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Original Article

GC-MS Phytochemical Profiling of Kaidarya Siddha Narikela Taila: Mechanistic Insights into Khalitya (Non-Specific Hairfall) Management

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ABSTRACT

Background: Non-Specific Hairfall (NSHF), classified as *Khalitya* in *Ayurveda* (NAMC FA-3, ICD-11 TM2), has a significant global burden. *Kaidarya siddha Narikela Taila* (KNT) is a formulation prepared with *Narikela Taila* (*Cocos nucifera*) and *Kaidarya kashaya* (decoction of *Murraya koenigii*), widely utilised in the management of *Khalitya*. **Aim and Objectives:** To identify and analyse the phytochemical profile of *Kaidarya siddha Narikela Taila* (KNT) by Gas Chromatography-Mass Spectrometry (GC-MS) and correlate it to relevant pathways in NSHF pathophysiology. **Materials and Methods:** KNT was prepared as per Ayurvedic Pharmacopoeia Standards at GMP-certified KLE Ayurveda Pharmacy, Belagavi. GC-MS analysis was done using Shimadzu QP2020 (hexane extract, 1 µL injection, helium carrier 1.0 mL/min, oven: 70-280ºC) at Kerala Forest Research Institute (KFRI), Kerala, India, with compound identification against the NIST20 spectral library. The mapping of bioactivity was based on indexed scientific literature. **Results:** 27 compounds were detected, with dominance of Dodecanoic acid (Lauric acid, 19.33%), Rac-glycerol-1,3-dilaurate (15.21%), 1-Hydroxy-3-(octanoyloxy)propan-2-yl decanoate (combined isomers, 21.71%), 1-Decanoyl-3-dodecanoylglycerol (combined isomers, 13.03%), and 2-(Decanoyloxy) propane-1,3-diyl dioctanoate (9.65%). 12 distinct pharmacological activities, directly relevant to hair fall, were identified, spanning from antioxidant, anti-inflammatory, anti-microbial, anti-androgenic, hair follicle protection and promotion and scalp penetration enhancement. **Conclusion:** GC-MS analysis reveals potential mechanisms of KNT in *Khalitya* and suggests mechanistic hypotheses that need further experimental validation for therapeutic applications.

Keywords: Alopecia, GC-MS, *kaidarya*, *Narikela taila*, Phytochemical Profiling.

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INTRODUCTION

Hair loss, or Alopecia, is one of the concerning dermatological conditions, affecting up to 50% of men and 40-50% women by age 50 (Iyengar and Li, 2025). A particular subset called Non-Specific Hairfall (NSHF) that is characterised by diffuse hair loss has a multifactorial aetiology that includes nutritional deficiency, hormone imbalances, lifestyle factors and stress (Walter, 2022). At the root of NSHF lies a complex pathophysiology of androgenic dysregulation influenced by the activity of 5 α- reductase, oxidative stress at the level of follicles, disruption in the signalling axes of the anagen phase, imbalance in the scalp microbiome and long-standing perifollicular inflammation (Chen *et al*., 2025; Du *et al*., 2024; Ho *et al*., 2024; Owecka *et al*., 2024). It results in hair loss, which has a profound effect on the psyche, personality of an individual and their social interactions, leading to diminished quality of life (Aukerman and Jafferany, 2023). NSHF clinically presents as telogen effluvium in the majority of cases, followed by female pattern hair loss and alopecia areata, with underlying Androgenetic Alopecia (AGA) affecting 70% of men and 40% of women (Monil *et al*., 2023). A study into the prevalence in India showed that AGA was seen in 58% of males aged 30-50 years (Krupa *et al*., 2009), and 85.5% of females were diagnosed as cases of telogen effluvium (Karakoyun *et al*., 2025).

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Currently available pharmacological interventions, particularly topical minoxidil and oral finasteride, have shown encouraging results in specific androgenetic presentations, but are riddled with undesirable adverse effects such as loss of libido, impotence, gynecomastia, regrowth dependency, hypotension, mood and cognitive disturbances, among others, limiting their use (Mysore, 2012; Suchonwanit *et al*., 2019).

Loss of hair is described in detail as *Kesha patana* under *Khalitya* (NAMC FA-3, ICD-11 TM2-SN71) in Ayurvedic literature. NAMC FA-3 describes *Khalitya* as a disorder characterised by the falling of scalp hair, due to the aggravated *vata* and *pitta* affecting the hair roots, followed by closure of the hair root. Oils processed with herbs are well known to maintain hair health and prevent hair fall. More than a thousand plant species with anti-oxidant, anti-inflammatory, neuroprotective, adaptogenic, and immunomodulatory effects have been explored for potential benefits in hair health. One such herb is *Murraya koenigii*, which is a source of several bioactive compounds, possesses alkaloids, flavonoids, and volatile phenolics that exhibit immunomodulatory, anti-oxidant, anti-microbial, anti-carcinogenic and anti-angiogenic properties. *M. koenigii* and its derivatives are proven to mitigate oxidative stress, neurotoxicity, neuroinflammation and cognitive dysfunction (Balakrishnan *et al*., 2020; Bhupatiraju *et al*., 2023; Mani *et al*., 2012). Medicated oils serve as lipid vehicles to deliver bioactive constituents. Controlled heating ensures enhancement of bioactive principles and improves bioavailability, which has been proven by *Taila Paka Vidhi* (Lahorkar *et al*., 2009; Singh and Chaudhary, 2011).

Kaidarya Siddha Narikela Taila (KNT) is a synergistic combination of the pharmacologically rich *M. koenigii* processed in *Narikela Taila* (Bangre *et al*., 2022), a saturated Medium-Chain Fatty Acid (MCFA)-rich lipid base with well-established anti-microbial and hair conditioning properties (Wang *et al*., 2015).

Gas Chromatography-Mass Spectrometry (GC-MS) is the standard technique for accurate analysis and quantification of lipophilic semivolatile and volatile phytochemicals. It provides a scientific evaluation of individual compounds by precise spectral evaluation and retention time-based separation (Lytovchenko *et al*., 2009; Ferretti *et al*., 2025). Although used widely, and studies showing its therapeutic efficacy exist, there is no published literature on the GC MS characterisation of *Kaidarya Siddha Narikela Taila*. The present investigation aims to document the GC-MS phytochemical profile of KNT and systematically correlate the identified bioactive compounds with established molecular mechanisms in the pathophysiology of NSHF, thereby providing preliminary mechanistic data mapping the therapeutic delivery context of a topically applied medicated oil.

MATERIALS AND METHODS

Preparation and Physicochemical Characterisation

The *Kaidarya Siddha Narikela Taila* was prepared at GMP-certified KLE Ayurveda Pharmacy, Belagavi, in accordance with the standards of the Ayurvedic pharmacopoeia of India. The ingredients and quantity used are listed in Table 1. The prepared KNT was subjected to standard physicochemical characterisation, including organoleptic evaluation, loss on drying, saponification value, iodine value, refractive index, specific gravity, acid value and rancidity as per API guidelines, with results listed in Table 2. The GC-MS analysis was carried out at the Centre for Analytical Instrumentation-Kerala (CAI-K), Kerala Forest Research Institute (KFRI) at Peechi, Thrissur, Kerala.

GC-MS Analysis

Sample preparation

KNT was extracted with HPLC-grade hexane (1:10, v/v), centrifuged and the clear supernatant after filtration through a 0.45 μM PTFE membrane syringe filter was used for GCMS injection.

Instrumental parameters

Analysis of KNT was done on a Shimadzu GCMS-QP2020 NX system, attached with an AOC-20i autosampler, a highly coveted instrument for accurate qualitative and quantitative analysis owing to high sensitivity and analytical reliability of identified bioactive compounds. The GC capillary column was filled with a carrier gas, helium, at a flow rate of 1.00 mL/min (linear velocity-36.7 cm/sec). The injection temperature was 280°C, split mode with a split ratio of 20:1 and injection volume 1.0 μL. The temperature in the column was programmed as follows: 70°C initially (hold 0 min), increased at 8°C/min to 260°C, then 4°C/min to 280°C (hold 5 min). The temperature of the ion source and interface was 220°C and 280°C, respectively. The detection by the mass spectrometer was in full scan mode (m/z 50-500) with an event time of 0.30 sec.

Compound Identification

The compounds were identified based on (i) retention time, (ii) molecular ion peak and fragmentation pattern, and (iii) comparison with NIST20 reference library. The similarity index of ≥70% was accepted, in line with standard guidelines. The relative abundance of every compound was calculated as a percentage area under the curve with respect to the Total Ion Chromatogram (TIC) area.

The present study represents a single-run GC-MS profiling exercise intended to identify the phytochemical constituents of KNT. Replicate analysis and validated quantitative methods are recommended for confirmation of individual compound concentrations in future studies.

Bioactivity mapping

A targeted literature review was conducted across PubMed, Scopus, and Web of Science, utilising IUPAC or common name with terms including 'hair', 'alopecia', 'antioxidant', 'anti-inflammatory', 'anti-microbial', 'hair follicle', and 'scalp'. Inclusion criteria: Indexed peer-reviewed publications reporting *in vitro, in vivo*, or clinical evidence of pharmacological activity of identified compound or a structural analogue. Exclusion criteria: non-indexed sources, review articles cited as sole primary evidence.

Ethical Statement

Ethical approval was not required for the present study as there was no involvement of human or animal subjects.

Statistical Analysis

No formal statistical analysis was performed. The study was conducted as a single-run GC-MS profiling exercise, and area percentages reported represent semi-quantitative relative abundance values from the total ion chromatogram, not absolute quantification. Future studies should include replicate injections (minimum n=3) to report mean±SD of relative peak areas, and validated quantitative GC-MS methods for individual compounds of pharmacological interest.

RESULTS

Physicochemical Parameters of KNT

KNT is a dull, greenish-yellow oil with a pleasant odour. The specific gravity and refractive index are within normal limits. The saponification value of 203.341 confirms the predominance of medium-chain fatty acid glycerides. An iodine value of 55.613 points to a low degree of unsaturation, whereas the low acid value of 2.794 mg KOH/g and a negative Kries test indicate lipid stability and absence of rancidity, which in turn validate the quality of KNT.

GC-MS Chromatographic Profile

A total of 27 chromatographic peaks were obtained across a Total Ion Chromatogram (TIC) with retention times spanning from 5.764 to 35.672 min (Figure 1). Every peak was successfully matched against the NIST 20 spectral library with similarity indices ranging from 72 to 97. The identified compounds, with peak areas, area percentages, molecular formula, compound class, and bioactivity, are shown in Table 3.

DISCUSSION

The present study is a phytochemical profiling investigation. It characterises the compositional landscape of KNT and maps identified compounds to pharmacological mechanisms reported in indexed literature. The pharmacological activities described herein are literature derived attributes of individual compounds or structurally analogous molecules. They are not experimentally validated in the context of KNT as a formulation. The discussion provides a mechanistic rationale for future experimental investigation and is driven towards hypothesis- generation.

Kaidarya Siddha Narikela Taila is a medicated oleaginous formulation that has been prepared for the management of *Khalitya* in accordance with the *Taila Paka Vidhi* explained in *Sharangadhara Samhita*. It consists of *Kaidarya Kashaya* (decoction of *M. koenigii*) processed with *Narikela Taila* (coconut oil). *Khalitya* (hairfall) is a precipitation of vitiated p*itta*, with involvement of *vata, kapha* and *rakta* in the *keshabhumi* (scalp), making *abhyanga* especially relevant in its management.

A traditionally relevant drug, *Kaidarya* (*Murraya koenigii*) with its *katu* (pungent), *tikta* (bitter), *kashaya* (astringent) *rasa, laghu* (light), *sheeta* (cold) *guna* (property), *sheeta* (cold) *virya* (potency), *katu* (pungent) *vipaka* (biotransformation), along with *keshya* (beneficial for hair), *rasayana* (rejuvenating), *vishahara* (anti-toxic) and *krimihara* (anti-microbial) actions, supports the scalp environment and antioxidant, anti-inflammatory and anti-microbial activity of *M. koenigii* makes it ideal for utilisation in hairfall (Abeysinghe *et al*., 2021; Javagal *et al*., 2021). *Narikela Taila* is inherently soothing and nourishing. It helps to reduce dryness, provides lubrication and scalp comfort and also has demonstrated improvement in hair fibre properties and porosity (Kaushik *et al*., 2022). The processing of *Kaidarya Kashaya* in *Narikela Taila* potentiates the medicinal action, enhances bioavailability, and gives an effective ayurvedic preparation that acts on scalp balance and hairfall. In addition, this study aims to put forth an evidence-based mode of action of *Kaidarya Siddha Narikela Taila* in the management of *Khalitya* and related disorders.

The GC-MS Analysis of *Kaidarya Siddha Narikela Taila* yielded 27 compounds in total, listed in Table 3. The compositional groups identified showed a complex phytochemical profile with the presence of Medium-Chain Fatty Acids (MCFAs) and their esters, glyceride esters, phenolic compounds, terpenoids, lactones and pyranones. The diverse portfolio of the compounds and their reported pharmacological actions of anti-oxidant, anti-inflammatory, anti-microbial, emollient, hair follicle protecting and hair growth promoting activities emphasises the pharmacological value of the sample. The bioactivity profile summary is listed in Table 4.

Medium-chain fatty acids

The phytochemical profile of KNT shows a striking quantitative dominance of medium-chain fatty acids, namely dodecanoic acid (Lauric acid) at 19.33%, along with n-decanoic acid (Capric acid) at 2.22% and Octanoic acid (Caprylic acid) at 2.97%. This MCFA triad represents a pharmacologically relevant cluster whose constituents have been reported to address multiple axes of NSHF pathophysiology (Khoramnia *et al*., 2013). Lauric acid, a low molecular weight straight-chain fatty acid, has been reported to have high affinity for hair proteins, enabling deep penetration into the hair cortex and reducing protein loss from the shaft (Rele and Mohile, 2003).

Lauric acid has been reported to modulate the hair follicle *in vitro*, with evidence of anagen prolongation and catagen suppression (Gu *et al*., 2022). It's presence in KNT suggests a potential contribution to follicular cycle regulation. It also has been reported to inhibit the growth of *Malassezia furfur*, which is implicated in seborrheic dermatitis-associated hairfall. It has also demonstrated antimicrobial activity against *Staphylococcus aureus* and gram-positive scalp pathogens in experimental models, with proposed mechanisms including phospholipid bilayer disruption and inhibition of bacterial signal transduction, suggesting potential relevance to folliculitis and perifollicular inflammation (Douglas *et al*., 2025; Qingyan *et al*., 2024; Rouse *et al*., 2005).

n-Decanoic acid (Capric acid) augments the anti-microbial activity of lauric acid by its anti-bacterial and anti-fungal activity (Akula *et al*., 2021). Capric acid has been reported to exhibit anti-inflammatory activity via negative modulation of the NLRP3 inflammasome pathway. This mechanism, if operative in the scalp microenvironment, may help limit hair follicle damage driven by inflammation and pyroptosis (Liu *et al*., 2022; Wang *et al*., 2022). It has been reported as a mitochondrial antioxidant that may mitigate ROS production; this neuroprotective activity suggests a possible role in supporting follicular cycle regulation, warranting experimental confirmation in a follicular model (Aanaimuthu *et al*., 2025).

Octanoic acid (Caprylic acid) has demonstrated antifungal, (Akula *et al*., 2021) anti-inflammatory, and neuroprotective activities in experimental models. It has been reported to suppress nitric oxide production and may contribute to maintaining perifollicular innervation, (Aanaimuthu *et al*., 2025; Nukaga *et al*., 2024), though this requires validation in a scalp-specific context.

Tetradecanoic acid (Myristic acid) has been reported to exhibit anti-biofilm activity against *Staphylococcus* species, with suggested relevance to follicular microenvironments (Kim *et al*., 2022; Yuyama *et al*., 2020).

Glyceride Esters

Glyceride esters (mono-, di- and triglycerides of MCFAs) constitute the dominant fraction by combined area percentage (54.39%) and are the phytochemicals with the quantitatively largest component class in KNT. It includes: Rac-glycerol-1,3-dilaurate (15.21%), 2 positional isomers of 1-Hydroxy-3-(octanoyloxy)propan-2-yl decanoate (8.13% and 13.58% respectively), 1-Decanoyl-3-dodecanoylglycerol (2.53% and 10.50%), 2-(Decanoyloxy)propane-1,3-diyl dioctanoate (9.65%), Glyceryl dilaurate (0.79%) and Trilaurin (2.48%). These compounds are likely products of transesterification and partial glycerolysis during the *Taila Paka* process, and may contribute pharmacological activity beyond serving as simple lipid carriers (Ginsburg *et al*., 2024).

The predominant pharmacological actions exhibited are transfollicular penetration enhancement, occlusive moisturisation and anti-microbial activity. Structurally analogous glyceride esters have been reported to act as penetration enhancers by interpolating into the stratum corneum and increasing lipid bilayer fluidity, potentially facilitating deeper follicular drug delivery; direct evidence for KNT glycerides in this role warrants experimental confirmation. Structurally analogous glyceride esters have demonstrated scalp penetration-enhancing activity to the dermal papilla and bulge region in experimental models, suggesting a possible role in supporting follicular stem cell access to bioactive constituents. This scalp penetration-enhancing activity is vital for the expression of antioxidant, anti-inflammatory, anti-androgenic, and hair growth promotion activities of compounds at the level of the target tissue (Haque and Talukder, 2018; Hosmer *et al*., 2009; Ibrahim and Li, 2009; Schafer *et al*., 2023). This glyceride fraction potentiates the pharmacological actions of the entire formulation, which can be correlated to the ayurvedic postulate that *sukshma, snigdha guna* of *taila* enables deep tissue penetration.

These glyceride esters are proposed to provide occlusive moisturisation by creating a semi-occlusive lipid film, which reduces the transepidermal water loss from the scalp surface (Kundu *et al*., 2026). They may help address scalp barrier dysfunction associated with xerosis and a proinflammatory scalp microenvironment, both of which have been implicated in NSHF (Mughni *et al*., 2025). In addition, glyceryl dilaurate, which closely resembles mono and diglycerides derived from lauric acid, exhibits anti-acne activity, which has relevance in comedo-associated hair follicle obstruction. This glyceride class shows broad-spectrum antimicrobial activity. Rac-glycerol-1,3-dilaurate and related dilaurate diglycerides may amplify total antimicrobial potency and are proposed to act as sustained-release reservoirs for Lauric acid, potentially maintaining active concentrations at

Table 1: Ingredients of *Kaidarya Siddha Narikela Taila*.

Sl. No.	Ingredient	Drug	Latin Name	Part Used	Proportion
1.	*Sneha Dravya* (Oil base)	*Narikela Taila*	*Cocos nucifera*	Oil	1 Part
2.	*Drava Dravya* (Kashaya-Decoction)	*Kaidarya Kashaya*	*Murraya koenigii*	Leaves	4 Parts

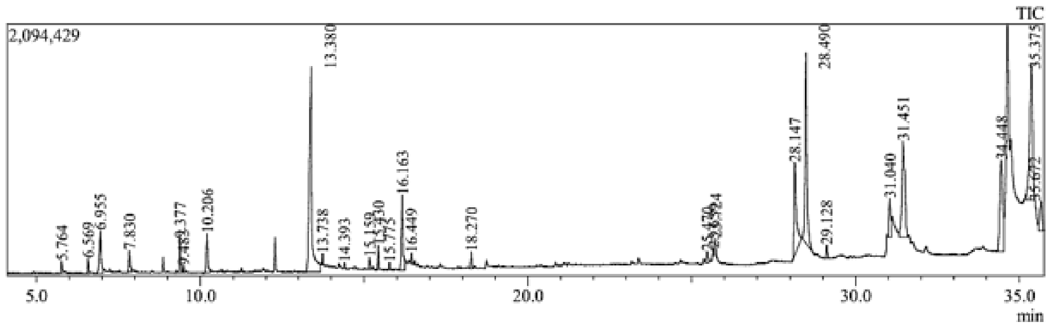


Figure 1: The Chromatogram of GC-MS Analysis of KNT. The oil was extracted with HPLC-grade hexane (1:10, v/v) and analysed on a Shimadzu GCMS-QP2020 NX system using a helium carrier gas (1.00 mL/min), with a split injection (20:1; 1.0 µL; 280ºC), and programmed column temperature ramp from 70ºC to 280ºC. Detection was in full scan mode (m/z 50-500). Compounds were identified by retention time, fragmentation pattern, and NIST20 library matching (similarity index ≥70%); relative abundance expressed as percentage TIC area.

Table 2: Organoleptic and Physico-Chemical Parameters of *Kaidarya Siddha Narikela Taila* Documented.

Parameters	Characters
Description	Dull, Greenish Yellow Colour, Pleasant Odour, Oily to Touch
Loss on drying at 110ºC	0.425%
Saponification value	203.341
Iodine value	55.613
Refractive index	1.463
Specific gravity	0.913
Acid value	2.794 mg/KOH
Rancidity	Negative

the follicular level after application; this pharmacokinetic role warrants direct experimental investigation (Yoon *et al*., 2018). This can be understood as the sustained effect of regular *taila* application, which promotes scalp health.

2 phenolic compounds- 4-Vinylphenol and 2-Methoxy-4-vinylphenol, derived from the thermal decarboxylation of p-coumaric acid and ferulic acid, respectively, represent the phytochemical signature of *M. koenigii* in the formulation. 2-Methoxy-4-vinylphenol has been reported to exhibit antioxidant activity through free radical scavenging, anti-inflammatory activity via COX-2 inhibition and NF-κB pathway suppression (Jeong *et al*., 2011), antiproliferative activity, and broad-spectrum antimicrobial activity in experimental models. The presence of antioxidant phenolics in KNT suggests a potential capacity to counteract accumulated ROS at the follicular level. Oxidative stress has been associated with premature catagen entry and telogen effluvium, making this a pharmacologically relevant hypothesis warranting *in vitro* validation in the spectrum of NSHF (Aroor *et al*., 2023; Parithy *et al*., 2021). 4-Vinylphenol has been reported to exhibit anti-angiogenic activity via PI3K/AKT targeting (Yue *et al*., 2015). This may be of relevance in inflammatory NSHF presentations characterised by pathological angiogenesis, though its effect in the scalp microenvironment remains to be directly investigated.

Squalene, a physiological precursor to sterol biosynthesis, is a linear triterpene that has immense therapeutic importance in the spectrum of trichology. As a constituent of human sebum, squalene has been reported to support dermal papilla cell viability under oxidative stress conditions, suggesting a potential protective role at the hair follicle level (Lin *et al*., 2013). Squalene is reported as one of the most potent singlet oxygen quenchers (Kohno *et al*., 1995; Yao *et al*., 2024) and may help prevent lipid peroxidation. This suggests a potential role in counteracting the oxidative follicular damage implicated in NSHF (Du *et al*., 2023; Özdemir *et al*., 2026).

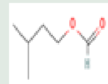
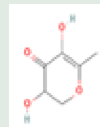
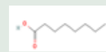
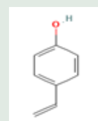
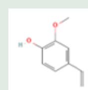
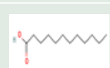
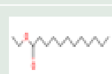
1,1,4,7-Tetramethyldecahydro-1H-cyclopropa(e)azulene-4,7-diol is a sesquiterpene that has been associated with a dual profile of anti-inflammatory and anti-androgenic activity, in structurally related analogues, raising the hypothesis of DHT-pathway modulation. By this dual nature, it can address both androgenic and inflammatory axes of NSHF simultaneously (Brooks *et al*., 1986; Ma *et al*., 2023), making an *in vitro* 5α-reductase inhibitory assay indispensable to understand its contribution to androgenic modulation.

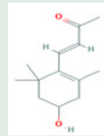
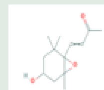
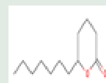
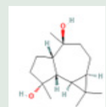
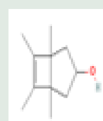
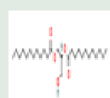
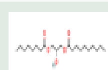
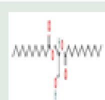
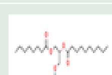
4-Hydroxy-β-ionone, a lipid-soluble, degraded carotene from the leaf of *M. koenigii*, has been reported to show antioxidant activity, it may help protect sebaceous scalp lipids from peroxidative degradation, potentially attenuating the downstream inflammatory cascade, a hypothesis that requires experimental confirmation (Jourdain *et al*., 2023; Kang *et al*., 2013). The antiproliferative activity (Luetragoon *et al*., 2020) of the β-scaffold may contribute to its anti-inflammatory activity.

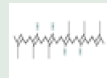
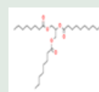
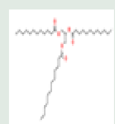
endo-1,5,6,7-Tetramethylbicyclo[3.2.0]hept-6-en-3-ol, a rigid, bicyclic monterpenoid alcohol from *M. koenigii*, is a metabolically stable compound with antioxidant and antibacterial activities.

DDMP (4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-) is a unique compound with significant documented evidence in hair growth-promoting activity. It is produced during the

Table 3: Details of Compounds detected in GCMS analysis with their Retention Time and their Activity.

Sl. No.	Name of the compound	Retention time	Area	Area%	Height	Height%	A/H	Structure	Chemical Formula	Compound Class	Activity of Compound
1.	1-Butanol, 3-methyl-, formate	5.764	233448	0.50	96156	0.92	2.43		$C_6H_{12}O_2$	Formate ester	Anti-bacterial (Sánchez-Hernández *et al.*, 2023), Anti-fungal (Shehata *et al.*, 2024)
2.	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	6.569	266100	0.57	122418	1.17	2.17		$C_6H_8O_4$	Hydroxypyranone	Antioxidant (Chen *et al.*, 2021), Hair-promoting activity (Jang *et al.*, 2022)
3.	Octanoic acid (Caprylic acid)	6.955	1393255	2.97	357055	3.42	3.90		$C_8H_{16}O_2$	Carboxylic acid (MCFA)	Antifungal (Aso *et al.*, 2021), Antibacterial (Hsu *et al.*, 2026; Lin *et al.*, 2023), Anti-inflammatory(Tang *et al.*, 2025), Neuroprotective (Altinoz *et al.*, 2020)
4.	4-Vinylphenol	7.830	498146	1.06	177601	1.70	2.80		C_8H_8O	Vinyl phenol	Anti-angiogenic (Yue *et al.*, 2015)
5.	2-Methoxy-4-vinylphenol	9.377	592673	1.26	280299	2.69	2.11		$C_9H_{10}O_2$	Methoxyphenol	Anti-inflammatory (Asami *et al.*, 2023), Anti-proliferative (Jeong and Jeong, 2010), Anti-oxidant (Shin *et al.*, 2019), Anti-microbial (Pintado *et al.*, 2024)
6.	Ethyl 2-(5-methyl-5-v inyltetrahydrofuran-2-yl) propan-2-yl carbonate	9.483	104174	0.22	54239	0.52	1.92		$C_{13}H_{22}O_4$	Cyclic ether ester	Unreported bioactivity
7.	n-Decanoic acid (Capric acid)	10.206	1041334	2.22	326411	3.13	3.19		$C_{10}H_{20}O_2$	Medium-chain saturated fatty acid (MCFA)	Anti-microbial (anti-bacterial(W. C. Huang *et al.*, 2014), anti-fungal(Bhattacharyya *et al.*, 2020), Anti-inflammatory(Huang *et al.*, 2014), Anti-oxidant(Mett and Müller, 2021), Neuroprotective(Sanguanphun *et al.*, 2022), Anti-cancer(Altinoz *et al.*, 2020)
8.	Dodecanoic acid (Lauric acid)	13.380	9069040	19.33	1706462	16.35	5.31		$C_{12}H_{24}O_2$	Medium-chain saturated fatty acid (MCFA)	Anti-microbial (Borrelli *et al.*, 2021; M *et al.*, 2024), Anti-inflammatory (Moore *et al.*, 2020), Anti-cancer (M *et al.*, 2024), Anti-hairfall (Z. Huang *et al.*, 2025), Anti-tumorigenic (Roopashree *et al.*, 2021), Anti-oxidant (M *et al.*, 2024)
9.	Dodecanoic acid, ethyl ester (Ethyl laurate)	13.738	157878	0.34	91065	0.87	1.73		$C_{14}H_{28}O_2$	Medium-chain fatty acid ethyl ester	Anti-microbial (Laqui-Estaña *et al.*, 2024; Nigussie *et al.*, 2021)

Sl. No.	Name of the compound	Retention time	Area	Area%	Height	Height%	A/H	Structure	Chemical Formula	Compound Class	Activity of Compound
10.	4-Hydroxy-.beta.-ionone	14.393	104444	0.22	49040	0.47	2.13		$C_{13}H_{20}O_2$	Ionone derivative	Parent β-ionone shows Anti-oxidant, Anti-inflammatory (Aloum *et al.*, 2020), Anti cancer/ Anti-proliferative (Aloum *et al.*, 2020; Ansari and Emami, 2016)
11.	3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxa bicyclo[4.1.0]hept-1-yl)	15.159	231759	0.49	100155	0.96	2.31		$C_{13}H_{20}O_3$	Monoterpene epoxide	Anti-microbial (Tabe *et al.*, 2026)
12.	.delta.-Dodecalactone	15.430	370626	0.79	197295	1.89	1.88		$C_{12}H_{22}O_2$	δ-Lactone	Anti-fungal, Anti-bacterial (Yang *et al.*, 2011)
13.	1,1,4,7-Tetram ethyldecahydro-1H-cyclo propa[e]azulene-4,7-diol	15.775	114191	0.24	57983	0.56	1.97		$C_{15}H_{26}O_2$	Sesquiterpene diol	Anti-inflammatory, anti-androgenic potential.
14.	Tetradecanoic acid (Myristic acid)	16.163	2034064	4.33	620633	5.95	3.28		$C_{14}H_{28}O_2$	Long-chain fatty acid	Anti-microbial (Juárez-Rodríguez *et al.*, 2021)
15.	endo-1,5,6, 7-Tetramethylbicyclo[3.2.0] hept-6-en-3-ol	16.449	193636	0.41	85050	0.82	2.28		$C_{11}H_{18}O$	Bicyclic monoterpenoid	Anti-oxidant (Ait benlabchir *et al.*, 2024), Anti-bacterial (Chebbac *et al.*, 2023)
16.	2H-Pyran-2-one, tetrahydro-6-nonyl- (delta-tetradecalactone)	18.270	265613	0.57	136268	1.31	1.95		$C_{14}H_{26}O_2$	δ-Lactone	Anti-microbial (Sato *et al.*, 2024)
17.	Dodecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	25.470	322302	0.69	90162	0.86	3.57		$C_{27}H_{52}O_5$	Diglyceride	Emollient(Hosmer *et al.*, 2009)
18.	Decanoic acid, 2-hydroxy-3-[(1-oxooctyl)oxy]propyl ester	25.659	108411	0.23	55251	0.53	1.96		$C_{21}H_{40}O_5$	Mixed medium-chain triglyceride (MCT)	Emollient, Penetration enhancer(88-91(Haque and Talukder, 2018; Hosmer *et al.*, 2009; Ibrahim and Li, 2009; Schafer *et al.*, 2023)
19.	Glyceryl dilaurate	25.724	370434	0.79	142310	1.36	2.60		$C_{27}H_{52}O_5$	Diglyceride	Anti-microbial (M *et al.*, 2024), Anti-acne (W. C. Huang *et al.*, 2014), Skin penetration enhancer (Roopashree *et al.*, 2021), occlusive moisturiser (Moore *et al.*, 2020)
20.	1-Hydroxy-3-(octanoyloxy) propan-2-yl decanoate	28.147	3816812	8.13	769016	7.37	4.96		$C_{21}H_{40}O_5$	Monoglyceride	Broad spectrum anti-microbial (Hyldgaard *et al.*, 2012; Thormar *et al.*, 2006; Yoon *et al.*, 2018), Skin/Scalp penetration enhancer, Emollient (Thormar *et al.*, 2006)
21.	1-Hydroxy-3-(octanoyloxy) propan-2-yl decanoate (isomer)	28.490	6372783	13.58	1584655	15.19	4.02		$C_{21}H_{40}O_5$	Mixed monoglyceride	Anti-bacterial (Hyldgaard *et al.*, 2012; Yoon *et al.*, 2018), Anti-fungal (Thormar *et al.*, 2006), Penetration enhancer, occlusive moisturiser (Moore *et al.*, 2020)

Sl. No.	Name of the compound	Retention time	Area	Area%	Height	Height%	A/H	Structure	Chemical Formula	Compound Class	Activity of Compound
22.	Squalene	29.128	319334	0.68	110474	1.06	2.89		$C_{30}H_{50}$	Triterpene	Anti-oxidant (Z. R. Huang *et al.*, 2009), Anti-inflammatory (X. Du *et al.*, 2023), Hair follicle protection (Cheng *et al.*, 2024), Hepatoprotective and Cardioprotective (Soumyashri C H, 2026), Anti-cancer (Z. R. Huang *et al.*, 2009)
23.	1-Decanoyl-3-dodecanoylglycerol	31.040	1188147	2.53	317866	3.05	3.74	-	$C_{25}H_{48}O_5$	Diglyceride	Emollient (Soumyashri C H, 2026), Class activity of anti-microbial (M *et al.*, 2024) and occlusive moisturiser (Roopashree *et al.*, 2021)
24.	1-Decanoyl-3-dodecanoylglycerol (isomer)	31.451	4927829	10.50	795985	7.63	6.19	-	$C_{25}H_{48}O_5$	Diglyceride	Emollient (Soumyashri C H, 2026), Class activity of anti-microbial (M *et al.*, 2024) and occlusive moisturiser (Roopashree *et al.*, 2021)
25.	2-(Decanoyloxy)propane-1,3-diyl dioctanoate	34.448	4527844	9.65	754848	7.23	6.00		$C_{29}H_{54}O_6$	Triglyceride	Emollient, occlusive moisturiser (Roopashree *et al.*, 2021), penetration enhancer, Anti-microbial (W. C. Huang *et al.*, 2014)
26.	Rac-glycerol-1,3-dilaurate	35.375	7139674	15.21	1116543	10.70	6.39	-	$C_{27}H_{52}O_5$	Diglyceride	Anti-microbial (M *et al.*, 2024)
27.	Dodecanoic acid, 1,2,3-propanetriyl ester (Trilaurin)	35.672	1163387	2.48	238723	2.29	4.87		$C_{39}H_{74}O_6$	Triglyceride	Anti-microbial (M *et al.*, 2024),

Maillard reaction in the lipid-aqueous interface. DDMP has been reported to act on the follicular regenerative matrix. It is proposed to support the proliferation of hair follicle keratinocytes and follicle elongation (Hwang *et al.*, 2013; Jang *et al.*, 2022).

It has been reported to promote hair follicle keratinocyte proliferation and support follicle elongation, potentially by protecting actively proliferating cells from ROS-mediated DNA damage (Hwang *et al.*, 2013; Jang *et al.*, 2022).

The triad of DDMP, Lauric acid, and Squalene may be responsible for anagen induction, maintenance, and mitogenic activity of hair follicles, reflecting the pharmacological importance of KNT in the mitigation of NSHF.

δ-Dodecalactone and δ-Tetradecalactone are macrolactones with a distinctive anti-microbial mechanism (Sato *et al.*, 2024). Triggered by the pH, they release the hydroxy fatty acid inside the microbial cell and disrupt the microorganism. The relatively alkaline pH of the follicular canal has been proposed to facilitate site-specific antimicrobial activity of pH-triggered lactones, though direct evidence in the follicular context is limited (Adav *et al.*, 2025; Kaden *et al.*, 2020).

Pharmacology and NSHF pathophysiology

The phytochemical profile of KNT demonstrates a confluence of multi-target mechanisms that can address the pathophysiology of NSHF.

Androgenic axis

The sesquiterpene diol is proposed to modulate the androgenic axis, its suggested 5α-reductase inhibitory activity, if confirmed, may contribute to limiting DHT-mediated follicular miniaturisation.

Oxidative stress axis

7 compounds have been reported to contribute antioxidant activity through mechanisms including direct scavenging, singlet oxygen quenching, and mitochondrial ROS reduction, suggesting a multi-point antioxidant profile for KNT at the follicular level.

Inflammatory axis

7 compounds-Octanoic acid, 2-Methoxy-4-vinylphenol, n-Decanoic acid, Dodecanoic acid, 4-Hydroxy-β.-ionone; 1,1,4,7-Tetramethyldecahydro-1H-cyclopropa[e]azulene-4,7-diol; Squalene has been individually

Table 4: Common Activity of the Compounds.

Sl. No.	Activity	Number	Name of the Compound
1.	Anti-Oxidant	7	4H-Pyran-4-one; 2,3-dihydro-3,5-dihydroxy-6-methyl-; 2-Methoxy-4-vinylphenol; n-Decanoic acid; Dodecanoic acid; 4-Hydroxy-.beta.-ionone; endo-1,5,6,7-Tetramethylbicyclo[3.2.0]hept-6-en-3-ol; Squalene
2.	Anti-Cancer/ Anti-proliferative	4	n-Decanoic acid, Dodecanoic acid, 4-Hydroxy-.beta.-ionone, Squalene
3.	Anti-Inflammatory	7	Octanoic acid, 2-Methoxy-4-vinylphenol, n-Decanoic acid; Dodecanoic acid; 4-Hydroxy-.beta.-ionone; 1,1,4,7-Tetramethyldecahydro-1H-cyclopropa[e]azulene-4,7-diol; Squalene
4.	Anti-Bacterial	6	1-Butanol, 3-methyl-, formate; Octanoic acid; n-Decanoic acid; .delta.-Dodecalactone; endo-1,5,6,7-Tetramethylbicyclo[3.2.0]hept-6-en-3-ol; 1-Hydroxy-3-(octanoyloxy)propan-2-yl decanoate
5.	Anti-Fungal	5	1-Butanol, 3-methyl-, formate; Octanoic acid; n-Decanoic acid; .delta.-Dodecalactone;1-Hydroxy-3-(octanoyloxy)propan-2-yl decanoate
6.	Anti-Microbial (broad-spectrum)	13	2-Methoxy-4-vinylphenol; n-Decanoic acid; Dodecanoic acid; Dodecanoic acid, ethyl ester; 3-Buten-2-one, 4-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl); Tetradecanoic acid; Glyceryl dilaurate; 1-Hydroxy-3-(octanoyloxy)propan-2-yl decanoate; 1-Decanoyl-3-dodecanoylglycerol; 2-(Decanoyloxy)propane-1,3-diyl dioctanoate; Rac-glycerol-1,3-dilaurate; Dodecanoic acid, 1,2,3-propanetriyl ester
7.	Hair-growth promoting	1	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
8.	Occlusive moisturiser	4	Glyceryl dilaurate; 1-Hydroxy-3-(octanoyloxy)propan-2-yl decanoate; 1-Decanoyl-3-dodecanoylglycerol; 2-(Decanoyloxy)propane-1,3-diyl dioctanoate
9.	Skin/Scalp Penetration Enhancer	3	Glyceryl dilaurate; 1-Hydroxy-3-(octanoyloxy)propan-2-yl decanoate; 2-(Decanoyloxy)propane-1,3-diyl dioctanoate
10.	Hair follicle protection	1	Squalene
11.	Anti-hairfall	1	Dodecanoic acid
12.	Anti-androgenic	1	1,1,4,7-Tetramethyldecahydro-1H-cyclopropa(e)azulene-4,7-diol

reported to address perifollicular inflammation through mechanisms including pro-inflammatory cytokine suppression (TNF-α, IL-1β, IL-6), NLRP3 inflammasome inhibition, and reduction of follicle-damaging inflammatory mediators, collectively suggesting a multi-target anti-inflammatory hypothesis for KNT in hair and scalp health.

Scalp microbiome axis

15 compounds have demonstrated antimicrobial activity in experimental models across bacterial and fungal origins implicated in scalp barrier dysbiosis.

Hair follicle cycle axis

Lauric acid (reported anagen prolongation), Squalene (reported dermal papilla protection), and DDMP (reported keratinocyte mitogenesis) form a proposed triad addressing specific phases of the hair follicle cycle-a hypothesis warranting validation in a follicular cycle model.

Transdermal delivery axis

The glyceride ester fraction is proposed to contribute to follicular bioavailability of active compounds through penetration enhancement, and may support scalp health through occlusive moisturisation, both roles reported for structurally analogous compounds in the literature.

To sum up, the compounds analysed through GC-MS analysis of KNT provide a pharmacologically grounded hypothesis framework for the potential utility of KNT across the above axes in the management of *Khalitya*, offering a mechanistic rationale consistent with the classical *Keshya, Twachya*, and *Balya* properties ascribed to KNT, pending experimental and clinical validation.

LIMITATIONS

GC-MS analysis was performed as a single-run exercise without replicate injections. Future studies should report mean ± SD of peak areas. All pharmacological inferences are based on literature-reported activities of isolated compounds and not on *in* *vitro, in vivo*, or clinical validation of KNT as a whole formulation. These limitations define the scope of the present work as an exploratory, hypothesis-generating investigation.

CONCLUSION

The GC-MS profiling of *Kaidarya Siddha Narikela Taila* identified 27 bioactive compounds spanning medium-chain fatty acids, glyceride esters, phenolics, terpenoids, and lactones. The pharmacological activities reported in literature for these compounds collectively address antioxidant, anti-inflammatory, antimicrobial, anti-androgenic, penetration-enhancing, and hair-growth-promoting mechanisms that are relevant to one or more pathophysiological axes of *Khalitya*/NSHF. These findings constitute a mechanistic hypothesis framework for the therapeutic utility of KNT and support its further investigation through *in vitro, in vivo*, and clinical studies. The study positions KNT as a promising candidate for evidence-based validation in trichology, bridging classical Ayurvedic formulation science with contemporary molecular pharmacology.

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ABBREVIATIONS

ICD-11: International Classification of Diseases 11th Revision; **AGA:** Androgenetic Alopecia; **PTFE:** Polytetrafluoroethylene; **TIC:** Total Ion Chromatogram; **KFRI:** Kerala Forest Research Institute; **CAI-K:** Centre for Analytical Instrumentation-Kerala; **API:** Ayurvedic Pharmacopoeia of India; **DDMP:** 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-; **MCT:** Medium-chain triglyceride; **DHT:** Dihydrotestosterone; **DNA:** Deoxyribonucleic acid; **CRF:** Central Research Facility. **NAMC:** National Ayurveda Morbidity Code, **GC-MS:** Gas Chromatography - Mass Spectrometry, **GMP:** Good Manufacturing Practice, **KNT:** Kaidarya siddha Narikela Taila, RT: Retention Time, **A/H:** Area/Height ratio, **ROS:** Reactive Oxygen Species, **TNF-α:** Tumour Necrosis Factor-alpha, **IL-1β:** Interleukin-1 beta, **IL-6:** Interleukin-6, **NF-κB:** Nuclear Factor kappa B, **COX-2:** Cyclooxygenase-2, **VEGF:** Vascular Endothelial Growth Factor, **NIST:** National Institute of Standards and Technology., **HPLC:** High-Performance Liquid Chromatography; **NSHF:** Non Specific hair fall; **MCFA:** Medium-Chain Fatty Acid.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

AUTHORS CONTRIBUTION

Sanyogeeta Ajay Dixit: Research concept and design, Collection and/or assembly of data, Data analysis and interpretation, Writing the article, Critical revision of the article, Final approval of the article. **Pankaj Sharma:** Research concept and design, Collection and/or assembly of data, Data analysis and interpretation, Writing the article, Critical revision of the article, Final approval of the article. **Pradnya Prakash Hemke:** Collection and/or assembly of data, Data analysis and interpretation, Critical revision of the article. **Kashavva Veerabasayya Hiremath:** Critical revision of the article, Final approval of the article. **Susmita Devgonda Shedbale:** Data analysis and interpretation, Writing the article. **Namrata Bhagaje:** Critical revision of the article, Final approval of the article. **Monika Yadav:** Data analysis and interpretation, Writing the article, Critical revision of the article.

SUMMARY

Hair loss, especially non-specific hair fall, is a multifactorial condition driven by hormonal imbalance, oxidative stress, inflammation, microbiome disruption, and lifestyle factors, with major psychosocial impact. This study evaluates *Kaidarya Siddha Narikela Taila*, an Ayurvedic medicated oil prepared with *Murraya koenigii* in coconut oil, for its potential in *Khalitya* management. GC-MS analysis identified 27 bioactive compounds, including medium-chain fatty acids, glyceride esters, phenolics, terpenoids, and lactones, many with antioxidant, anti-inflammatory, antimicrobial, and hair-growth-promoting properties. The findings suggest that KNT may support scalp health, follicular delivery, and hair preservation through multiple mechanistic pathways, warranting further preclinical and clinical validation.

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