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Original Research Article

GC-MS Analysis of Hexane Extracts from the Roots, Stems, and Leaves of *Hyptis suaveolens*: Organ-Specific Phytochemical Profiling

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KEYWORDS
Hyptis suaveolens,
GC–MS profiling,
Phytochemical analysis,
Hexane extract,
Organ-specific,
Lamiaceae,
Volatile compounds.

ABSTRACT
Phytochemical characterization of medicinal plants is essential for elucidating their bioactive constituents and supporting their ethnopharmacological applications. *Hyptis suaveolens* (L.) Poit. (Family *Lamiaceae*) is widely utilized in traditional medicine for the management of infectious, inflammatory, and febrile conditions. However, comparative organ-specific chemical profiling of its non-polar extracts remains limited. This study aimed to characterize and compare the volatile and semi-volatile constituents of hexane extracts obtained from the roots, stems, and leaves of *Hyptis suaveolens* collected in Kano, Nigeria using Gas Chromatography–Mass Spectrometry. Plant organs were air-dried, pulverized, and macerated in hexane, and the extracts were analyzed using Agilent 7890A GC system coupled to a 5975C mass selective detector. Compound identification was performed by comparison with the NIST spectral library using a similarity index ≥ 80%. GC–MS analysis revealed distinct organ-specific phytochemical distributions. The root extract was dominated by bicyclic and heterocyclic compounds, notably cis-7-oxabicyclo[4.3.0]nonan-8-one (24.535%) and 2-butynedioic acid, di-2-propenyl ester (21.555%). The stem extract was characterized predominantly by fatty acid methyl esters, with hexadecanoic acid methyl ester (27.757%) and 10-octadecenoic acid methyl ester (20.790%) as the major constituents. Similarly, the leaves extract was rich in fatty acid derivatives, particularly pentadecanoic acid, 14-methyl-, methyl ester (29.898%) and 9-octadecenoic acid methyl ester (21.847%), alongside the diterpenoid phytol (6.989%). These findings demonstrate pronounced organ-specific variation in lipophilic secondary metabolites of *H. suaveolens*, highlighting the chemical diversity of this species. The study provides phytochemical data for *H. suaveolens* from Kano Nigeria and establishes a basis for future bioassay-guided fractionation and pharmacological investigations.

CITATION
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INTRODUCTION

Phytochemical analysis of medicinal plants is fundamental for elucidating their chemical composition and providing scientific validation for their traditional therapeutic applications. *Hyptis suaveolens* (L.) Poit., commonly known as bush mint, is widely distributed

across tropical and subtropical regions and is extensively used in ethnomedicine for the treatment of febrile conditions, infectious diseases, gastrointestinal disorders, and inflammatory ailments. Previous studies have reported that *H. suaveolens* contains diverse classes of secondary metabolites, including flavonoids, alkaloids, saponins, tannins, terpenoids, and phenolic compounds (Ojeaburu, and Uanseoje; 2025, Amaka *et al*., 2018; Ghaffari *et al*., 2014). Investigations involving essential oil analysis and preliminary phytochemical screening further indicate that the plant's chemical composition may vary depending on geographical origin, extraction solvent, and the specific plant organ examined (Mishra *et al*., 2021).

Despite these contributions, several gaps remain in the existing literature. Many studies have focused primarily on essential oils or single plant organs—most commonly the leaves while integrated comparative profiling of roots, stems, and leaves within a unified analytical framework remains limited. In addition, environmental and ecological factors can influence the biosynthesis and accumulation of secondary metabolites; however, region-specific phytochemical data for several populations of *H. suaveolens*, particularly those from Nigeria, remain insufficiently documented (Starlin *et al*., 2019). Furthermore, earlier investigations often relied on preliminary phytochemical screening methods that provide only broad classification of metabolite groups without detailed compound-level identification.

Gas Chromatography–Mass Spectrometry (GC–MS) is a well-established analytical technique for the identification and characterization of volatile and semi-volatile compounds in complex plant extracts. The use of non-polar solvents such as hexane is particularly advantageous for extracting lipophilic constituents, including volatile and semi-volatile metabolites that may not be efficiently recovered using polar solvents. Nevertheless, systematic GC–MS-based comparative profiling of non-polar extracts from multiple anatomical parts of *H. suaveolens* collected in Nigeria has not been comprehensively reported.

Accordingly, the present study undertakes a GC–MS characterization of hexane extracts derived from the roots, stems, and leaves of *H. suaveolens* collected in Nigeria. By performing a comparative analysis of different plant organs under standardized experimental conditions, this study aims to generate organ-specific and region-specific phytochemical data and to contribute to a more comprehensive understanding of the chemical diversity of this medicinal plant.

MATERIALS AND METHODS

Collection of Plant Sample

A plant *Hyptis suaveolens* was collected, identified and authenticated by the Department of Plant Bioresources, Bioresource Development Centre, National Biotechnology Development Agency (NABDA), Nigeria. A voucher specimen was subsequently prepared and deposited in the herbarium of the Department of Plant Bioresources, Bioresource Development Centre, NABDA, and assigned the voucher number NABDA/BDC/PBR/2024/019.

Preparation of Hexane Extract

Twenty grams (20g) of the powdered sample material were macerated in 200 mL of hexane for 72 hours with intermittent agitation. Following the extraction period, the mixture was filtered through Whatman No. 1 filter paper, and the solvent was subsequently removed under reduced pressure using a rotary evaporator to yield the hexane extract.

Gas Chromatography-Mass spectrometry (GC-MS) Analysis

GC–MS analysis of the hexane extracts of *Hyptis suaveolens* was performed at the Chemistry Analytical Laboratory, Yobe State University, using an Agilent 7890A gas chromatograph coupled to a 5975C mass selective detector fitted with an HP-5MS capillary column. Helium served as the carrier gas at a flow rate of 1 mL/min, and 1 µL of each extract was injected in splitless mode at an injector temperature of 250°C. The oven temperature was programmed from 80°C (2 min hold) to 240°C at 12°C/min with a final hold of 6 min. Mass spectra were recorded under electron ionization at 70 eV over an m/z range of 50–500, with source and interface temperatures maintained at 230°C and 250°C, respectively. Compound identification was accomplished using the NIST 14 spectral library with a minimum similarity index of 80%, and retention times were confirmed with literature data to ensure analytical reliability.

RESULTS AND DISCUSSION

Root Extract of *Hyptis suaveolens*

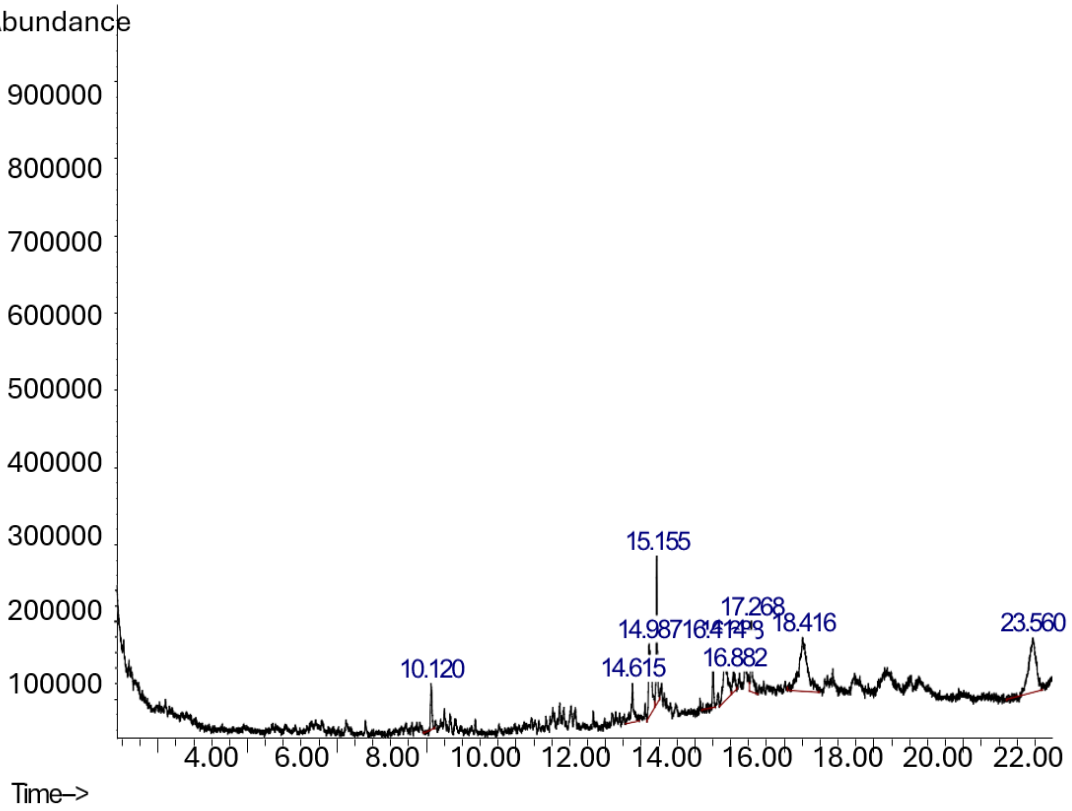

Figure 1: Chromatogram Showing GC-MS Result of Hexane Root Extract of *Hyptis suaveolens*

Table 1: Compounds Identified from the Hexane Root Extract of *Hyptis suaveolens*

Peak	Compounds	RT (Mins)	Area %	MW
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	10.120	3.380	206
2	Benzene, (2-methylpropoxy)-	14.615	5.486	150
3	3-Tridecen-1-yne, (E)-	14.987	11.560	176
4	1H-Pyrrole-2,5-dione, 2,5-dihydro-1-(3,5-dimethylphenyl)-	15.155	10.295	201
5	2-Methyl-Z,Z-3,13-octadecadienol	16.414	3.662	280
6	9-Oxabicyclo[6.1.0]nonane	16.688	10.158	126
7	Bicyclo[2.2.2]octane, 1-chloro-	16.882	2.574	144
8	9-octadecanoic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester	17.268	6.796	464
9	cis-7-Oxabicyclo[4.3.0]nonan-8-one	18.416	24.535	140
10	2-Butynedioic acid, di-2-propenyl ester	23.560	21.555	194

Stem Extract of *Hyptis Suaveolens*

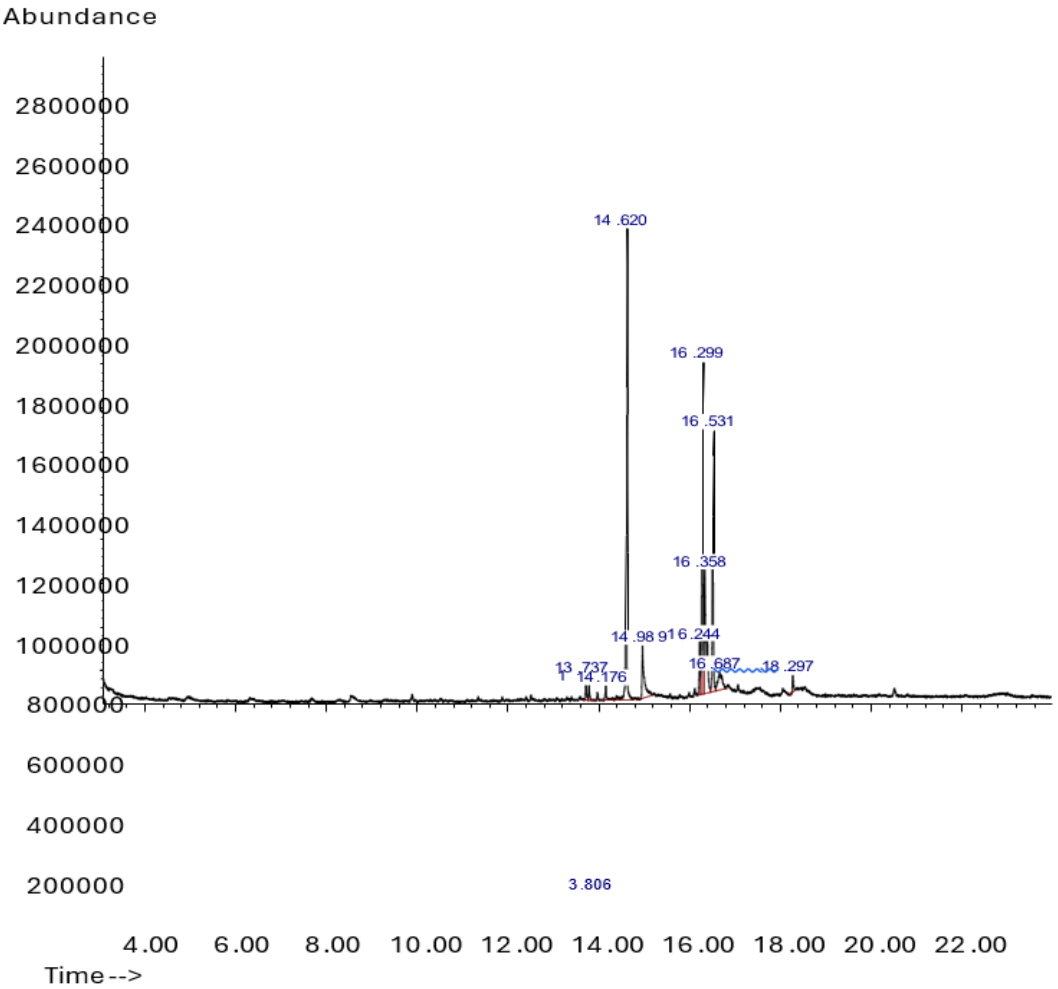

Figure 2: Chromatogram Showing GC-MS Result of Hexane Stem Extract of *Hyptis suaveolens*

Table 2: Compounds Identified from the Hexane Stem Extract of *Hyptis Suaveolens*

Peak	Compounds	RT (Mins)	Area %	MW
1	1,12-Tridecadiene	13.737	1.752	180
2	Bicyclo[2.2.1]heptane, endo-2-methyl-exo-2 acetoxy	13.806	1.177	168
3	1,3-Cycloheptadiene	14.176	1.277	94
4	Hexadecanoic acid, methyl ester	14.620	27.757	270
5	n-Hexadecanoic acid	14.989	7.103	256
6	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	16.244	3.448	294
7	10-Octadecenoic acid, methyl ester	16.299	20.790	296
8	9-Octadecenoic acid, methyl ester	16.358	15.576	296
9	Methyl stearate	16.531	15.528	298
10	Eicosanoic acid, methyl ester	16.687	4.469	326
11	Dimethyl palmitanine	18.297	1.124	269

Leaves Extract of *Hyptis suaveolens*

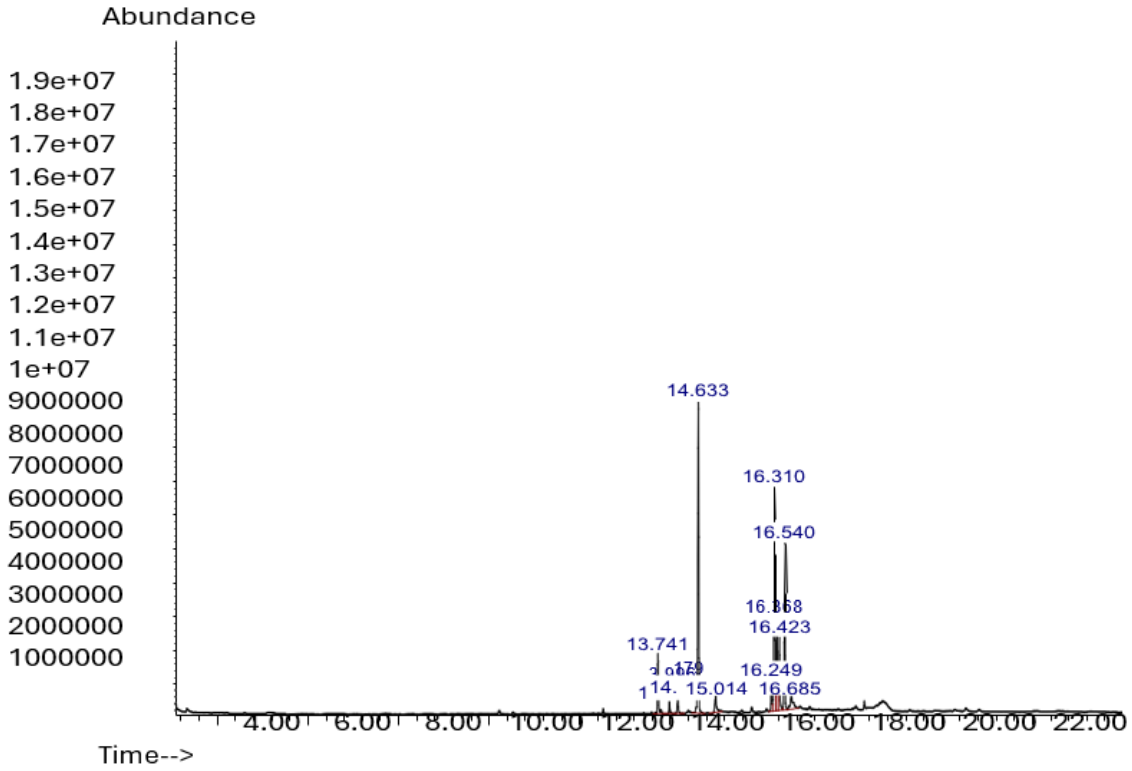

Figure 3: Chromatogram Showing GC-MS Result of Hexane Leaves Extract of *Hyptis suaveolens*

Table 3: Compounds Identified from the Hexane Leaves Extract of *Hyptis Suaveolens*

Peak	Compounds	RT (Mins)	Area %	MW
1	Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, (1α,2β,5α)-	13.741	5.861	138
2	3,4-Octadiene, 7-methyl-	13.996	1.037	124
3	1-Hexadecyne	14.179	1.855	222
4	Pentadecanoic acid, 14-methyl-, methyl ester	14.633	29.898	270
5	n-Hexadecanoic acid	15.014	2.649	256
6	Methyl 5,12-octadecadienoate	16.249	2.753	294
7	9-Octadecenoic acid (Z)-, methyl ester	16.310	21.847	296
8	9-Octadecenoic acid, methyl ester	16.368	9.171	296
9	Phytol	16.423	6.989	296
10	Methyl stearate	16.540	14.447	298
11	9,12-Octadecadienoic acid (Z,Z)-	16.685	3.493	280

Discussion

The GC–MS analysis of the hexane extracts of *Hyptis suaveolens* root, stem, and leaves revealed a chemically diverse profile dominated largely by lipophilic constituents, including fatty acid methyl esters, long-chain hydrocarbons, terpenoids, bicyclic compounds, and aromatic derivatives (Tables 1-3, Figures 1–3)). The predominance of non-polar secondary metabolites across all plant parts reflects the extraction selectivity of hexane and is consistent with earlier phytochemical investigations of *H. suaveolens* and related *Lamiaceae* species (Iwalewa *et al*., 2008; Osho *et al*., 2020; Ezeonu *et al*., 2018). This findings provide a detailed chemical list of the volatile and semi-volatile fractions of the plant and demonstrate organ specific variation in metabolite distribution.

In the hexane root extract of *Hyptis suaveolens* (Table 1, Figure 1), cis-7-oxabicyclo[4.3.0]nonan-8-one (24.535%) and 2-butynedioic acid, di-2-propenyl ester (21.555%) were the most abundant constituents, followed by 3-tridecen-1-yne, (E)- (11.560%), 1H-pyrrole-2,5-dione, 2,5-dihydro-1-(3,5-dimethylphenyl)- (10.295%), and 9-oxabicyclo[6.1.0]nonane (10.158%). Additional components included benzene, (2-methylpropoxy)- (5.486%), 9-octadecanoic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester (6.796%), phenol, 2,6-bis(1,1-dimethylethyl)- (3.380%), and 2-methyl-Z,Z-3,13-octadecadienol (3.662%). The root extract therefore

exhibited a profile enriched with bicyclic ketones, unsaturated esters, heterocyclic derivatives, and minor phenolic constituents, distinguishing it from the other plant parts.

The hexane stem extract (Table 2, Figure 2) was characterized predominantly by fatty acid methyl esters, with hexadecanoic acid, methyl ester (27.757%) and 10-octadecenoic acid, methyl ester (20.79%) as major components. Other significant constituents included 9-octadecenoic acid, methyl ester (15.58%), methyl stearate (15.53%), 9,12-octadecadienoic acid (Z,Z)-, methyl ester (3.448%), and eicosanoic acid, methyl ester (4.47%) (Adeleke *et al*., 2021). Minor compounds such as dimethyl palmitanine (1.12%), 1,3-cycloheptadiene (1.28%), and bicyclo[2.2.1]heptane, endo-2-methyl-exo-2-acetoxy (1.18%) were also detected. The stem extract thus displayed a strong predominance of saturated and unsaturated long-chain fatty acid derivatives, with relatively fewer heterocyclic or bicyclic compounds compared to the root. Structurally related bicyclic ketones, esters, and heterocyclic derivatives have previously been reported in *H. suaveolens* extracts (Ezeonu *et al*., 2018),

Similarly, the hexane leaves extract (Table 3, Figure 3) was dominated by fatty acid esters, particularly pentadecanoic acid, 14-methyl-, methyl ester (29.898%), 9-octadecenoic acid (Z)-, methyl esters, and 9-octadecenoic acid, methyl esters (21.847% and 9.171%), and methyl stearate (14.447%). Additional constituents included phytol (6.989%), bicyclo[3.1.1]heptane, 2,6,6-trimethyl- (camphene; 5.861%), n-hexadecanoic acid (2.649%), 9,12-octadecadienoic acid (Z,Z) (3.493%), and minor hydrocarbons such as 3,4-octadiene, 7-methyl- and 1-hexadecyne. The leaves therefore combined fatty acid derivatives with notable terpenoid components, contributing to a chemically rich but distinct profile compared to the stem and root.

Comparative analysis shows that fatty acid methyl esters were present in all plant parts, with the root relatively enriched in bicyclic and heterocyclic compounds, the stem dominated by long-chain saturated and unsaturated esters, and the leaves containing both fatty acid derivatives and notable terpenoids such as phytol and camphene, highlighting organ-specific metabolite distribution in *Hyptis suaveolens*. These variations reflect organ specific metabolite patterns, which can inform targeted bioassay-guided fractionation and isolation of compounds. This study presents a comprehensive chemical profile of *H. suaveolens* hexanolic extracts, providing a valuable framework for future phytochemical and pharmacological research.

CONCLUSION

GC–MS analysis of hexane extracts from the roots, stems, and leaves of *Hyptis suaveolens* revealed distinct organ-specific differences in lipophilic phytochemical composition. The root extract was characterized mainly by bicyclic ketones, heterocyclic derivatives, and unsaturated esters, whereas the stem and leaf extracts were dominated by fatty acid methyl esters, with the leaves exhibiting the highest abundance of these compounds. These results highlight the chemical diversity of *H. suaveolens* and provide organ-specific phytochemical data for populations from Nigeria. However, the study is limited to GC–MS-based chemical profiling and does not include biological activity evaluation. Therefore, further studies involving bioassay-guided fractionation and isolation of active compounds are recommended to determine the pharmacological relevance of these constituents.

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