phytochemicals were selected for their multifunctional benefits in skin health, particularly antioxidant defense, anti-inflammation, and photoprotection

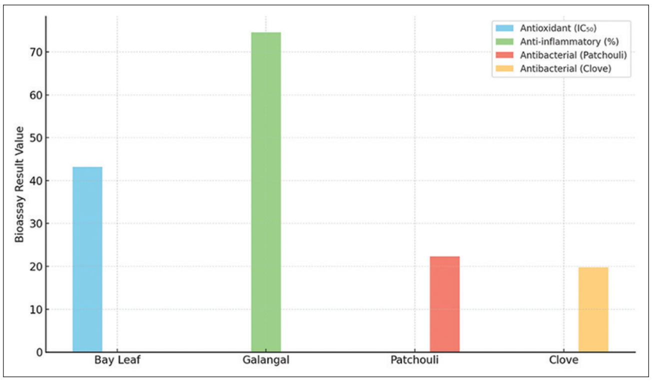

Fig. 5: Comparative bar chart showing bioassay results of the four botanical extracts. Results include antioxidant (IC50), anti-inflammatory (% inhibition), and antibacterial (zone of inhibition in mm). Bars represent mean±standard deviation from triplicate measurements. Statistically significant differences were observed across all tested extracts (p<0.05, one-way analysis of variance)

antimicrobial effectiveness and its contribution to the sensory profile of cosmetic products, enhancing their aromatic appeal.

Galangal (*A. galanga*)

The Galangal extract exhibited high levels of 1′-acetoxychavicol acetate, a compound associated with potent anti-inflammatory activity through modulation of biochemical pathways. In addition, the presence of galangin, a flavonoid with ultraviolet (UV)-protective and antioxidative properties, supports its inclusion in anti-aging and photoprotective skincare formulations.

Clove (*S. aromaticum*)

Caryophyllene oxide was found to be the dominant compound in the clove extract. Known for its broad functionality, this sesquiterpene oxide contributes to anti-inflammatory, antifungal, and skin-penetration-enhancing properties. It also plays a crucial role in stabilizing volatile components in fragrance formulations, making it valuable in product development (Fig. 4 and Table 3).

DISCUSSION

The discovery of distinctive phytochemicals through GC-MS analysis underscores the promising role of aromatic plants as emerging assets in

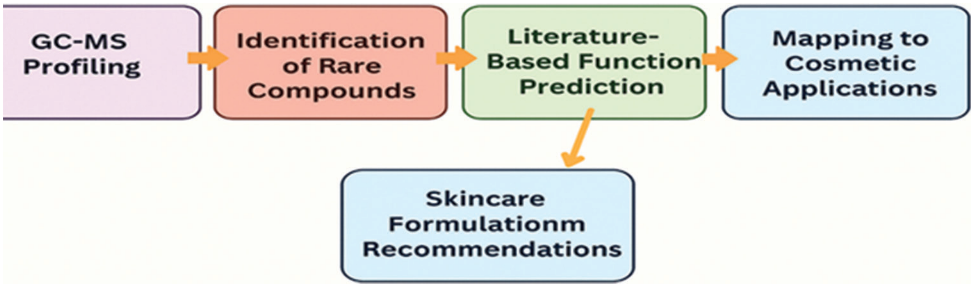

Fig. 6: Conceptual flowchart outlining the research workflow from gas chromatography–mass spectrometry-based identification of rare phytochemicals to biological validation and their potential integration into botanical skincare

cosmetic science. Among the standout compounds, 1′-acetoxychavicol acetate, found abundantly in *A. galanga*, exhibited significant anti-inflammatory potential. This activity is likely mediated through interference with cyclooxygenase and nitric oxide signalling pathways, reflecting trends consistent with in vitro experimental findings [2,4,16,33].

An unexpected yet notable outcome was the identification of azulene in *P. cablin*. Conventionally associated with *Matricaria Chamomilla*, azulene's anti-inflammatory and skin-calming effects are well documented. Its presence in Patchouli expands the phytochemical map of this plant and reinforces its potential application in formulations designed for sensitive or irritation-prone skin [7,12,21,34].

In the case of *C. tamala*, the identification of elemicin introduces new possibilities for its cosmetic utilization. As a phenylpropanoid with antioxidant attributes, elemicin contributes functional benefits. However, its chemical resemblance to myristicin suggests that thorough toxicological evaluations are necessary before broader commercial use [3,23,30,33]. Despite this, its fragrance and antioxidant traits position it well for inclusion in herbal and aromatic skincare lines [16,27,32].

Galangin, also detected in Galangal, displayed a dual role in supporting skin health through antioxidant defense and UV protection. This polyphenolic flavonoid shares structural similarities with well-known compounds used in anti-aging products, enhancing its utility in skin-repair and sun care formulations [6,22,24,25,26,27,32].

Collectively, these compounds demonstrate a synergistic set of bioactivities, including anti-inflammatory, antimicrobial, and photoprotective functions, that align well with the current demand for effective, plant-based, and clean-label skincare solutions. Their application could drive a new wave of science-backed, naturally derived cosmeceutical products that cater to both efficacy and consumer preference (Fig. 5) [10,19].

CONCLUSION

This study confirms the presence of distinctive, biologically active compounds in four commonly utilized aromatic plants-*P. cablin* (Patchouli), *C. tamala* (Bay Leaf), *A. galanga* (Galangal), and *S. aromaticum* (Clove). The detection of key phytochemicals such as azulene, 1′-acetoxychavicol acetate, and elemicin underscores their promising functionality in skincare, offering anti-inflammatory, antioxidant, antimicrobial, and UV-protective benefits.

The findings provide a scientific rationale for revisiting underexplored botanicals in the context of modern skincare formulation. Incorporating these compounds into clean-label, plant-based cosmeceuticals aligns with consumer demand for natural and multifunctional ingredients. Future research should focus on formulation stability, bioavailability, and clinical validation to support their integration into commercial skincare products (Fig. 6).

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AUTHOR'S CONTRIBUTION

Both authors contributed equally.

DATA AVAILABILITY STATEMENT

All data generated or analyzed during this study are included in this published article and its supplementary materials. Additional data can be obtained from the corresponding author upon reasonable request.

CONFLICTS OF INTEREST

The authors declare no conflict of interest. The study was conducted independently, without any financial or personal affiliations influencing the outcomes.

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