



RESEARCH ARTICLE

# Unveiling the fragrance compounds of *Jasminum auriculatum* genotypes through GC-MS and FTIR techniques

S Naveen<sup>1</sup>, S P Thamarai Selvi<sup>2\*</sup>, S Karthikeyan<sup>2\*</sup>, R Renuka<sup>3</sup>, B Vinoth Kumar<sup>4</sup> & S P Mirunalini<sup>1</sup>

<sup>1</sup>Department of Floriculture and Landscape Architecture, Horticultural College and Research Institute, Tamil Nadu Agricultural University, Coimbatore 641 003, Tamil Nadu, India

<sup>2</sup>Department of Floriculture & Landscape Architecture, Tamil Nadu Agricultural University, Coimbatore 641 003, Tamil Nadu, India

<sup>3</sup>Department of Plant Biotechnology, Centre for Plant Molecular Biology and Biotechnology, Tamil Nadu Agricultural University, Coimbatore 641 003, Tamil Nadu, India

<sup>4</sup>Krishi Vigyan Kendra Vijayanagar, Ooty 643 001, Tamil Nadu, India

\*Correspondence email - [thamaraiselvi.sp@tnau.ac.in](mailto:thamaraiselvi.sp@tnau.ac.in)

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## Abstract

*Jasminum auriculatum* Vahl, a species valued and commonly cultivated for its fragrant flowers, holds significant cultural and commercial value in India. Tamil Nadu is the leading state cultivating *Jasminum* spp. for perfumery industries; also holds a niche market for use as loose flowers in garland making and worship. There are three released varieties of *J. auriculatum* viz., CO.1 Mullai, CO.2 Mullai and Pacha Mullai widely cultivated among the jasmine farmers of Tamil Nadu. Besides the above varieties, from the germplasm collection of TNAU, a promising genotype, *Pacha Mullai*, has been identified and recognized for its distinctive, green-tinged buds and superior agronomic traits. This genotype will be a promising alternative to the already cultivated Mullai types. Hence this study was conducted to investigate the phytochemical composition and aromatic profile of Pacha Mullai in comparison to CO.1 Mullai using Gas Chromatography-Mass Spectrometry (GC-MS) and Fourier Transform Infrared Spectroscopy (FT-IR). The GC-MS analysis revealed that Pacha Mullai exhibited a higher peak area percentage for several bioactive compounds such as squalene, phytol and  $\beta$ -sitosterol, indicating a richer presence of antioxidant, antimicrobial and fragrance-contributing metabolites. Notably, unique compounds like  $\alpha$ -farnesene and phenylethyl alcohol in Pacha Mullai were strongly associated with enhanced aroma and fragrance persistence. FT-IR spectral analysis confirmed the presence of functional groups such as O-H, C-H and C=O, with distinctive peaks in Pacha Mullai indicating additional methyl group vibrations, possibly contributing to its longer shelf life and chemical stability. The distinct metabolite profile and structural attributes affirm that Pacha Mullai not only offers a unique and intense fragrance but also improved post-harvest longevity, making it a superior genotype for commercial cultivation. While CO.1 Mullai retains its relevance for traditional use, Pacha Mullai demonstrates superior phytochemical richness, aromatic complexity and post-harvest potential, supporting its recommendation for commercial cultivation, particularly in the perfumery, cosmetic and floriculture industries.

**Keywords:** FT-IR spectroscopy; fragrance compounds; *Jasminum auriculatum*; pacha mullai; GC-MS analysis

## Introduction

Jasmine (*Jasminum* spp.) is one of the remuneratively prized and significant traditional flower crops in India. It belongs to the family Oleaceae, an aromatic flower cultivated since immemorial and it is valued as the most revered flower in our country for its attractive and fragrant flowers. Jasmine flowers are popularly used in the preparation of garlands and hair adornments for women, used in religious and ceremonial occasions and for extracting perfumery oil used in the cosmetic and perfumery industries. Jasmine cultivation in India spans approximately 23800 hectares, with an annual production of 204790 kilograms. India is the world's largest jasmine oil exporter, accounting over 40 percent of total world exports. It has extensive application in aromatherapy as jasmine

“fragrance” and it is effective in treating depression, nervous exhaustion and stress. It is also widely used in the medicinal and pharmaceutical industries. *J. sambac*, *J. grandiflorum*, *J. auriculatum* and *J. multiflorum* are the key jasmine species cultivated commercially in Tamil Nadu, Karnataka, Andhra Pradesh, Uttar Pradesh and parts of Bihar and West Bengal (1).

Among the Indian states, Tamil Nadu is the leading producer contributing 173870 kg from 16800 thousand hectares, accounting for the most of the nation's output. Major jasmine producing regions within Tamil Nadu include Erode, Coimbatore, Dindigul, Madurai, Salem, Virudhunagar and Trichy districts, where favourable agro-climatic conditions support extensive cultivation (2). Research at Tamil Nadu Agricultural University has identified promising and lesser

known eco types of *J. auriculatum*. The culture “Pacha Mullai” is an ecotype known for its unique bud and stalk colouration of green. The green-tinged flower buds of the Pacha Mullai occupy a niche market in Tamil Nadu, making it a compelling choice for commercial cultivation in regions where jasmine holds cultural and economic significance (3). It is a climber grown as shrub with small dark green oval-shaped leaves and silky-white powdery flowers in clusters. Leaves are opposite and ashy velvet above with trifoliate or simple auricles; the latter remotely separated from the pseudo-stipules. Side leaflets are very small in relation to the central ones. Flowers are borne in many-flowered cymes and highly fragrant; flowers are tinged with “greenish white” in colour both in petals as well as pedicel and hence called with the vernacular name of ‘Pacha Mullai’ (3).

The other unique traits of ‘Pacha Mullai’ are its superior yield, enhanced floral traits and relatively higher tolerance to gall mite (*Aceria jasmini*, Eriophyidae), a major pest of *J. auriculatum* that causes significant economic losses by reducing the marketable quality of the flowers (3). Its attributes to align well with market demands, offering both agronomic benefits to growers and aesthetic appeal to consumers. Due to its higher productivity, better pest resistance and unique market appeal, Pacha Mullai proves to be a superior choice compared to existing variety CO.1 Mullai for commercial jasmine cultivation (3).

This study aims to compare the newly identified green-tinged genotype of *Jasminum auriculatum*, Pacha Mullai with the commercially cultivated CO.1 Mullai variety, focusing on fragrance intensity and phytochemical composition. The research seeks to evaluate the variations in aromatic profiles as well as to determine whether the new genotype exhibits a significantly enhanced fragrance output.

## Materials and Methods

The *Jasminum* genotypes included in this study comprised of the green-tinged *J. auriculatum*, Pacha Mullai (Ja-GT-1) genotype and the CO.1 Mullai (Ja-15) variety, both of which were evolved at Tamil Nadu Agricultural University (TNAU) (Figure 1). Fully opened fresh flowers from both genotypes were collected during the morning hours from the Jasmine germplasm maintained at the Department of Floriculture and Landscaping, TNAU, Coimbatore District, Tamil Nadu, India, during the 2024-2025.

### Preparation of liquid nitrogen flowers extract

The fragrance compounds were extracted from flower samples of a highly fragrant Pacha Mullai and CO.1 Mullai (check variety). Flower samples, each weighing 50 grams were thoroughly cleaned and ground into a fine powder using liquid nitrogen. The powdered material was transferred to a conical flask and mixed with an equal volume of ethyl acetate. The mixture was agitated at 100 ppm in an orbital shaker for 96 hours at 28 °C. The blend was filtered through Whatman No. 3 filter paper. The filtrate was concentrated using a rotary flash evaporator at 55 °C and 80 RPM. The resulting concentrated extract was reconstituted in 1 ml of HPLC-grade methanol, filtered through a PVDF hydrophilic membrane (0.22 µm pore size, Himedia) and prepared for GC-MS analysis (4).

### GC-MS analysis

Volatile compounds of the liquid nitrogen extract of Jasmine flowers were identified by GC-MS using an Agilent Technologies model 7890A gas chromatograph fitted with a Mass Selective Detector model 5975C (MSD) operating in electron ionization (70 V) with the ion source temperature at 250 °C. For the analysis of this extract, a capillary column Agilent DB5MS (30 mm × 0.25 mm × 0.25 µm) was utilized. Helium (99.9 %) was utilized as high-purity carrier gas employed, with the flow rate of ml/min. The injector mode was split (1:60) and the injection volume was one litre. The oven temperature program initiated at 100 °C and held constant for 0.5 min and then rise to 140 °C at 20 °C/min, holding constant for a minute and then continued to 280 °C at 11 °C/min in 20 min (4).

### Analysis with Fourier transform infrared spectroscopy (FTIR)

Analyses were carried out using Thermo Scientific Nicolet iS5 FT-IR Spectrometer. The spectrum was recorded for wavenumbers between 4000 cm<sup>-1</sup> and 400 cm<sup>-1</sup>.

### Identification of bioactive compounds

The peaks were characterized using databases viz., the Wiley Mass Spectral Library (W9N11) and the National Institute of Standards and Technology (NIST) for the identification of volatile compounds. Information regarding the biological activities of the compounds was gathered from Dr. Duke's Phytochemical and Ethno botanical Databases. The molecular weight and formula of the compounds were validated using PubChem.

### Statistical analysis

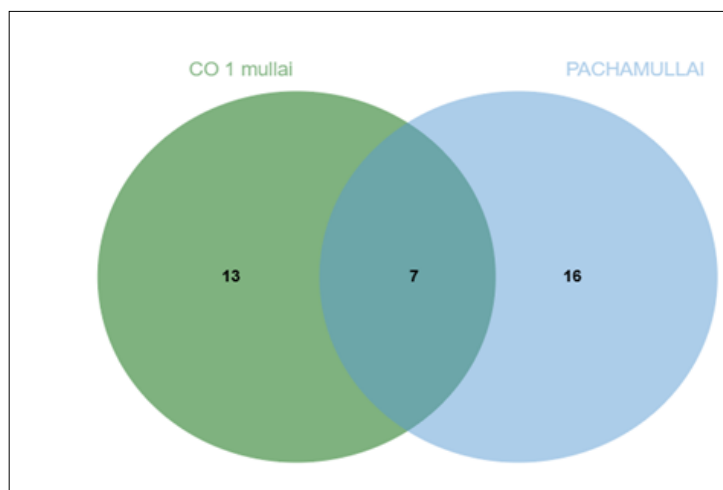
Mass Hunter software was employed for peak area measurement and data processing. The identification of fragments was determined by comparison of their mass spectra to those found in the NIST Wiley 2008 library. A Venn diagram illustrating the significant metabolites along with their interactions was created using jvenn software (Fig. 1).

## Results

The presence of various secondary metabolites and phytochemical components was revealed by GC-MS analysis in the floral extracts of CO.1 Mullai and Pacha Mullai. The identification of these phytochemicals was confirmed through the examination of peak area and properties of the metabolites. These metabolites were confirmed by the NIST (National Institute of Standards and Technology) database.

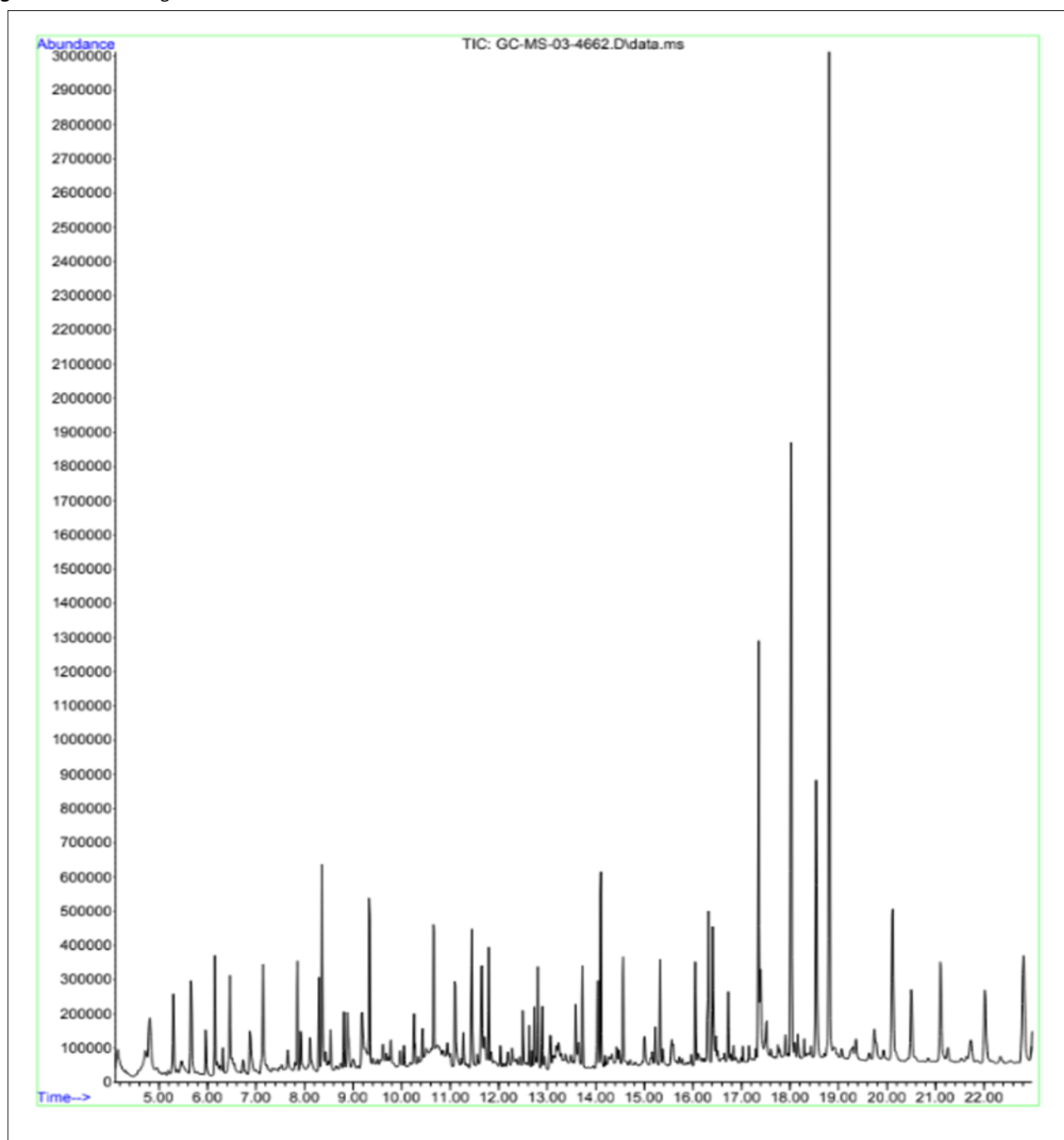
The metabolite profiles of flower extracts are represented in the Fig. 2 and 3. The GC-MS analysis of floral extracts, revealed the presence of diverse phytochemicals with important biological properties. Among the two cultures, Pacha Mullai extract consistently exhibited higher peak area percentages for key metabolites compared to the CO.1 Mullai, indicating an enhanced production of bioactive compounds. This increase suggests that the Pacha Mullai possessed higher level of antioxidant, antifungal and antimicrobial activities, which could be of significant interest for further phytochemical exploration.

The common compounds which were present in CO.1 Mullai and Pacha Mullai include Squalene, heptacosane, beta sitosterol, nanosane, petacosane, glycerol palmitate and phytol. (Table 1).

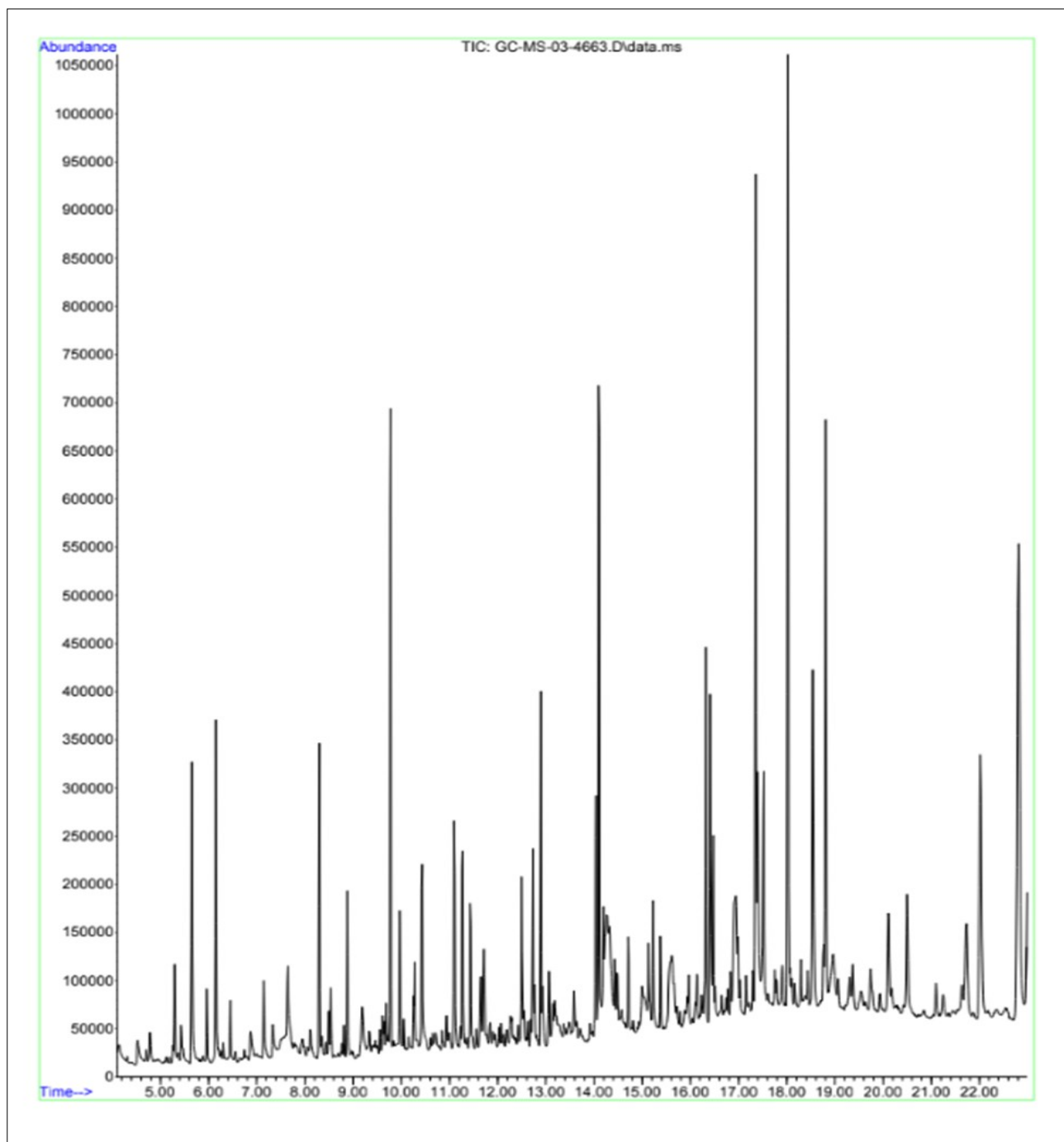


Statistical investigation (jvenn software)

**Fig. 1.** Metabolic divergence: Distinct and shared metabolites between CO.1 Mullai and Pacha Mullai.



**Fig. 2.** Metabolite profiling of VOC's in flowers of *J. auriculatum* CO.1 Mullai.



**Fig. 3.** Metabolite profiling of VOC's in flowers of *J. auriculatum* Pacha Mullai.

**Table 1.** Phytochemical compounds in common identified in flower extracts of *J. auriculatum* CO.1 Mullai and Pacha Mullai

| S. No. | Compound name      | Molecular formula                              | Retention time | Biological activity                                                                                                                               | Reference |
|--------|--------------------|------------------------------------------------|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| 1      | Squalene           | C <sub>30</sub> H <sub>50</sub>                | 18.0184        | Antibacterial, antioxidant, Antitumor, cancer preventive, Immunostimulant                                                                         | 3         |
| 2      | Heptacosane        | C <sub>27</sub> H <sub>56</sub>                | 17.352         | Antioxidant, antibacterial, antimalarial, antidermatophytic effects                                                                               | 4         |
| 3      | Beta Sitosterol    | C <sub>29</sub> H <sub>50</sub> O              | 22.807         | Antioxidant, antimicrobial, angiogenic, antioxidant, immunomodulatory, antidiabetic, anti-inflammatory, anticancer and antinociceptive activities | 5         |
| 4      | Nanosane           | C <sub>29</sub> H <sub>60</sub>                | 18.541         | Antimicrobial potential                                                                                                                           | 6         |
| 5      | Petacosane         | C <sub>25</sub> H <sub>52</sub>                | 16.319         | Antibacterial                                                                                                                                     | 7         |
| 6      | Glycerol Palmitate | C <sub>19</sub> H <sub>38</sub> O <sub>4</sub> | 16.407         | Cytotoxic and antiviral; pro-inflammatory                                                                                                         | 8         |
| 7      | Phytol             | C <sub>20</sub> H <sub>40</sub> O              | 14.097         | Antioxidant, autophagy- and apoptosis-, antinociceptive, anti-inflammatory, immune-modulating and antimicrobial                                   | 9         |

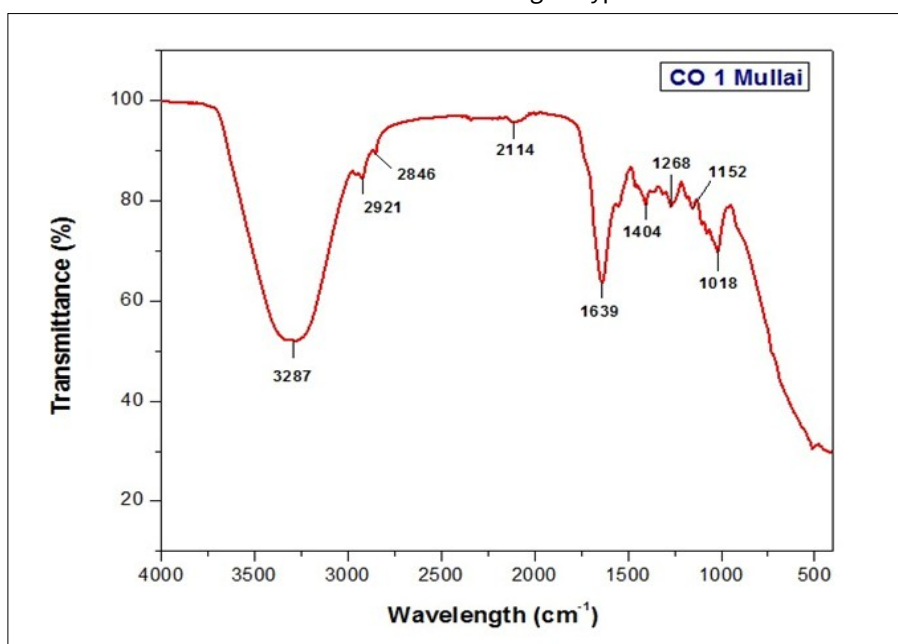
The FTIR analysis of the CO.1 Mullai flower identified various functional groups based on absorption bands (Fig. 4). The peaks at 3287.07  $\text{cm}^{-1}$  and 2921.63  $\text{cm}^{-1}$  indicate O-H stretching (alcohols, phenols) and C-H stretching (alkanes), respectively. The 2114.56  $\text{cm}^{-1}$  peak suggests the presence of C-C bonds (alkynes) and nitriles. The 1639.20  $\text{cm}^{-1}$  peak corresponds to C=C bonds in alkenes and aromatic rings, while 1404.89  $\text{cm}^{-1}$  indicates  $\text{CH}_2$  groups (alkanes). Functional groups such as ethers, esters and carboxylic acids are confirmed by the 1268.93  $\text{cm}^{-1}$  (C-O stretching) peak. The 1152.26  $\text{cm}^{-1}$  peak corresponds to C-O stretching (alcohols, esters) and 1018.23  $\text{cm}^{-1}$  suggests C-N stretching (amines).

FTIR analysis of the green-tinged *Jasminum auriculatum* flower identified various functional groups when compared to CO.1 Mullai (Fig. 5). The absorption bands at 2918.73  $\text{cm}^{-1}$  and 2851.24  $\text{cm}^{-1}$  indicate C-H stretching (alkanes), while 3290.93  $\text{cm}^{-1}$  corresponds to O-H bonds (alcohols, phenols). The peak at 2115.53  $\text{cm}^{-1}$  suggests C-N bonds (alkenes, nitriles) and 1636.30  $\text{cm}^{-1}$

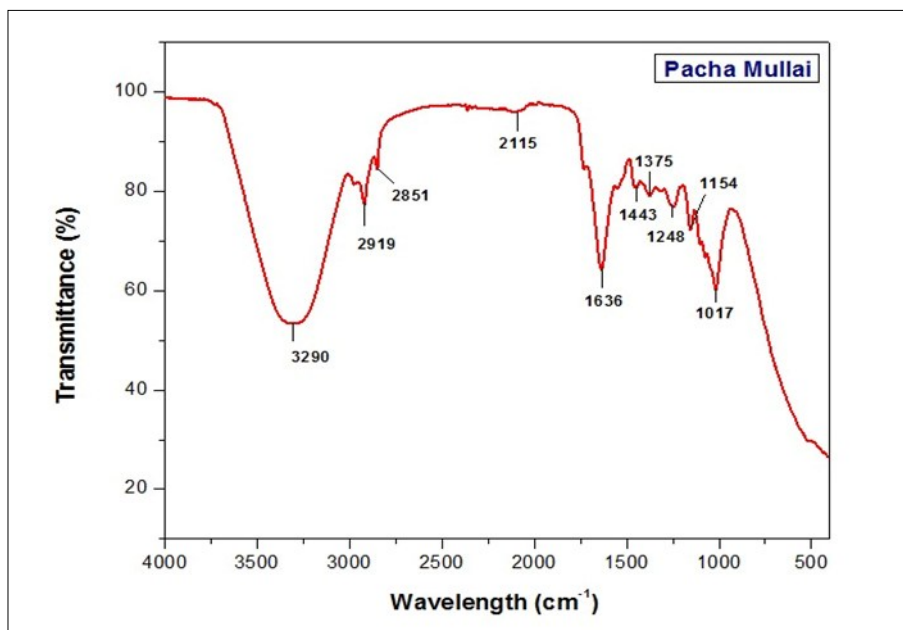
$\text{cm}^{-1}$  represents C=C bonds (alkenes, aromatic rings). Additional peaks confirm  $\text{CH}_2$  bending (1443.46  $\text{cm}^{-1}$ , alkanes), C-H bonds (1375.00  $\text{cm}^{-1}$ , methyl groups) and C-O stretching (1248.68  $\text{cm}^{-1}$  for ethers, esters, carboxylic acids; 1154.19  $\text{cm}^{-1}$  for alcohols, esters). The 1017.27  $\text{cm}^{-1}$  peak indicates C-N stretching (amines) (Table 2, 3).

## Discussion

In the present study, though both genotypes demonstrated the presence of several bioactive compounds with significant therapeutic potential, a notable variation in metabolite profiles was observed between the CO.1 Mullai and Pacha Mullai. Pacha Mullai exhibited a higher peak area percentage in chromatographic analysis, indicating an enhanced production of phytochemicals. The major compounds and their biological activities as reported by earlier references have proved significant cosmetic and pharmaceutical properties for both these genotypes of *J. auriculatum*.



**Fig. 4.** FT-IR spectrum of CO.1 Mullai flower extract for identification of functional groups.



**Fig. 5.** FT-IR spectrum of Pacha Mullai flower extract for identification of functional groups.

**Table 2.** Phytochemical compounds identified in flower extracts of *J.auriculatum* (CO.1 Mullai)

| S No | Compound name                                      | Molecular formula                                              | Retention time (%) | Biological activity                                                                         | Reference                    |
|------|----------------------------------------------------|----------------------------------------------------------------|--------------------|---------------------------------------------------------------------------------------------|------------------------------|
| 1    | Octacosane                                         | C <sub>28</sub> H <sub>58</sub>                                | 18.541             | Anti-inflammatory                                                                           | 10                           |
| 6    | 2,7-Octadiene-1,6-Diol,2,6-Dimethyl-               | C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>                 | 8.353              | Antifungal, Antibacterial, Antimicrobial, Emulsifier, Perfumery Industry                    | 11                           |
| 8    | Farnesol, Acetate                                  | C <sub>17</sub> H <sub>28</sub> O <sub>2</sub>                 | 21.096             | Antimicrobial, Antitumor, Nervous and cardiovascular system, Metabolic and hepatic effects. | 12                           |
| 9    | Benzofuran, 2,3-Dihydro-                           | C <sub>8</sub> H <sub>8</sub> O                                | 7.142              | Antifungal and antibacterial activity                                                       | 13                           |
| 10   | Cycloheptasiloxane, Tetradecamethyl-               | C <sub>14</sub> H <sub>42</sub> O <sub>7</sub>                 | 9.331              | Antidiabetic agent                                                                          | 14                           |
| 11   | 4H-Pyran-4-One, 2,3-Dihydro-3,5-Dihydroxy-6-Methyl | C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>                   | 6.464              | Antioxidant                                                                                 | 15                           |
| 12   | 2,6,10-Dodecatrien-1-OL, 3,7,11-Trimethyl-         | C <sub>15</sub> H <sub>26</sub> O                              | 11.453             | Antifungal and antimicrobial                                                                | 16                           |
| 16   | 3-Amino-3-(4-Methoxy-Phenyl)-Propionic Acid        | C <sub>10</sub> H <sub>13</sub> NO <sub>3</sub>                | 9.186              | anti-inflammatory                                                                           | National library of medicine |
| 17   | 4-((1E)-3-Hydroxy-1-Propenyl)-2-Methoxyphenyl      | C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>                 | 11.653             | Antioxidant , anti-inflammatory                                                             | 17                           |
| 18   | P-Cresol                                           | C <sub>7</sub> H <sub>8</sub> O                                | 5.653              | Aroma profiling                                                                             | National library of medicine |
| 20   | Cyclononasiloxane, Octadecamethyl                  | C <sub>18</sub> H <sub>54</sub> O <sub>9</sub> Si <sub>9</sub> | 14.563             | Antifungal                                                                                  | 18                           |

**Table 3.** Phytochemical compounds identified in flower extracts of *J. auriculatum* (Pacha Mullai)

| S No | Compound name                                                                  | Molecular formula                              | Retention time( %) | Biological activity                                                                                                                  | References                   |
|------|--------------------------------------------------------------------------------|------------------------------------------------|--------------------|--------------------------------------------------------------------------------------------------------------------------------------|------------------------------|
| \    | Alpha.-Farnesene                                                               | C <sub>15</sub> H <sub>24</sub>                | 9.755              | Armo profiling                                                                                                                       | National library of medicine |
| 7    | Stigmasterol                                                                   | C <sub>29</sub> H <sub>48</sub> O              | 22.018             | Anti-diabetic effects                                                                                                                | 19                           |
| 8    | 9,19-Cyclolanostan-3-OL, 24-Methylene-, (3.Beta.)                              | C <sub>31</sub> H <sub>52</sub> O              | 16.941             | Anti-HIV compound used to Prevent the HIV virus                                                                                      | 20                           |
| 11   | Methyl 18-Methylnonadecanoate                                                  | C <sub>21</sub> H <sub>42</sub> O <sub>2</sub> | 15.374             | Antimicrobial                                                                                                                        | 21                           |
| 13   | Hexadecanoic Acid, Methyl Ester                                                | C <sub>17</sub> H <sub>34</sub> O <sub>2</sub> | 12.896             | Antioxidant; Nematicide; Pesticide; Antibacterial; Antifungal; Antiarthritic; Antitumor; Anticancer; Anticoronary; Anti-inflammatory | 22                           |
| 14   | Phenylethyl Alcohol                                                            | C <sub>8</sub> H <sub>10</sub> O               | 6.153              | Aroma profiling                                                                                                                      | 23                           |
| 15   | Tetracosanoic Acid, Methyl Ester                                               | C <sub>25</sub> H <sub>50</sub> O <sub>2</sub> | 17.518             | Antibacterial, antifungal                                                                                                            | 24                           |
| 16   | 6-Octadecenoic Acid, Methyl Ester, (Z)-                                        | C <sub>19</sub> H <sub>36</sub> O <sub>2</sub> | 14.041             | Antifungal, antibacterial, antimicrobial, emulsifier, perfumery industry                                                             | 25                           |
| 17   | 9,12,15-Octadecatrienoic Acid, (Z,Z,Z)-                                        | C <sub>18</sub> H <sub>30</sub> O <sub>2</sub> | 12.730             | Anti-inflammatory, Hypocholesterolemic, Cancer preventive, Hepatoprotective, Antibacterial, antiarthritic, Anticoronary              | 26                           |
| 18   | Pentadeca-2,3,6,9,12,13-Hexaen-8-One, 2,5,5,11,11,14-Hexamethyl-               | C <sub>21</sub> H <sub>30</sub> O              | 10.430             | Antibacterial activity                                                                                                               | 27                           |
| 20   | Bicyclo[3.2.0]Heptane-2,6-Diol, 5-(2-Hydroxyethyl)-3,3-Dimethyl-6-Vinyl-, (Z)- | C <sub>13</sub> H <sub>22</sub> O <sub>3</sub> | 11.275             | Antimicrobial, Antifungal, Antioxidant                                                                                               | 28                           |

The compounds commonly found in both CO.1 Mullai and Pacha Mullai varieties include several bioactive constituents. These shared compounds may play key roles in the pharmacological properties of the two jasmine types, contributing to their fragrance, therapeutic potential and overall phytochemical profile. Squalene, a compound identified in *Cassia italica*, is known for its antibacterial, antioxidant, antitumor, cancer-preventive and immunostimulant properties (5). Heptacosane, detected in *Salvia palestina*, exhibits antioxidant, antibacterial, antimalarial and antidermatophytic activities (6).  $\beta$ -Sitosterol, a phytochemical widely distributed in the plant kingdom, demonstrates a broad spectrum of biological activities, including antioxidant, antimicrobial, angiogenic, immunomodulatory, antidiabetic, anti-inflammatory, anticancer and antinociceptive effects (7). Nonacosane, found in *Senecio asirensis*, has shown notable antimicrobial potential (8). Pentacosane, present in the Ayurvedic formulation *Talisapatradi Churnam*, possesses antibacterial activity (9). Glycerol 1-palmitate, reported in *Jatropha curcas*, exhibits cytotoxic, antiviral and pro-inflammatory effects (10). Phytol is also recognized for its antioxidant, anti-inflammatory, antinociceptive and immunomodulatory properties (11).

The key phytochemicals identified in CO.1 Mullai include several bioactive compounds with diverse therapeutic and industrial applications. Octacosane, previously reported in *Maranthas pumilum*, is recognized as a potential anti-inflammatory biomarker (12). The compound 2,7-octadiene-1,6-diol, 2,6-dimethyl exhibits antifungal, antibacterial and emulsifying properties, making it valuable for antimicrobial uses and in the perfumery industry (13). Farnesol acetate, found in *Vachellia farnesiana*, is known for its antimicrobial, antitumor, neurological, cardiovascular, metabolic and hepatoprotective benefits (14). Additionally, 2, 3-dihydrobenzofuran, reported in *Tagetes patula*, displays strong antifungal and antibacterial activity (15). Cycloheptasiloxane, tetradecamethyl-identified in *Aitchisonia rosea*-has demonstrated antidiabetic potential (16). The compound 4H-pyran-4-one, 2, 3-dihydro-3, 5-dihydroxy-6-methyl, found in rice, is known for its antioxidant properties (17). Furthermore, 2, 6, 10-dodecatrien-1-ol, 3, 7, 11-trimethyl exhibits both antifungal and antimicrobial effects (18). The compound 4-((1E)-3-hydroxy-1-propenyl)-2-methoxyphenyl, which can result from microbial transformation of dietary phenols or be present in fermented foods, has antioxidant and anti-inflammatory properties (19). Lastly, cyclononasiloxane, octadecamethyl-reported in *Zingiber griffithii*-has demonstrated notable antifungal potential (20).

In this study, a significant variation in metabolite profiles was observed between CO.1 Mullai and Pacha Mullai. Notably, Pacha Mullai exhibited a higher peak area percentage in the chromatographic analysis, suggesting an increased production of phytochemically active compounds. Several bioactive constituents were detected in Pacha Mullai, many of which are associated with important pharmacological and therapeutic effects. Among the prominent compounds identified,  $\alpha$ -farnesene, a volatile compound known for its contribution to aroma profiling (National Library of Medicine) was noteworthy. Stigmasterol, commonly found in vegetable fats and oils, has demonstrated antidiabetic properties (21). Another major compound, 9, 19-Cyclolanostan-3-ol, 24-methylene- ( $\beta$ ), reported in *Senecio asirensis*, is known for its anti-HIV activity and

is being explored as a potential agent for HIV prevention (22). While Methyl 18-Methylnonadecanoate has been linked to antibacterial activity (23). Hexadecanoic acid, methyl ester, found in *Pistia stratiotes*, exhibits a wide range of bioactivities including antioxidant, nematocidal, pesticidal, antibacterial, antifungal, antiarthritic, antitumor, anticancer, anti-inflammatory and anticoronary effects (24). Phenylethyl alcohol, commonly present in Damask rose and hybrid roses, plays a significant role in fragrance and aroma development (25). Tetracosanoic acid, methyl ester and 6-octadecenoic acid, methyl ester-both reported in *Cenchrus setigerus*-demonstrate antibacterial, antifungal and emulsifying properties, with additional applications in the perfumery industry. These compounds are also known for their anti-inflammatory, hypocholesterolemic, cancer-preventive, hepatoprotective and antiarthritic effects (9, 25). 6-Octadecenoic Acid, Methyl Ester, (Z)- these compounds are also known for their Anti-inflammatory,

Hypocholesterolemic, Cancer preventive, Hepatoprotective, Antibacterial, antiarthritic, Anticoronary (28). Furthermore, pentadeca-2, 3, 6, 9, 12, 13-hexaen-8-one, 2, 5, 5, 11, 11, 14-hexamethyl-, reported in *Shepherdia argentea*, is recognized for its antimicrobial, antifungal and antioxidant properties (29). Finally, bicycloheptane hydroxyethyl has also been identified for its antimicrobial, antifungal and antioxidant activities (30).

Fourier Transform Infrared (FT-IR) spectroscopy alongside functional theory calculations to investigate the vibrational characteristics of two plant samples, CO.1 Mullai and Pacha Mullai, revealed distinct absorption bands that correspond to various functional groups present in the samples. Both plant types exhibited prominent O-H stretching vibrations in the range of 3287-3291  $\text{cm}^{-1}$ , which is indicative of alcohol or phenolic compounds (31). Additionally, C-H stretching vibrations attributed to alkanes were observed around 2918-2921  $\text{cm}^{-1}$  (32).

FT-IR spectral analysis showing absorption bands near 2114-2115  $\text{cm}^{-1}$ , suggest the presence of C-C or C-N stretching vibrations, typically associated with alkynes or nitriles (33). The C=C stretching vibrations, characteristic of alkenes or aromatic rings, appear in both samples around 1636-1639  $\text{cm}^{-1}$  (34). In addition, bending vibrations of  $\text{CH}_2$  groups and, along with C-O stretching modes (35), indicate the presence of ethers, esters, carboxylic acids (36) and alcohols (37). The spectrum also displays C-N stretching vibrations, confirming the presence of amines (38). A notable feature unique to Pacha Mullai was the presence of an additional absorption peak at 2851  $\text{cm}^{-1}$ , suggesting minor but significant compositional differences between the two samples.

Moreover, an additional C-H bending vibration at 1375  $\text{cm}^{-1}$  is observed in the Pacha Mullai sample, which is characteristic of methyl group vibrations. This distinguishes it from the CO.1 Mullai sample and suggests a distinct chemical composition. The presence of this methyl group may contribute to enhanced hydrophobic interactions, structural stability and biological activity, potentially influencing the plant's medicinal or ecological properties (Table 4, 5). However, further biochemical and pharmacological studies are necessary to validate the functional role of this methyl substitution. The present study has unveiled the fragrance compounds of the new genotype Pacha Mullai making it a potential crop for cultivation by Jasmine growers.

**Table 4.** FT-IR spectrum peak values and functional groups in the flower extracts of *J. auriculatum* (CO.1 Mullai)

| S No | Vibration assignment (V) (cm <sup>-1</sup> ) | Absorption band                                     | Reference |
|------|----------------------------------------------|-----------------------------------------------------|-----------|
| 1    | 3287.07 cm <sup>-1</sup>                     | O - H stretching (alcohols, phenols)                | 29        |
| 2    | 2921.63 cm <sup>-1</sup>                     | C - H stretching (alkanes)                          | 30        |
| 3    | 2114.56 cm <sup>-1</sup>                     | C-C or C-N stretching (alkynes, nitriles)           | 31        |
| 4    | 1639.21 cm <sup>-1</sup>                     | C = C stretching (alkenes, aromatic rings)          | 32        |
| 5    | 1404.89 cm <sup>-1</sup>                     | CH <sub>2</sub> bending (alkanes)                   | 33        |
| 6    | 1268.93 cm <sup>-1</sup>                     | C - O stretching (ethers, esters, carboxylic acids) | 34        |
| 7    | 1152.26 cm <sup>-1</sup>                     | C - O stretching (alcohols, esters)                 | 35        |
| 8    | 1018.23 cm <sup>-1</sup>                     | C - N stretching (amines)                           | 36        |

**Table 5.** FT-IR spectrum peak values and functional groups in the flower extracts *J. auriculatum* (Pacha Mullai)

| S No | Vibration assignment (V) (cm <sup>-1</sup> ) | Absorption band                                     | References |
|------|----------------------------------------------|-----------------------------------------------------|------------|
| 1    | 3290.93 cm <sup>-1</sup>                     | O - H stretching (alcohols, phenols)                | 29         |
| 2    | 2918.73 cm <sup>-1</sup>                     | C - H stretching (alkanes)                          | 30         |
| 3    | 2115.53 cm <sup>-1</sup>                     | C-C or C-N stretching (alkynes, nitriles)           | 31         |
| 4    | 1636.30 cm <sup>-1</sup>                     | C = C stretching (alkenes, aromatic rings)          | 32         |
| 5    | 1443.46 cm <sup>-1</sup>                     | CH <sub>2</sub> bending (alkanes)                   | 33         |
| 6    | 1248.68 cm <sup>-1</sup>                     | C - O stretching (ethers, esters, carboxylic acids) | 34         |
| 7    | 1154.19 cm <sup>-1</sup>                     | C - O stretching (alcohols, esters)                 | 35         |
| 8    | 1017.27 cm <sup>-1</sup>                     | C - N stretching (amines)                           | 36         |
| 9    | 2851.24 cm <sup>-1</sup>                     | C - H stretching (alkanes)                          | 37         |
| 10   | 1375.00 cm <sup>-1</sup>                     | C - H bending (methyl groups)                       | 37         |

## Conclusion

Based on the comparative analysis of CO.1 Mullai and Pacha Mullai, it is evident that Pacha Mullai demonstrates superior overall performance. The small graph analysis clearly indicates that Pacha Mullai excels in key attributes such as fragrance intensity, shelf life and post-harvest quality. These findings suggest that Pacha Mullai is a potential genotype of *Jasminum auriculatum* for both commercial and ornamental purpose, offering enhanced aesthetic and economic value.

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## Authors' contributions

SN has written the whole manuscript. SPT guided in providing technical support to write the manuscript in a proper format and approved the final manuscript. SK guided in providing technical support to write the manuscript in a proper format and approved the final manuscript. RR guided to write the manuscript in a proper format and approved the final manuscript. SVK guided to write the manuscript in a proper format and approved the final manuscript. SM guided to write the manuscript in a proper format and approved the final 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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