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RESEARCH ARTICLE

Phytochemical diversity and volatile metabolite profiling in *Jasminum auriculatum* varieties and mutants

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Abstract

Phytochemical diversity and volatile metabolite profiling are essential for understanding the medicinal and industrial potential of aromatic plants. *Jasminum auriculatum* Vahl., widely valued for its fragrance and traditional therapeutic uses, remains underexplored for mutation-induced variation in phytochemical composition. The present study reports original experimental work aimed at characterising the phytochemical diversity and volatile metabolite shifts induced through mutation breeding in *J. auriculatum*. Two varieties, CO.1 Mullai and Muthu Mullai, along with their mutants, CO.1 MM-HY (2) and MMM-TM (1), were analysed. Fully bloomed fresh flowers were subjected to hexane extraction and extracts were profiled using gas chromatography-mass spectrometry (GC-MS) to identify and quantify volatile and bioactive compounds. The analysis revealed significant qualitative and quantitative variation between parental genotypes and mutants, suggesting mutation-induced reprogramming of metabolic pathways. Notable compounds such as cis-jasmone, phenylethyl alcohol, phytol, benzofuran, linolenic acid and 4H-pyran-4-one were consistently detected, though with variable abundance across genotypes. Mutants displayed elevated levels of pharmacologically important metabolites including 1,2-cyclopentanedione, benzyl β-D-glucoside, trans-cinnamic acid and squalene. The pharmacological significance of these metabolites was inferred from previously reported literature, where they have been associated with antioxidant, antimicrobial, anti-inflammatory, cytotoxic and antiproliferative activities. Overall, the study demonstrates that induced mutation broadens the phytochemical spectrum of *J. auriculatum*, enhancing its potential beyond ornamental value. These findings provide a foundation for exploiting its bioactive compounds in perfumery, cosmetics and pharmaceutical industries. Further biochemical validation and functional assays are warranted to substantiate the observed pharmacological potential.

Keywords: bioactive metabolites; ecotype and mutants; GC-MS analysis; *Jasminum auriculatum*; phytochemical profiling; volatile compounds

Introduction

Jasmines are one of the oldest flowering species cultivated mainly for their unique fragrance. They have many commercial applications in perfumery and natural cosmetic product formulation and are utilised for producing floral wax, flavoured tea and essential oils. Around 200 species of *Jasminum* are known to be distributed throughout the tropical and subtropical regions of the globe. Many of the intensely scented species, such as *J. sambac*, *J. grandiflorum* and *J. auriculatum*, are cultivated extensively in many Eurasian countries primarily for producing attars and other perfumery products (1, 2). *J. auriculatum* is a small evergreen shrub, approximately 1 m to 1.5 m high; the foliage is glossy, bright green, about 2 - 3 inches long, oppositely and pinnately compound with five to nine leaflets. The species flowers during April to August. The petals are either five or more than five lobed, white sweet-scented and extremely fragrant. *J. auriculatum* is used in traditional medicines, viz. Ayurveda, Siddha and Unani (3). Research have identified diverse classes of phytochemicals in *Jasminum auriculatum*, including terpenoids (cis-jasmone, linalool), flavonoids (rutin, quercetin), alkaloids, fatty acids (linolenic, palmitic, stearic acids) and phenolic acids (benzoic acid, cinnamic acid derivatives). These metabolites are reported to exhibit antioxidant, antimicrobial, wound-healing and anti-inflammatory activities, supporting the therapeutic value of the species (4, 5).

Roots of *J. auriculatum* are useful in skin diseases, especially for ringworm. Flowers are useful in treating a burning sensation. Leaves, roots and flowers are also useful in stomatopathy, antiseptic, emollient, anthelmintic, ulcers, leprosy, skin diseases and wounds (6). Flowers are also used as a

flavouring agent in foods such as frozen dairy desserts, beverages, gelatines, puddings *etc.* Flowers also possess beneficial effects such as aphrodisiac, anti-septic and are widely used in aromatherapy (7). Gas chromatography has a very wide field of applications. One of its major applications is in the separation and analysis of multi-component mixtures such as essential oils, hydrocarbons and solvents. GC-MS is exclusively used for the analysis of esters, fatty acids, alcohols, aldehydes, terpenes etc. (8). Intrinsically, with the use of the flame ionization detector and the electron capture detector (which have very high sensitivities), gas chromatography can quantify materials which are present at very low concentrations. A knowledge of the chemical constituents of plants is desirable not only for the discovery of therapeutic agents but also for disclosing new sources of economic phytocompounds for the synthesis of complex chemical substances. To identify a variety of bioactive compounds, GC-MS analysis was performed on the flowers of *J. auriculatum* mutants along with the parent varieties, CO.1 Mullai and Muthu Mullai.

Materials and Methods

Collection of plant samples

This experiment was conducted at the Department of Floriculture and Landscape Architecture, Tamil Nadu Agricultural University (TNAU), Coimbatore, during 2024-2025. In this study, CO.1 Mullai, an improved TNAU variety and Muthu Mullai, an ecotype of *J. auriculatum* were used along with two promising mutants viz. CO.1 MM-HY (2) (high yielding mutant of CO.1 Mullai) and MMM-TM (1) (tall mutant of Muthu Mullai) were selected for this study based on their superior floral traits including longer corolla tube length, higher flower yield and greater concrete recovery percentage, which make them commercially important for perfumery and ornamental use (Fig 1A-D).

Preparation of extract

Fully bloomed fresh flowers free from pests and diseases were harvested and graded. Twenty grams of flowers were weighed, corolla tubes were removed and the petals were subjected to cold extraction using hexane (80 mL) and the sample was kept at room temperature for one hour. The hexane layer was decanted using Whatman filter paper. Again, 60 mL of hexane was added to the flower sample and the extraction process was repeated. Hexane (non-polar) was selected to extract volatile and lipophilic constituents (terpenoids, hydrocarbons, fatty acids, squalene) that are efficiently recovered and directly analysed by GC-MS without derivatisation. Cold maceration was preferred over Soxhlet to preserve thermo-labile floral volatiles (e.g. cis-jasmone, phenylethyl alcohol), as prolonged heating can cause degradation or loss of aroma compounds. Polar solvents such as methanol or acetone were avoided since they predominantly extract non-volatile, hydrophilic metabolites. The extracts were subjected to rotary evaporation to remove the excess solvent.

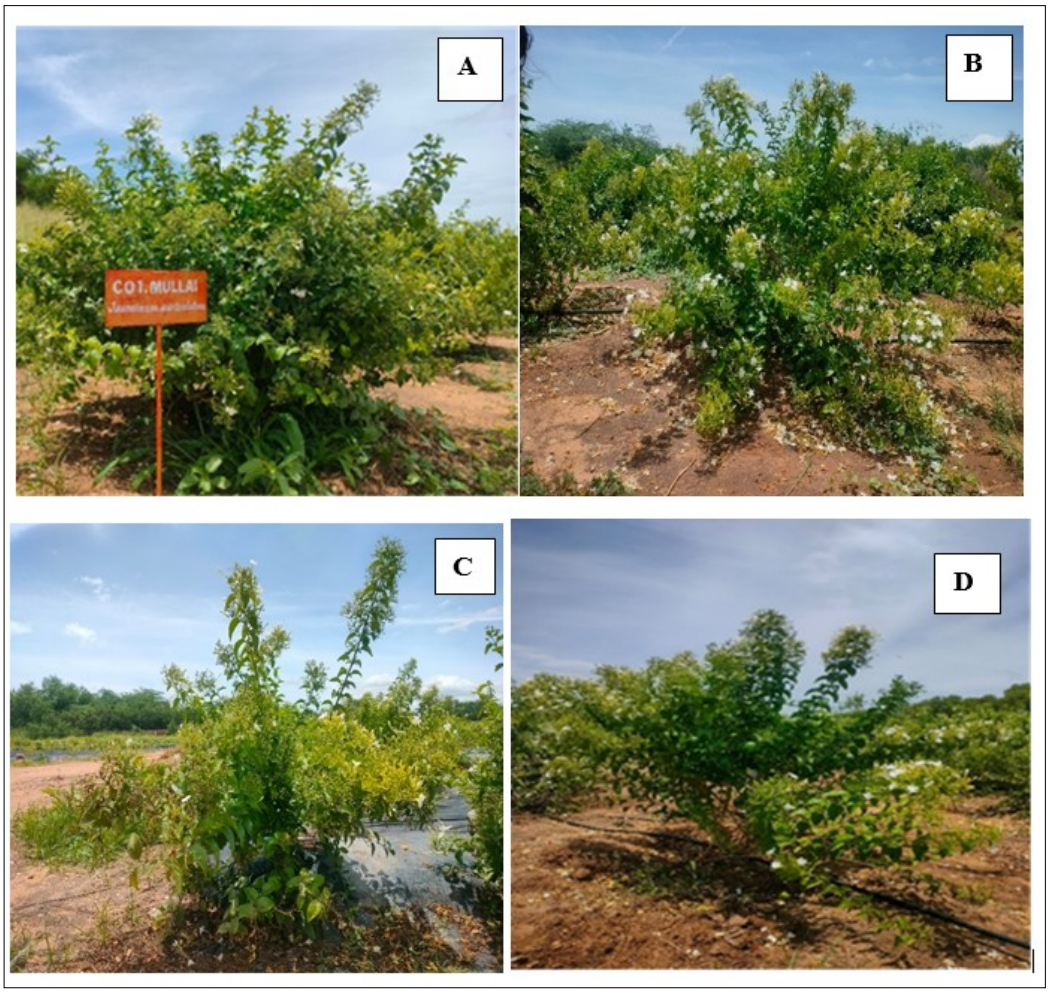


Fig. 1. *Jasminum auriculatum* varieties and mutants **A.** CO.1 Mullai (Parent), **B.** CO.1 MM-HY (2) (High yielding mutant of CO.1 Mullai), **C.** Muthu Mullai (Parent), **D.** MMM-TM (1) (Tall mutant of Muthu Mullai).

Gas chromatography and mass spectroscopy (GC-MS)

The solvent-free flower samples were dissolved in HPLC-grade methanol. The samples were analysed using Gas Chromatography (GC) equipped with Mass Spectroscopy (MS) (Agilent GC 7890A/ MS 5975C). The column temperature was kept at 60 °C for 1.36 min, later increased to 325 °C and maintained for 23 min. The injector temperature was set at 280 °C [split mode 100:1; injection volume 1mL; the flow rate of a helium carrier gas was set to 1ml/min (with a total run time of 23 min)]. Mass spectra were set from the range m/z 50 to 350. The chromatogram of the sample was confirmed by comparing its mass with the spectral database. Compounds detected were identified using the NIST (National Institute of Standards and Technology) mass spectral database. The concentration of each compound was determined based on the peak area percentage derived from the chromatograms. For each compound, the peak area was integrated and the relative abundance was expressed as a percentage of the total peak area in the sample. The higher concentration of common compounds in the mutant lines was confirmed by comparing the peak area percentages between the parent varieties and mutant lines. To ensure accuracy, all measurements were performed in triplicate and the results were averaged.

Statistical analysis

To identify the variations in volatile compound emission between the floral samples of the parent varieties and mutant lines, a hierarchical clustering heat map and peak area analysis were carried out using Metaboanalyst software (Fig. 2). A Venn diagram depicting the significant metabolites and their intersections was generated using the jVenn software tool (Fig. 3).

Results and Discussion

The phytochemical screening of *J. auriculatum* mutants CO.1 MM-HY (2) and MMM-TM 1, along with the parents CO.1 Mullai and Muthu Mullai, led to the identification of major volatile compounds (Fig. 4-7). Among these, five compounds, viz. phenylethyl alcohol, phytol, 4H-pyran-4-one, 2-cyclopenten-1-one (cis-jasmone) and ethyl tetra methyl cyclopentadiene, were consistently detected across the mutants and parents. The present work demonstrates that induced mutants of *J. auriculatum* accumulate higher levels of key volatile compounds (e.g. squalene, linolenic acid, 4H-pyran-4-one) and also produce unique metabolites absent in the parents.

Notably, 2-cyclopenten-1-one (cis-jasmone) was detected at 100 % in both CO.1 Mullai and Muthu Mullai, indicating its stable presence in the parent genotypes. Among the two mutants, the compound was present abundantly in CO.1 MM-HY (2) (44.59 %) compared to MMM-TM (1) (35.77 %). The compounds, viz. phenylethyl alcohol and ethyl tetra methyl cyclopentadiene, were also found to be higher in the parent genotypes compared to mutants. CO.1 Mullai had a 26.35 % peak area percentage and the ecotype had 9.52 % of phenylethyl alcohol. Among the mutants, MMM-TM (1) had the highest percentage (5.81 %). In the case of ethyl tetra methyl cyclopentadiene, CO.1 Mullai and Muthu Mullai had 34.82 % and 24.62 % peak area, respectively. Among the mutants, CO.1 MM-HY (2) registered 9.78 % and MMM-TM (1) had 7.76 % (Table 1). It was observed that the compound 4H-pyran-4-one was highest in mutants compared to the parent genotypes. Among the mutants, MMM-TM (1) had the highest percentage (80.55 %) and CO.1 MM-HY (2) had 61.97 %.

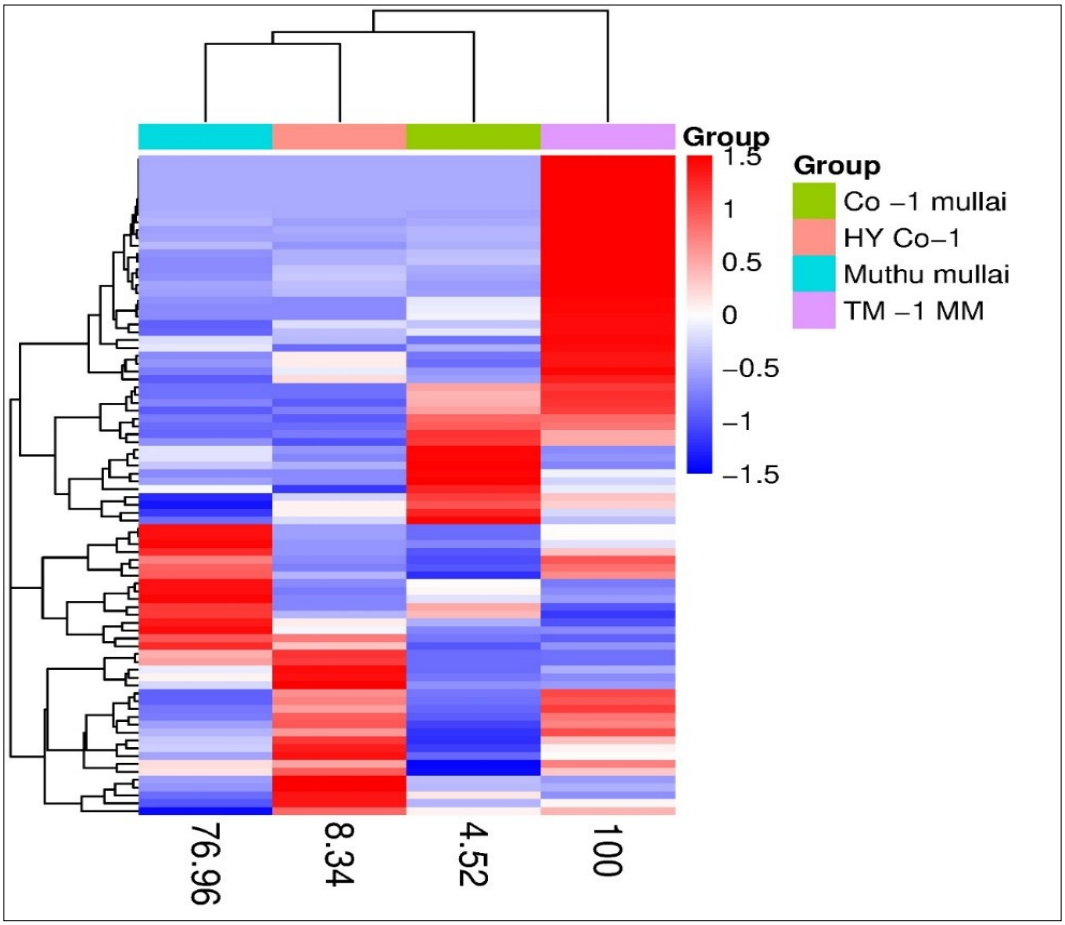


Fig. 2. Heat map analysis of metabolites peak area (%) in the parental and mutant lines of *J. auriculatum.*

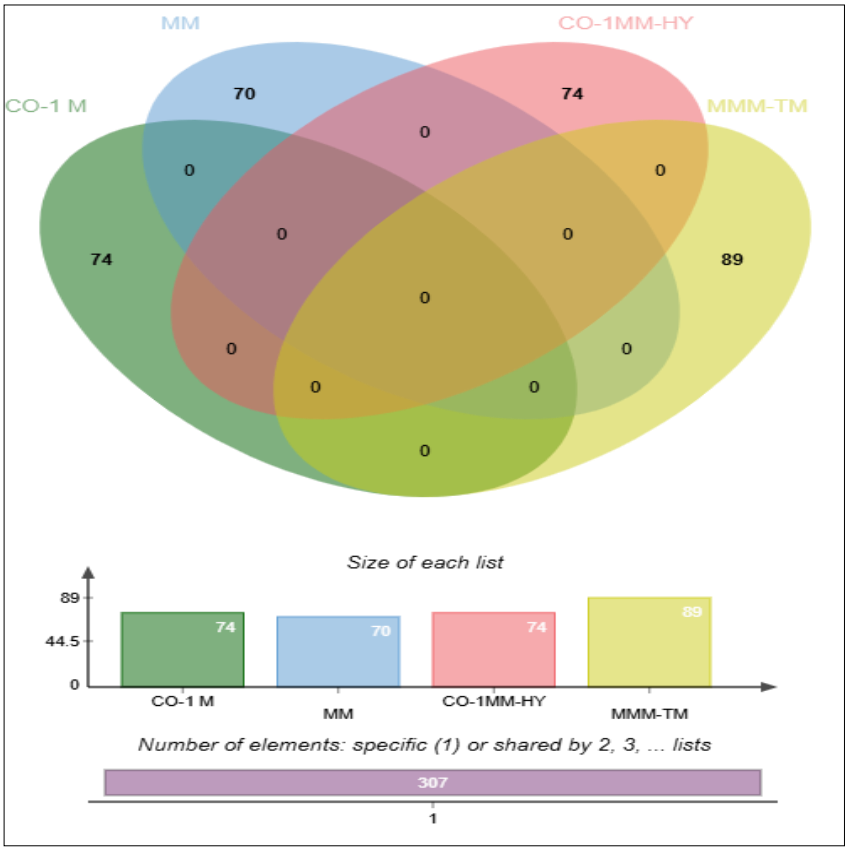


Fig. 3. Venn diagram of parental and mutant lines of *J. auriculatum.*

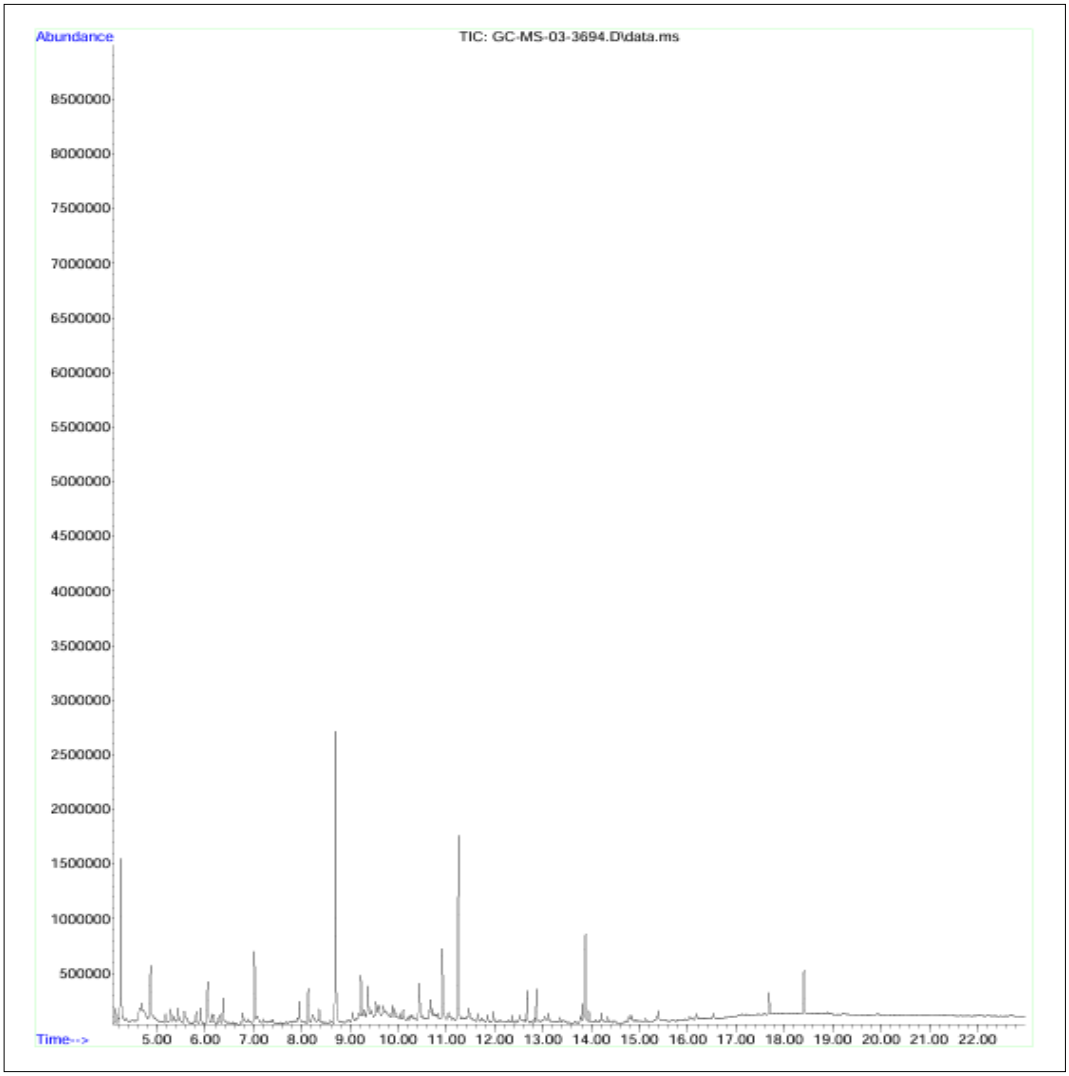


Fig. 4. GCMS chromatogram of volatile compounds of CO.1 Mullai (Parent).

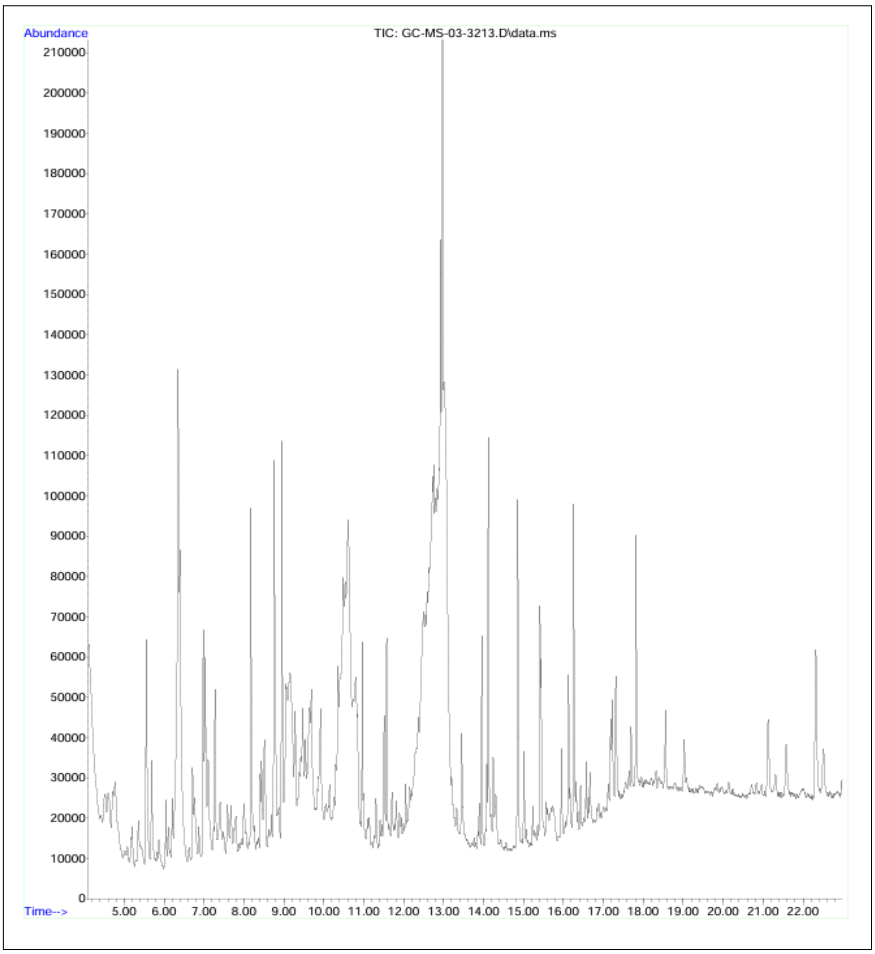


Fig. 5. GCMS chromatogram of volatile compounds CO.1 MM-HY (2) (Mutant).

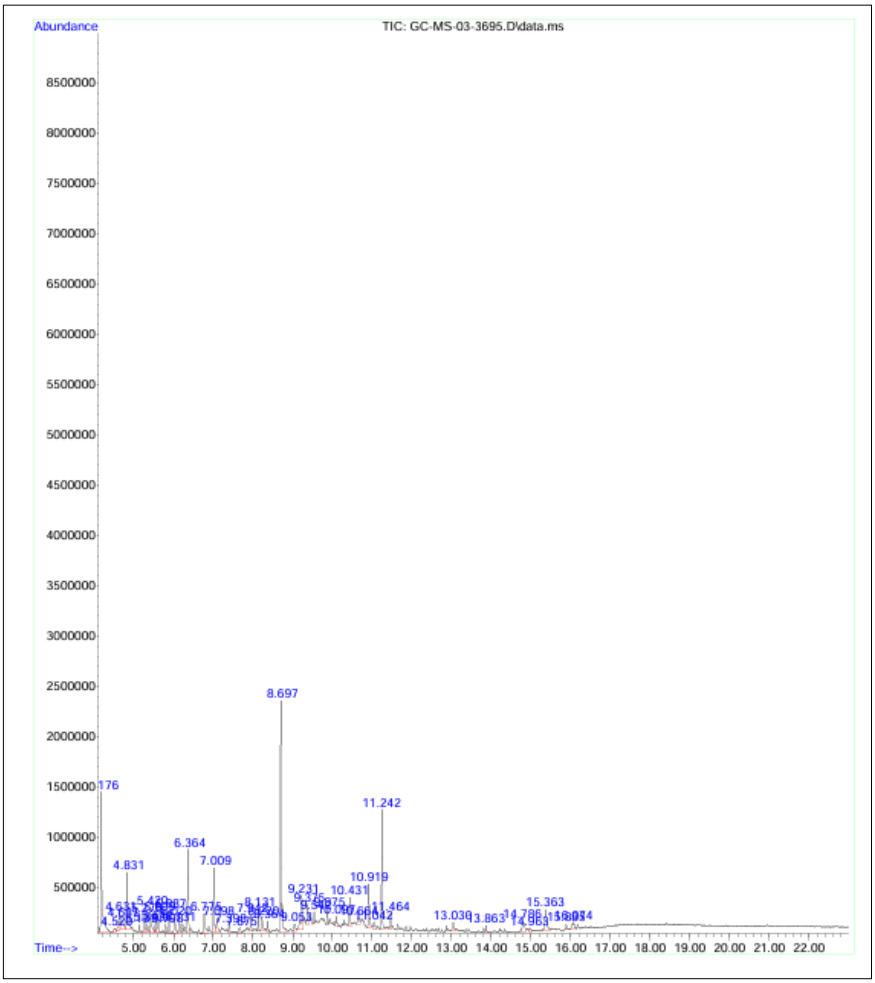


Fig. 6. GC-MS chromatogram of volatile compounds of Muthu Mullai (Parent).

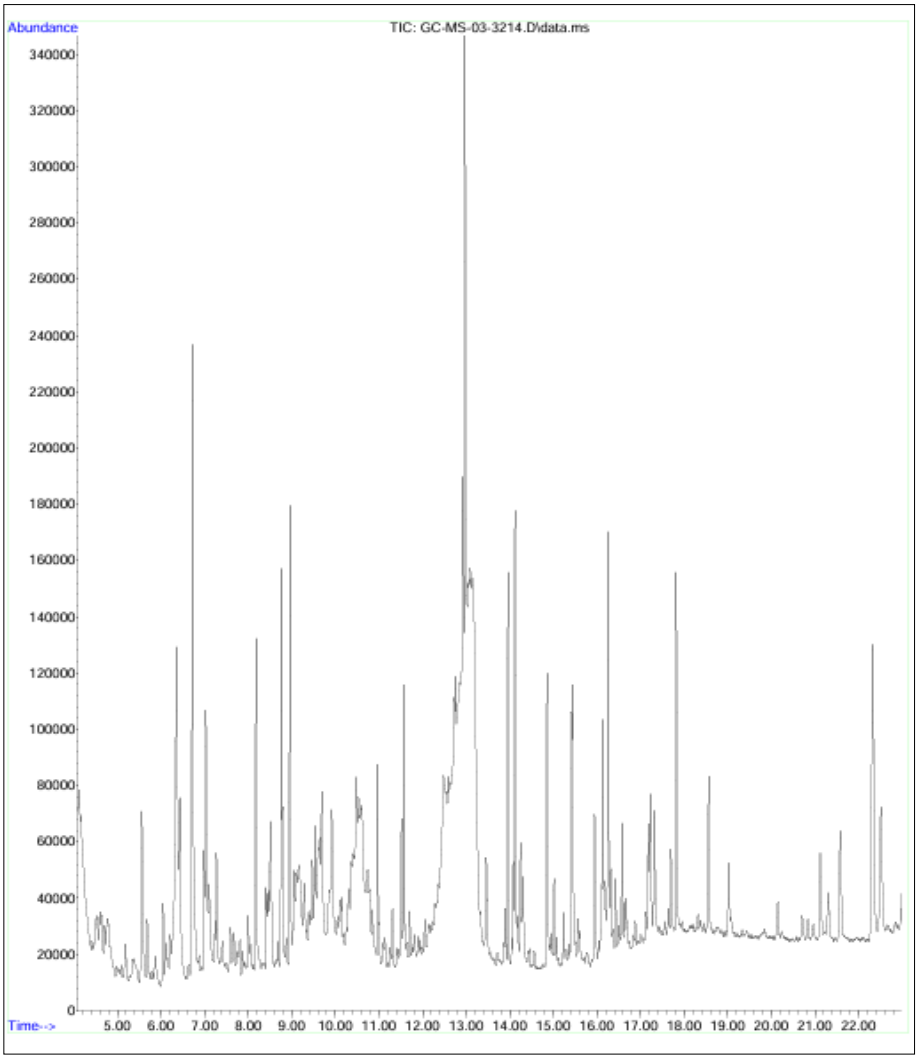


Fig. 7. GC-MS chromatogram of volatile compounds of MMM-TM (1)(Mutant).

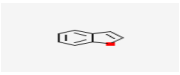
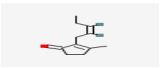
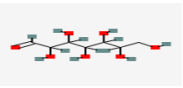
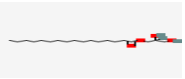
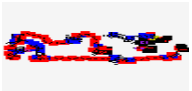
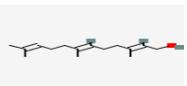
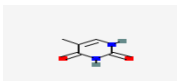
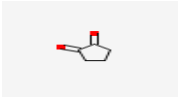
Peak area percentage of the compound phytol was found to be maximum in CO.1 Mullai (39.65 %), followed by MMM-TM (1) (28.63 %) and least in the Muthu Mullai (3.69 %).

The phytocompounds 1,2-cyclopentanedione (100 %) and benzofuran (51.81 %) were found to be the highest in MMM-TM (1). However, these compounds were absent in CO.1 MM-HY (2). Muthu Mullai had registered the highest peak area percentage for 1,2-cyclopentanedione (76.96 %) and benzofuran (32.45 %). Squalene was found to be highest in MMM-TM (1) (38.81 %), while it was absent in the parent line and present in lower levels in CO.1 Mullai (8.25 %). Oxalic acid was exclusively detected in Muthu Mullai and its mutant, with a significantly higher peak area in the parent line (57.12 %) and a lower level in its mutant (9.33 %). Interestingly, certain unique compounds were predominantly associated with the mutant lines. For instance 9,12,15-octadecatrienoic acid (linolenic acid) was highly abundant in MMM -TM (1) (45.85 %), followed by CO.1 MM-HY (2) (22.77 %), whereas it was completely absent in Muthu Mullai and present at minimal levels in CO.1 Mullai (6.51 %). A similar pattern was observed for benzoic acid, which was most prominent in CO.1 MM-HY (2) (28.33 %) and MMM-TM (1) (27.46 %), absent in Muthu Mullai and minimal in CO.1 Mullai. Conversely 2,6,10-dodecatrien-1-ol,3,7,11-trimethyl- was exclusively detected in variety and ecotype, with the highest level in CO.1 Mullai (70.19 %) and was absent in the mutants.

Additionally, compounds such as trans-cinnamic acid, octadecanoic acid, benzyl β-D-glucoside, tetradecanoic acid, d-glycero-d-ido-heptose, cyclohexanone and dodecanoic acid were exclusively detected in the mutant lines while they were absent in the parent genotypes. Among these compounds, trans-cinnamic acid exhibited the highest peak area percentage (42.3 %), followed by cyclohexanone (46.87 %), benzyl β-D-glucoside (36.54 %), octadecanoic acid (25.01 %), tetradecanoic acid (22.29 %) and dodecanoic acid (11.01 %). Furthermore, phytocompounds such as silane, n-hexadecanoic acid (palmitic acid) and thymine were identified in Muthu Mullai as well as in mutants and were absent in CO.1 Mullai. Among these compounds, silane recorded its highest level in Muthu Mullai (17.85 %) and n-hexadecanoic acid (palmitic acid) was abundant in MMM-TM (1) (46.32 %). Thymine followed a comparable distribution pattern across these genotypes. Overall, the observed variations in the qualitative and quantitative distribution of phytochemical constituents among the mutants and their parental genotypes strongly indicate mutation-induced metabolic reprogramming, which may have significant implications on the aromatic and therapeutic potential of *J. auriculatum.*

Phytochemical profiling of CO.1 and Muthu Mullai and their mutants has indicated that induced mutations have reprogrammed the metabolic profile, generating both enhancements and reductions in key phytoconstituents. Among the twenty-four major volatile compounds, five compounds, viz. phenylethyl alcohol, phytol, 4H-pyran-4-one, 2-cyclopenten-1-one (cis-jasmone) and ethyl tetra methyl cyclopentadiene, were consistently detected across the mutants and their parents. The

Table 1. Chemical compounds identified in flower extracts of *J. auriculatum* parental and mutant genotypes and Biochemical activity of phyto-compounds identified in floral extracts

S. No.	Molecular formula	Chemical structure	CO.1 Mullai Peak area %		Muthu Mullai Peak area %		Biochemical activity	Reference
			CO.1 Mullai (Parent)	CO.1 MM-HY (2) (Mutant)	Muthu Mullai (Parent)	MMM- TM-1 (Mutant)		
1	$C_{11}H_{18}$		34.82	9.78	24.62	7.76	Antimicrobial	(2)
2	$C_{18}H_{30}O_2$		6.51	22.77	a	45.85	Antimicrobial	(9)
3	$C_7H_6O_2$		1.71	28.33	a	27.46	Antioxidant	(10)
4	C_8H_8O		25.73	a	32.45	51.81	Anti-inflammatory and Antibacterial	(11)
5	$C_8H_{10}O$		26.35	4.09	9.52	5.81	Antioxidant and Antibacterial	(12)
6	$C_6H_6O_4$		12.12	61.97	37.53	80.55	Antioxidant	(13)
7	$C_{11}H_{16}O$		100.00	35.77	100.00	44.59	Anti-inflammatory effect	(14)
8	$C_9H_8O_2$		a	8.92	a	42.3	Antioxidants and Antimicrobial	(15)
9	$C_{16}H_{32}O_2$		a	22.62	0.41	46.32	Anticancer	(16)
10	$C_{20}H_{40}O$		39.65	9.13	3.69	28.63	Anti-inflammatory	(17)
11	$C_{13}H_{18}O_6$		a	20.57	a	36.54	Antioxidant and Antiproliferative	(18)
12	$C_7H_{14}O_7$		a	53.38	a	39.34	Immunosuppressant	(19)
13	$C_{19}H_{38}O_4$		2.92	18.79	2.39	53.04	Antidiabetic, Antioxidant and Anti-inflammatory	(20)
14	$C_{11}H_{18}$		34.82	9.78	24.62	7.76	Antimicrobial	(2)
15	$C_{30}H_{50}$		8.25	14.10	a	38.81	Antioxidant and Antimicrobial	(21)
16	$C_7H_{10}O_4$		a	a	57.12	9.33	Inhibits the production of uric acid	(22)
17	$C_{15}H_{26}O$		70.19	a	48.71	a	Antimicrobial	(23)
18	$C_5H_6N_2O_2$		a	17.22	9.56	23.14	Antioxidant, Antimicrobial, Antifungal and Antiseptic	(24)
19	$C_5H_6O_2$		65.25	a	76.96	100.00	Anticancer, Anti-inflammatory and Anti-microbial	(25)

compounds 2-cyclopenten-1-one (cis-jasmone), phenylethyl alcohol and ethyl tetra methyl cyclopentadiene were found to be highest in the parents compared to the mutants. On the other hand, the mutants registered the highest peaks for the compound 4H-pyran-4-one.

The compound 2 cyclopenten-1-one (cis-jasmone) was detected at 100 % in both CO.1 Mullai and Muthu Mullai. Abundance of cis-jasmone in CO.1 Mullai and Muthu Mullai reinforces the superior aromatic traits, which are highly valued for fragrance production. This compound also contributes to plant defence mechanisms and is being explored for topical anti-inflammatory applications (14, 26). The elevated levels of phenylethyl alcohol in the parental genotypes further highlight their suitability for perfumery and cosmetic industries, offering a stronger and more desirable aromatic profile compared to the mutant lines (12, 27). The increase in 4H-pyran-4-one in MMM-TM (1) indicates improved antioxidative and antimicrobial potential, which could extend the shelf-life of floral extracts (28). Ethyl tetra methyl cyclopentadiene, though less common in plant profiles, has been reported to exhibit antimicrobial effects (29).

The phytocompounds 1,2-cyclopentanedione, benzofuran and trans-cinnamic acid were found to be highest in the Muthu Mullai mutant MMM-TM (1). The detection of 1,2-cyclopentanedione at high levels in MMM-TM (1) supports the role of mutation in boosting anticancer and antimicrobial activities (24, 29). The higher concentrations of benzofuran, linolenic acid, squalene and trans-cinnamic acid in mutants point to enhanced antioxidant, anti-inflammatory, anti-microbial and dermal protective properties (15, 30-32). Trans-cinnamic acid is often linked to plant resistance mechanisms against microbial invasion and oxidative damage, further substantiating its functional significance in the studied varieties and their mutants.

Among the identified compounds, benzoic acid was detected with a considerable peak area, supporting its relevance as a natural antioxidant. Its presence aligns with previous findings, highlighting its ability to neutralise free radicals and enhance the shelf life of plant-derived extracts (10). The consistent detection of benzoic acid across genotypes suggests its conserved role in plant defence and preservation. Compounds such as octadecanoic acid, benzyl β-D-glucoside, tetradecanoic acid, d-glycero-d-ido-heptose, cyclohexanone and dodecanoic acid were exclusively detected in the mutant lines and absent in the parent genotypes. Octadecanoic acid (stearic acid) and tetradecanoic acid (myristic acid) are widely recognised for their antimicrobial and anti-inflammatory activities, contributing to the plant's defence system and potential therapeutic applications. Their presence suggests a stable fatty acid composition that could support both metabolic functions and commercial utilisation in cosmetics and nutraceuticals.

Fatty acids like palmitic acid (n-hexadecanoic acid) and phytol are well known for their anticancer and anti-inflammatory properties. Research indicates that the identified ecotype and its mutants could serve as valuable sources for bioactive lipid compounds. Squalene supports skin hydration owing to its anti-ageing properties (16, 17). It is an immune enhancer exhibiting antioxidant and antimicrobial activities by scavenging the reactive oxygen species; it prevents lipid peroxidation and reduces inflammation, thereby disrupting the microbial cell membranes and inhibiting bacterial and fungal growth (21). Silane, a miscellaneous mixed metal, possesses cytotoxic activity(33). The presence of oxalic acid adds value by indicating uric acid-inhibiting effects (21).

The appearance of unique compounds such as D-glycero-D-ido-heptose and benzyl β-D-glucoside in the mutants suggests mutation-induced alterations in sugar and glycoside biosynthesis pathways, potentially expanding their immunomodulatory and antiproliferative applications (18, 19). Overall, this comparative analysis demonstrates that while traditional ecotypes retain their hallmark aromatic qualities due to higher aromatic volatile compound content, the mutant lines display a broadened and enhanced phytochemical spectrum with potential pharmaceutical, nutraceutical and industrial applications. This highlights the significance of induced mutagenesis in diversifying and improving the bioactive profile of *J. auriculatum*. Further biochemical characterisation and functional validation are warranted to fully harness these promising traits.

Conclusion

This study demonstrates that induced mutation breeding alters the phytochemical and volatile metabolite profile of *J. auriculatum*, with mutants showing enhanced levels of pharmacologically significant compounds alongside variation in aroma traits. These results highlight the potential of mutants as sources for therapeutic, cosmetic and industrial applications. Future work should focus on targeted isolation of key metabolites, biochemical validation of their bioactivities and breeding strategies to develop elite genotypes with optimised phytochemical traits.

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Authors' contributions

AM experimented and prepared the first draft of the manuscript. NL conceived the idea, monitored the experiment and finalised the manuscript. GM conceived the idea and acquired resources for the experiments. SM and CK reviewed the manuscript. AT assisted in data collection. SP assisted in making draft manuscript. All authors read and approved the final version of the manuscript.

Compliance with ethical standards

Conflict of interest: Authors do not have any conflict of interests to declare.

Ethical issues: None

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