RESEARCH ARTICLE

# Analytical Approaches to Phytochemical Profiling of *Jasminum grandiflorum* White Pitchi genotype: FTIR and GC–MS Studies on Stem Extracts

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## ABSTRACT

Plants have long served as a rich source of raw materials for pharmaceuticals, contributing significantly to both traditional and modern medicine. The present study focused on the phytochemical profiling of stems from a novel White Flower Bud genotype of *Jasminum grandiflorum* L. (WF), aiming to explore its potential for pharmacological applications. Methanolic extracts of the stems were subjected to Gas Chromatography–Mass Spectrometry (GC–MS) analysis, which revealed the presence of 16 bioactive compounds. These identified compounds are known to exhibit diverse biological activities, including antimicrobial, antibacterial, antioxidant, and anticancer properties, underscoring their medicinal relevance. Compound identification was achieved through standard protocols and verified using Willey and NIST libraries, while Dr. Duke's Phytochemical and Ethnobotanical Databases were consulted to confirm their biological functions. Additionally, Fourier Transform Infrared (FTIR) spectroscopy was employed to detect the functional groups and structural features of these secondary metabolites, providing valuable qualitative and quantitative insights into the biomolecular composition. Phytochemical screening of stem and leaf extracts (using n-hexane, chloroform, ethanol, and aqueous solvents) confirmed the presence of tannins, saponins, flavonoids, alkaloids, and reducing sugars. However, their distribution varied across different extracts. The FTIR analysis supported these findings by revealing characteristic peaks corresponding to these metabolites. Overall, this investigation demonstrates that the novel *Jasminum grandiflorum* (White Flower type) genotype is a rich reservoir of bioactive compounds. The results highlight its promising role in the development of natural therapeutic agents and its potential contribution to the ongoing search for plant-based pharmaceutical resources.

**Keywords**: *Jasminum spp, GC-MS analysis, Phytochemicals, Stem extracts, FTIR, Bioactive compounds*

## INTRODUCTION:

Gas chromatograph-mass spectrometry (GC-MS) is a combined technique for the precise analysis of volatile compounds, including alcohols, acids, and esters, as well as detecting hydrocarbons with long and branched chains. It has been ethnobotanically reported that approximately 80% of the 122

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elements employed in modern healthcare products have been found to have similar activities to those registered for their respective original herbal drugs (Parnami & Lakhawat, 2022; Pipon, 2010). Herbal remedies are thus believed to meet approximately 80% of worldwide health needs, catering to millions residing in developing areas, especially rural ones. Historically, plant metabolites have been regarded as one of the most important sources of essential nutritional components. In recent times, restrictions on the development, promotion, and use of antibiotics derived from animals have shifted attention toward plant-based alternatives. Consequently, scientific interest has grown in plant metabolites as promising sources for alternative bioactive agents (Adamson *et al*., 2018). In the pharmaceutical field, the focus has increasingly turned to secondary plant metabolites due to their valuable roles in plant stress physiology, as well as their applications in nutrition and cosmetics. These secondary metabolites not only help plants mitigate stress but also serve as protective agents against toxicity (Ingle *et al*., 2016). Spectroscopic techniques are employed to detect the presence of such metabolites, providing valuable qualitative and quantitative information on biomolecular composition. FTIR is widely used to profile phytochemicals, producing signals that encompass a broad range of compounds detectable when whole cells are analysed. It is recognized as an exact analytical technique for identifying compound constituents and elucidating their structural characteristics (Hashimoto & Kameoka, 2008; Hussain *et al*., 2009). Foot-and-mouth disease (FMD) in animals is caused by the highly infectious foot-and-mouth disease virus (FMDV), which affects both wild animals and domesticated livestock, including cattle, buffaloes, pigs, goats, and sheep. The disease is characterized by fever, vesicular lesions, and sores on the feet, nose, tongue, or teats, with low mortality but high morbidity. Younus *et al*. (2017) employed the MTT assay [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide] to evaluate extracts of *Azadirachta indica*, *Moringa oleifera*, and *Morus alba* against FMDV, assessing their antiviral and cytotoxic activities. The present investigation was set up to evaluate the pharmaceutical properties of stem extracts from these three genotypes, thereby serving as a supplementary income source for jasmine farmers. FTIR was utilized to detect chemical compounds with potent antimicrobial and antioxidant properties.

## MATERIALS AND METHODS:

### *Plant Material Collection*

The Jasminum genotype studied included a white flower bud type of *Jasminum grandiflorum* (White Pitchi), developed at Tamil Nadu Agricultural University (TNAU). This genotype is distinctive among jasmine varieties, as most commercial cultivars typically produce buds with a white tinge. Fresh stem samples from *Jasminum* genotype were collected during 2023–2024 from the jasmine germplasm maintained at the Department of Floriculture and Landscaping, TNAU, Coimbatore District, Tamil Nadu, India.

**Fig 1: *Jasminum grandiflorum* (White budded flower type)**

### *Preparation of Methanolic Stem Extract*

The harvested stems were thoroughly cleaned, chopped into small pieces, and washed twice with deionized water. They were then air-dried in a cool, shaded environment. Once thoroughly dried, the stems were ground into a fine powder using a blender and stored in an airtight container for subsequent analysis (Guha *et al*., 2010; Sultana *et al*., 2009)

To extract the active constituents, 50 grams of the powdered material were placed in a 500 mL conical flask. A total of 300 mL of 70% methanol (methanol: water) was added, and the mixture was macerated at room temperature for three days with intermittent stirring (Salisu & Garba, 2008). The mixture was then filtered, and the filtrate was concentrated using a rotary evaporator (Brinkmann, R110). The concentrated extracts were stored in labelled vials and refrigerated at 4 °C for further analysis.

### *Gas Chromatography–Mass Spectrometry (GC-MS) Analysis*

Volatile components of the methanolic stem extract were analysed using an Agilent Technologies 7890A gas chromatograph coupled with a 5975C Mass Selective Detector (MSD), operating in electron ionization mode at 70 eV with the ion source temperature maintained at 250 °C. A DB-5MS capillary column (30 m × 0.25 mm × 0.25 µm, Agilent) was used, with helium (99.9%) as the carrier gas at a constant flow rate of 1 mL/min. Injection was performed in split mode (1:60) with an injection volume of 1 µL. The oven temperature was initially set at 100 °C and held for 0.5 minutes, then ramped to 140 °C at a rate of 20 °C/min and held for 1 minute, followed by a final increase to 280 °C at a rate of 11 °C/min over 20 minutes. Data acquisition and peak integration were performed using MassHunter software. Compound identification was performed by comparing the obtained mass spectra with those in the NIST Wiley 2008 and W9N11 libraries. Biological activities of the identified bioactive compounds were confirmed using Dr. Duke's Phytochemical and Ethnobotanical Databases, while molecular formula and weights were validated via PubChem.

### *ATR-FTIR (Attenuated Total Reflectance–Fourier Transform Infrared) Spectroscopy*

The powdered stem samples were analysed using ATR-FTIR spectroscopy with a Thermo Scientific Nicolet iS10 spectrometer equipped with a Germanium ATR crystal. The sample was firmly pressed against the crystal to ensure optimal contact. Infrared spectra were recorded over the wavenumber range of 4000–550 $cm^{-1}$. The infrared beam entered the crystal and generated evanescent waves, which interacted with the sample. The modified infrared signal was then collected by a detector for spectral interpretation.

## RESULTS & DISCUSSION:

The paramount importance of GC-MS applications lies in the determination of volatile organic compounds, such as alcohols or esters. The GC-MS also could discriminate long-chain aliphatic hydrocarbons from olefins and aromatics such as naphthene's or alkyl benzenes. GC-MS proved its worth in the aroma profiling of several *Jasminum* species (Ranchana *et al*., 2017) and in profiling metabolites and their biosynthetic pathways in putative mutants of *J. grandiflorum* (Soundarya *et al*., 2022). The study performed GC-MS analysis on stem extracts of Jasmine, revealing various phytochemical constituents. Retention time, molecular formulae,

**Table 1. Phytochemical compounds identified in the methanol extract of *J. grandiflorum* (White Flower type) stem**

| RT (min) | Chemical Compound | Molecular Formula | Molecular Weight (g/mol) | Area % |
|---|---|---|---|---|
| 5.1867 | Benzyl alcohol | $C_7H_8O$ | 108.14 | 2.02 |
| 6.3310 | 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- | $C_6H_8O_4$ | 144.13 | 1.49 |
| 8.5085 | Benzoic acid, 2-formyl-, methyl ester | $C_9H_8O_3$ | 164.16 | 3.43 |
| 8.9418 | Benzeneethanol, 4-hydroxy- | $C_8H_{10}O_2$ | 138.16 | 2.61 |
| 9.2528 | Dimethyl{bis[(2Z)-pent-2-en-1-yloxy]} silane | $C_{12}H_{24}O_2Si$ | 244.41 | 1.61 |
| 9.3084 | Doconexent | $C_{22}H_{32}O_2$ | 328.49 | 1.32 |
| 9.4084 | Benzo[b]thiophene 1,1-dioxide, 3-methyl- | $C_9H_8O_2S$ | 180.23 | 2.49 |
| 9.8639 | Homovanillyl alcohol | $C_9H_{12}O_3$ | 168.19 | 3.33 |
| 11.4859 | 4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol | $C_{10}H_{12}O_3$ | 180.20 | 5.53 |
| 11.7970 | Papaveroline, 1,2,3,4-tetrahydro-3-O-methyl- | $C_{17}H_{19}NO_4$ | 301.34 | 3.06 |
| 12.7413 | Hexadecanoic acid, methyl ester | $C_{17}H_{34}O_2$ | 270.45 | 2.91 |
| 13.8411 | 9,12-Octadecadienoic acid (Z, Z)-, methyl ester | $C_{19}H_{34}O_2$ | 294.48 | 13.39 |
| 17.7962 | Squalene | $C_{30}H_{50}$ | 410.72 | 1.68 |
| 20.1070 | Vitamin E | $C_{29}H_{50}O_2$ | 430.71 | 1.85 |
| 22.2512 | γ-Sitosterol | $C_{29}H_{50}O$ | 414.71 | 6.02 |

and peak area confirmed these phytochemicals. The present experimental outcomes are shown in Figure 2. The NIST Database predicted the compounds. The GC-MS of the sample revealed 9,12-Octadecadienoic acid (Z, Z)-, methyl ester (RT 13.8411 min) as the most dominant compound, covering 13.39% of the total peak area. Other major compounds were γ-Sitosterol (RT 22.2512 min, 6.02%), 4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol (RT 11.4859 min, 5.53%), Benzoic acid, 2-formyl-, methyl ester (RT 8.5085 min, 3.43%), and Homovanillyl alcohol (RT 9.8639 min, 3.33%). Also detected were several other important compounds including Papaveroline, 1,2,3,4-tetrahydro-3-O-methyl- (3.06%), Hexadecenoic acid, methyl ester (2.91%), and Benzene ethanol, 4-hydroxy- (2.61%). These chemical compositions reveal a heterogeneous composition dominated by fatty acid esters, phytosterols, and phenolic derivatives, which can significantly contribute to the bio-functional properties of the extract.

### *FTIR peak values and functional groups.*

In evaluating the FTIR of the stem extract of *Jasminum grandiflorum*, the hydroxyl group stretch finally arrived from the 3280/cm peak, confirming the presence of polyphenols in the stem macerates of *Jasminum grandiflorum* with a white flower bud type. Then again, at 2884/cm peak, the spectra were attributed to terpenes (C-H). At 2353/cm, C=N stretches were assigned to nitrites as per Table 2 and Fig. 3. At 1730/cm, thereby, stretches of C=O (carboxylic) were observed. Following this are alkaloids detected at 1514/cm, which are stressed through N-H stretching, while the peak at 1600/cm indicates the presence of primary amines (Table 2). The esters showed the presence of amines (C-N) or C-O stretches at 1232 $cm^{-1}$ and 1155 $cm^{-1}$, respectively (Fig. 3).

Various potential pharmacological properties are ascribed to the compounds identified from *Jasminum grandiflorum*. Those reported to show antioxidant activities within this study include homovanillyl alcohol (Benincasa *et al*., 2024; Bernini *et al*., 2019), (4-((1E)-3-hydroxy-1-propenyl)-2-methoxyphenol (Mahatheeranont, 2020) and octadecenoic acid, methyl ester (Yu *et al*., 2005). In the same way, hexadecenoic acid, methyl ester, has been reported to show antifungal activity (Sharma *et al*., 2021). Antimicrobial activities have been reported for benzoic acid, 4-ethoxy ethyl ester (Sheela & Uthayakumari, 2013), whereas antibacterial activities are attributed to hexadecenoic acid, methyl ester (Shaaban *et al*., 2021) and 9,12-octadecadienoic acid, methyl ester (Shoge & Amusan, 2020). Among the plant sterols, γ-sitosterol (Sundarraj *et al*., 2012) is one with its health benefits in anti-inflammation, lowering cholesterol, promoting cardiovascular health, and managing metabolic disorders; it could also retard cancer cell growth. Further, benzeneethanol, 4-hydroxy- (Li *et al*., 2018) has also exhibited nematicidal activity.

For FTIR analysis, stem powders of Jasminum grandiflorum were subjected to detect and document the functional groups present in different parts of the plant. Depending upon the peak portions that act as a fingerprint and functional groups, differences and similarities among the different parts of plants were identified. Functional groups were characterized in this study as C-O, N=O, C=O, C-N, C-H, and C-O and were recorded at their corresponding absorbance peaks. These functional groups are attributed to alkyl, anhydrides, deoxyribose, esters, and alcoholic group formations (Sohrabi & Ebrahiminezhad, 2020). The present work is in agreement with the results of

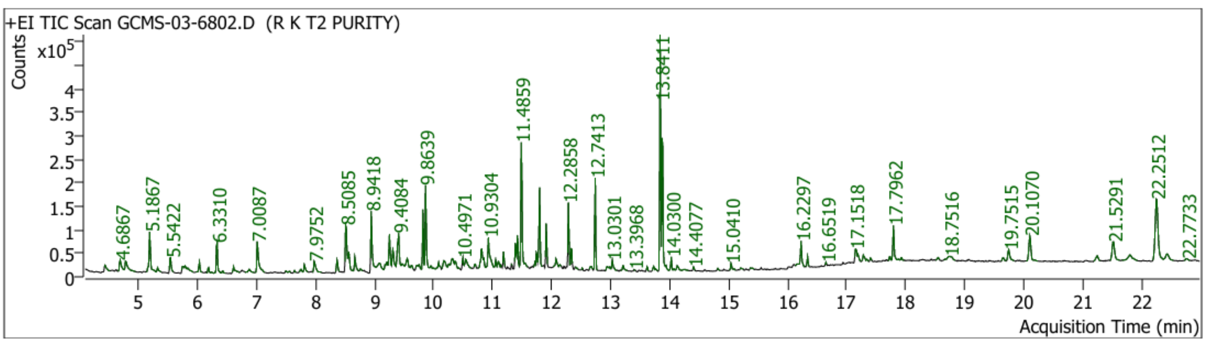


**Figure 2: GC-MS chromatogram of *J. grandiflorum* (WF) stem.**

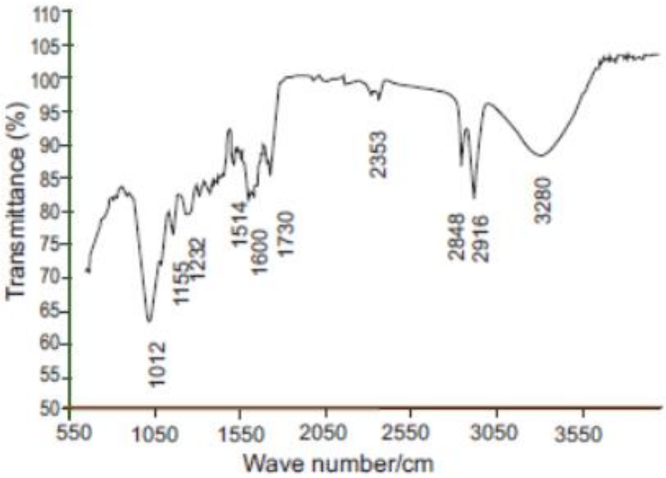


**Figure 3. *Jasminum grandiflorum* stem's FTIR spectra.**

**Table 2. FTIR peak values and functional groups**

| Wavenumber ($cm^{-1}$) | Bond / Compound | Functional Group / Possible Assignment |
|---|---|---|
| 3290 | O–H | Polyphenols |
| 3280 | – | – |
| 2916 | – | Phenols |
| 2848 | C–O | Carboxylic acid |
| 2353 | C≡N | Nitriles |
| 1730 | C=O | Saponins |
| 1631 | C=O | Flavonoids |
| 1602 | – | Alkenes |
| 1600 | – | Primary amines |
| 1514 | N–H | Alkaloids |
| 1454 | C–H | Terpenes |
| 1305 | S=O | Sulphate esters |
| 1232 | C–N | Amines |
| 1157 | C–O | Esters |
| 1155 | C–O | Esters |
| 1012 | C–O | Esters |

Mariswamy et al. (2012), who carried out FTIR analysis on *Aerva lanata* (L.) Juss. Ex Schult. Correspondingly, this study also supported the work of Maobe and Nyarango (2013) and that of Bobby et al. (2012), who reported that these groups exhibited relevant absorption values of peak intensities in the leaves of Utrica dioica as well as Albizia lebbeck Benth.

## CONCLUSION:

The current study revealed that the stems of *Jasminum grandiflorum* (White Flower bud type) are a rich biorepository of various bioactive compounds, as supported by GC–MS and FTIR analyses. GC–MS profiling revealed fatty acid esters, phytosterols, and phenolic derivatives as the primary components, most of which have been reported to exhibit antioxidant, antimicrobial, antifungal, antibacterial, anti-inflammatory, and nematicidal activities. Through FTIR spectroscopy, the functional groups present in phenols, terpenes, saponins, flavonoids, alkaloids, amines, esters, and carboxylic acids were identified, indicating the complex phytochemical nature of the extract. Thus, the stem extracts of *J. grandiflorum* can be promoted for their significance as natural therapeutic agents, thereby earning a position in the pharmaceutical, nutraceutical, and agro-industries.

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