Pharmacogn. Res., 2026; 18(4):1577-1581.
https://www.phcogres.com

Original Article

Comprehensive GC-MS Profiling of Bioactive Metabolites in *Syzygium samarangense* Root Extract

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ABSTRACT

Background/Aim: Gas Chromatography coupled on-line with Mass Spectrometry (GC-MS) is one of the best instrumental method to determine the secondary metabolites presented in the plant extracts. Comprehensive Gas Chromatography-Mass Spectrometry (GC-MS)-based metabolite profiling was performed to identify and characterize the bioactive compounds present in the root extract of *Syzygium samarangense*. **Materials and Methods:** The aqueous root extract was prepared and analyzed by GC-MS against the NIST/Wiley library to assign putative chemical identities. The selected major peaks were tentatively identified based on their retention indices and mass fragmentation patterns, and their relative abundances were estimated. **Results:** The chromatogram revealed the presence of several classes of secondary metabolites, including phenolic compounds, terpenoids, fatty acids, sterols, many of which are reported to possess antioxidant, anti-inflammatory, antimicrobial, and/or antidiabetic properties. The results provide a detailed chemical fingerprint of *Syzygium samarangense* root metabolites. **Conclusion:** The present findings highlighting its potential as a rich source of bioactive constituents for further pharmacological investigation and the possible development of natural-product-based therapeutics.

Keywords GC-MS Analysis, Metabolite Profiling, Secondary Metabolites, *Syzygium Samarangense*, *Terpenoids*.

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Received: 26-10-2025;
Revised: 16-01-2026;
Accepted: 03-03-2026.

INTRODUCTION

The plant *Syzygium samarangense* was traditionally used as a best medicine for many systemic diseases. Several researchers were documented the potential benefits of many phytoconstituents of this plant including flavonoids and anthocyanins. The pharmacological effect of various extracts of this plant already documented well also (Khamchan *et al*., 2018; Mahmoud *et al*., 2021; Sobeh *et al*., 2018). Myricitrin and 3,5-di-O-methyl gossypetin were isolated from the leaf of *Syzygium samarangense* and the anti-oxidative effect of these components were well documented (Sobeh *et al*., 2019). Several components of methanolic leaf extract of *Syzygium samarangense* were isolated. Most of the components belongs to flavonoid, tannins and polyphenols (Sobeh *et al*., 2018). Many older studies reported that, the plant *Syzygium samarangense* contains phenolic components as secondary metabolites with promising pharmacological activities (Hassan *et al*., 2022).

DOI: 10.5530/pres.20260193

Gas Chromatography coupled on-line with Mass Spectrometry (GC-MS) is one of the best instrumental method to determine the secondary metabolites presented in the plant extracts. The characterization of phytoconstituents through GC-MS can provide complete metabolite profile (Frolova *et al*., 2026). The GC-MS methods is modern technique, which can separate and identify the phytoconstituents in single step by using GC-MS library (Arifuzzaman *et al*., 2025). Hence, the present study was designed to investigate the important phytoconstituents present in the aqueous extract of root of *Syzygium samarangense* by using GC-MS method.

MATERIALS AND METHODS

Plant Collection and Authentication

The root of *Syzygium samarangense* was collected from surrounding village of Rajampet Kadapa, A.P, India in the month of September 2018. The root was further verified and authenticated as the root of *Syzygium samarangense* (Blume) Merr and L.M. Perry from the family of Myrtaceae by Dr. M.V. Suresh Babu Department of Botany, Govt Degree College, Rajampet, Kadapa, A.P, India and voucher specimen number was lodged (ANCP-MP-COL-01/2018-19).

Preparation of Aqueous extract of root of *Syzygium samarangense*

Fresh roots were collected and dried in the shade. The shade-dried roots of the plant (500 g) were powdered, sieved through a mesh of size 80 to obtain a powder of uniform size, soaked in cold water (cold percolation) for 3 days, and the aqueous extract were decanted. The solvent of the total liquid extract was evaporated by distillation to a concentrate over a water bath to a syrupy consistency and then evaporated to dryness under vacuum to give the dry extract (16%w/w yield). The extract was stored at 4°C for further analysis.

Phytochemical Screening

The crude aqueous extract subjected to preliminary phytochemical screening to identify the major phytochemical constituent's by using standard protocols. The Total Phenolic Content (TPC) and Total Flavonoid Content (TFC) were analysed by using the Folin-Ciocalteu reagent method with gallic acid as the standard and aluminum chloride colorimetric method with quercetin as the standard respectively, following a standard protocol with minor modifications (Arifuzzaman *et al*., 2025).

TPC determination

2 mg of the extract were dissolved in distilled water to obtain a stock concentration of 1 mg/mL. An aliquot of 0.5 mL of this extract was mixed with 2 mL of diluted Folin-Ciocalteu reagent and allowed to stand at 22 ± 2°C for 5 min. Subsequently, 2.5 mL of 7.5% (w/v) sodium carbonate solution was added, and the mixture was gently vortexed and incubated for 20 min for color development. The absorbance was measured at 760 nm using a UV-visible spectrophotometer. TPC was calculated from the gallic acid calibration curve and expressed as mg Gallic Acid Equivalents (GAE) per g of dry extract.

TFC determination

Briefly, 1.5 mL of the extract was mixed with 0.1 mL of 10% $AlCl_3$, followed by 0.1 mL of 1 M sodium acetate. After standing for 30 min, 1 mL of 1 M NaOH was added, and the volume was adjusted to 5 mL with double-distilled water. The reaction mixture was incubated for 15 min, and absorbance was recorded at 415 nm. TFC was calculated from the quercetin calibration curve and expressed as mg Quercetin Equivalents (QE) per gram of dry extract.

The TLC profiling was analysed as described by a previous study by using silica gel plates and the mobile phase n-hexane:ethyl acetate: glacial acetic acid (85:20:5 v/v/v). The extract was spotted onto the plate and developed in a saturated chamber until the solvent front reached an appropriate height. After drying, the chromatogram was visualized under UV light (Appamaraka *et al*., 2022).

GC-MS Analysis

The GC-MS analysis was carried out with 6890 N Agilent gas chromatograph attached with a JMS 600 H JEOL mass spectrometer. The phyto constituents present in the extract was separated on a fused capillary SPBI column, 30 m 0.32 mm, 0.25 µm film thicknesses in a temperature program initially 50 to 256°C with a rate of 4°C/min with 2 min hold. The injector was at 260°C and the flow speed of the carrier gas helium, was 1 mL/min. The EI mode JMS 600 H JEOL mass spectrometer had ionization volt of 70 Ev, electron emission of 100 Ma, ion source temperature of 250°C and analyzer temperature of 250°C. The extract was injected 1 µL manually in split mode with the ratio of sample in split mode was 20:1. GC-MS detection was based on the computer evaluation of mass spectra of samples through National Institute Standard and Technology (NIST), through comparison of peaks and retention time and computer matching as well as by following the characteristic fragmentation patterns of the mass spectra of particular class of compounds.

Statistical analysis

The research work is purely depending on phytochemical analysis of aqueous extract of root of *Syzygium samarangense*. Hence, only description of GC-MS results is included without any specific descriptive statistical analysis

RESULTS

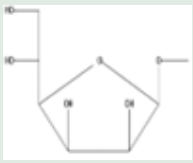
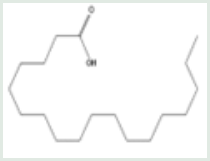
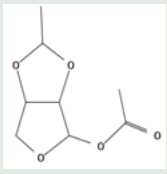
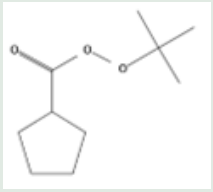
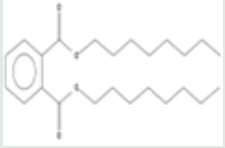
Preliminary phytochemical investigation revealed the presence of terpenoids, carbohydrates, lipids, and flavonoids. Quantitative analyses revealed a substantial Total Phenolic Content (TPC) ranging from 61.41 to 143.68 ppm and Total Flavonoid Content (TFC) between 45.76 and 148.53 ppm in the aqueous extract of the root. TLC analysis of the extract confirmed that the mobile phase n-hexane: ethyl acetate: glacial acetic acid in the ratio of 85:20:5 gave better separation, and three compounds were observed with R_f values of 0.36, 0.82, and 0.94 (Figure 1).

The aqueous extract of root of *Syzygium samarangense* was analyzed by GC-MS to detect various compounds with the help of NIST library. Totally 11 major compounds were identified which have been listed in Table 1. The chromatograph showed 48 peaks with 48 individual compounds (Figure 2).

DISCUSSION

GC-MS profiling of the *Syzygium samarangense* root extract revealed a diverse array of bioactive metabolites, predominantly therapeutic fatty acids, phytosterols, and terpenoids. These findings are consistent with comprehensive phytochemical reviews of the species, which report sterols among the major classes of metabolites found in *Syzygium samarangense* (Sandhiya and Amudha, 2025; Tarigan, 2021). The synergistic action of compounds such as n-hexadecanoic acid, squalene, lupeol, and eugenol imparts significant antimicrobial, anti-inflammatory,

Table 1: GC-MS profile of Phytoconstituents of *Syzygium samarangense* root.

Sl. No.	Retention Time	Peak area %	Name of the compound	Molecular formula	Molecular weight	Chemical structure	Nature of the compound
1.	7.045	2.796	1,4-Dioxane-2,5-Dione, 3,6- Dimethyl	$C_6H_8O_4$	144		Lactone derived from lactic acid
2.	18.360	37.943	Beta-D-Mannofuranoside, Methyl	$C_7H_{14}O_6$	194		Carbohydrate Derivative Acts as A Substrate for glucosidase
3.	19.610	13.547	N-Hexadecanoic Acid	$C_{16}H_{32}O_2$	256		Saturated Fatty acid known as Palmitic acid
4.	19.885	7.054	Octadecanoic acid	$C_{18}H_{36}O_2$	284		Saturated fatty acid known as Stearic acid
5.	20.265	1.441	1-O-Acetyl-Exo-2,3-O-Ethylidine-Beta -D-Erythrofuranose	$C_8H_{12}O_5$	188		Cyclic hemiacetal Carbohydrate Derivative
6.	20.371	3.077	Hexadecanoic Acid,1,1-Dimethylethyl Ester	$C_{20}H_{40}O_2$	312		Ester of Palmitic acid
7.	20.896	23.139	9-Oxanonanoic Acid	$C_9H_{16}O_3$	172		Medium-chain oxo-fatty acid, acetyl-CoA carboxylase inhibitor
8.	21.656	2.095	11-Tridecen-1-Ol	$C_{13}H_{26}O$	198		Fatty alcohol
9.	21.746	1.598	Hexadecanoic Acid,2-Hydroxy-Methyl Ester, Acetate	$C_{19}H_{36}O_4$	328		Esterified form of Palmitic acid
10.	21.846	2.133	T-Butyl Cyclopentane peroxy carboxylate	$C_{10}H_{18}O_3$	186		Hydrocarbon
11.	23.257	5.179	Di-N-Octyl phthalate	$C_{24}H_{38}O_4$	390		Esters of phthalic acid

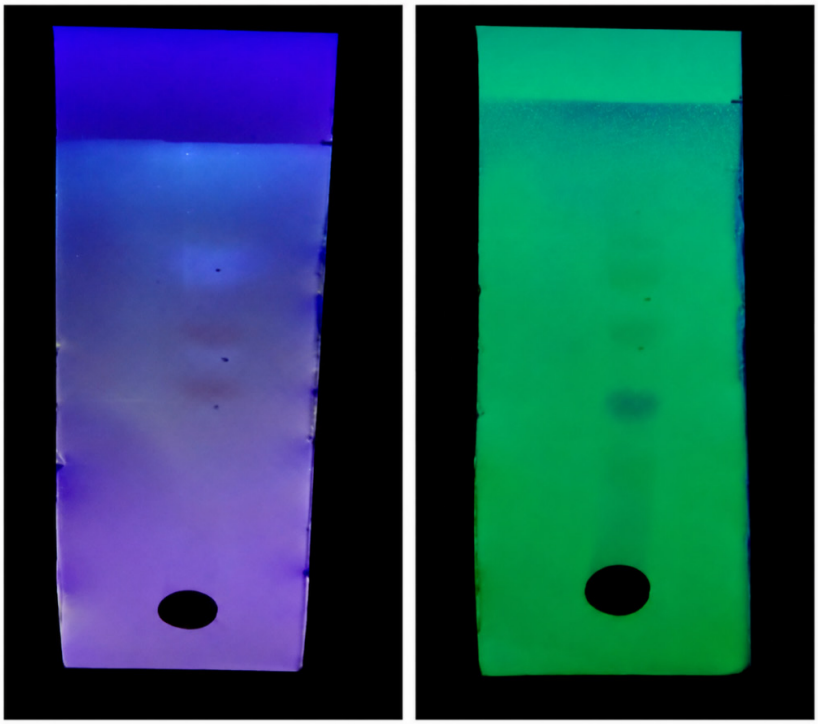


Figure 1: TLC analysis of aqueous extract of root of *Syzygium samarangense.*

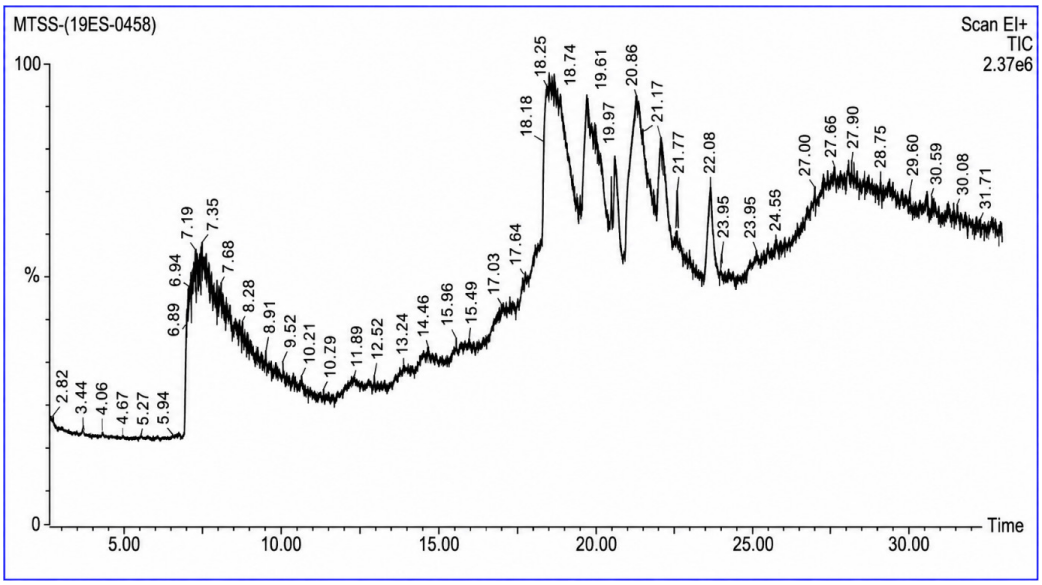


Figure 2: GC-MS spectral chromatogram of aqueous root extract of Syzygium samarangense.

and antioxidant properties to the root extract. These findings strongly validate the traditional ethnomedicinal applications of the plant roots and underscore their potential as a viable source of novel plant-based pharmacological therapeutics. Ultimately, this study advances the pharmacognostic understanding of *Syzygium samarangense* and supports the sustainable utilization of medicinal plant resources for human health benefits.

CONCLUSION

The findings from the present analysis indicate that *Syzygium samarangense* root extract possesses a diverse array of bioactive phytoconstituents that collectively support its traditional medicinal applications and pharmacological potential.

ACKNOWLEDGEMENT

The author acknowledges the Annamacharya College of Pharmacy, India faculty members and management for the laboratory facility provided to carry out possible research work.

ABBREVIATIONS

GC-MS: Gas Chromatography-Mass Spectrometry; **NIST:** National Institute of Standards and Technology; **TPC:** Total Phenolic Content; **TFC:** Total Flavonoid Content; **TLC:** Thin Layer Chromatography; **EI:** Electron Ionization; **eV:** Electron Volt.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ETHICAL STATEMENT

The present research work does not involve by using human or animal studies. Hence, ethics approval not applicable. The plant collection complied with relevant institutional and national guidelines.

SUMMARY

This study provides a comprehensive GC-MS-based phytochemical profiling of the aqueous root extract of *Syzygium samarangense*. The analysis identified 11 major bioactive metabolites-including therapeutic fatty acids, phytosterols, and terpenoids-confirming the plant's traditional medicinal value and its potential for developing natural therapeutics.

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Cite this article: Saleem TSM. Comprehensive GC-MS Profiling of Bioactive Metabolites in *Syzygium samarangense* Root Extract. Pharmacog Res. 2026;18(4):1577-81.