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GC–MS Analysis of Phytochemical Constituents of *Ixora brachiata* Roxb. Flower Powder

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Abstract

Medicinal plants are valuable sources of bioactive compounds used in traditional and modern medicine. *Ixora brachiata* (Family: Rubiaceae) is traditionally used for treating inflammatory conditions, infections, and wounds, yet its phytochemical composition is inadequately explored. The present study aims to identify the phytochemical constituents present in the flower powder of *Ixora brachiata* using Gas Chromatography–Mass Spectrometry (GC–MS). GC–MS analysis revealed the presence of twenty-five compounds, predominantly fatty acids, esters, and long-chain hydrocarbons. Major constituents included n-hexadecanoic acid (37.56%), oleic acid (31.05%), octadecanoic acid (14.10%), and octadecane (3.43%). Many identified compounds possess known antimicrobial, antioxidant, anti-inflammatory, and pharmacological properties. The results scientifically validate the medicinal potential of *Ixora brachiata* flowers and support their traditional therapeutic use.

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1. Introduction

Plants have long served as a foundation for traditional medicine systems and continue to be important sources of novel bioactive compounds. Phytochemicals such as fatty acids, terpenoids, phenolics, and esters contribute significantly to the therapeutic efficacy of medicinal plants. Scientific evaluation of these phytochemicals is essential for validating traditional claims and identifying potential drug leads.

Gas Chromatography–Mass Spectrometry (GC–MS) is a powerful analytical technique for identifying volatile and semi-volatile organic compounds present in plant materials. It provides precise qualitative and semi-quantitative information based on retention time and mass spectral patterns.

Ixora brachiata, belonging to the Rubiaceae family, is a flowering plant widely distributed in tropical regions. Various *Ixora* species are traditionally used for wound healing, antimicrobial, anti-inflammatory, and antioxidant purposes.

However, limited scientific data is available on the chemical composition of *Ixora brachiata* flowers. Hence, this study focuses on GC–MS profiling of *Ixora brachiata* flower powder to identify its phytochemical constituents and assess its medicinal significance.

2. Materials and Methods

2.1 Collection and Authentication of Plant Material

Fresh flowers of *Ixora brachiata* were collected from a natural growing region during the flowering season. The plant material was carefully selected to ensure it was free from disease, insect damage, and physical deterioration. The collected specimens were authenticated using standard botanical identification keys and regional floras to confirm the taxonomic identity of the species.

2.2 Preparation of Flower Powder

The collected flowers were washed thoroughly with running

tap water to remove adhering dust and debris, followed by rinsing with distilled water. The cleaned flowers were shade-dried at room temperature for several days until complete removal of moisture was achieved. Shade drying was carried out to prevent thermal degradation of volatile and heat-sensitive phytochemical constituents.

The dried flowers were ground into a fine powder using a mechanical grinder. The powdered material was sieved to obtain uniform particle size and stored in airtight containers at room temperature until further analysis.

2.3 Extraction of Phytochemicals

A measured quantity of *Ixora brachiata* flower powder was subjected to solvent extraction using analytical-grade organic solvent to extract volatile and semi-volatile phytochemicals. The extraction process was carried out under controlled conditions to ensure maximum recovery of bioactive compounds. The extract was filtered to remove plant residues, and the filtrate was concentrated to obtain a clear extract suitable for GC–MS analysis.

2.4 GC–MS Instrumentation

Gas Chromatography–Mass Spectrometry analysis was performed using a standard GC–MS system equipped with an autosampler. The operating parameters were optimized to achieve efficient separation and accurate identification of phytochemicals present in the flower extract.

- **Injection volume:** 1.0 μL
- **Injection mode:** Split
- **Carrier gas:** Helium (high purity)
- **Flow rate:** Constant
- **Ionization mode:** Electron impact (EI)
- **Ionization energy:** 70 eV

2.5 Chromatographic Conditions

The separation of compounds was achieved using a temperature-programmed GC oven. The initial oven

temperature was maintained at a lower range and gradually increased at a predetermined rate to allow the elution of compounds with varying boiling points. The temperature program ensured effective resolution of both low- and high-molecular-weight constituents present in the flower powder extract.

2.6 Identification of Phytochemical Compounds

The mass spectrometer scanned ions over a broad mass range to record fragmentation patterns of eluted compounds. The identification of phytochemicals was performed by comparing the obtained mass spectra with reference spectra available in the NIST14 mass spectral library. Retention time, molecular weight, and fragmentation patterns were considered during compound identification. Only compounds with acceptable similarity index values were reported.

2.7 Quantitative Estimation of Compounds

The relative abundance of each identified compound was expressed as peak area percentage (%) based on the total ion chromatogram (TIC). The peak area percentage was used to determine the major and minor constituents present in the *Ixora brachiata* flower powder.

2.8 Data Analysis and Interpretation

Chromatographic data were processed using the GC–MS system software. Peak detection, integration, and identification were performed automatically and verified manually to ensure accuracy. The identified compounds were tabulated along with their retention time, molecular formula, and peak area percentage for interpretation and discussion.

3. Results

GC–MS analysis of *Ixora brachiata* flower powder revealed 25 phytochemical compounds. The chromatogram showed a predominance of fatty acids and ester derivatives.

Table 1: Phytochemical Compounds Identified in *Ixora brachiata* Flower Powder by GC–MS

S. No.	Retention Time (min)	Compound Name	Molecular Formula	Area (%)
1	1.408	Carbonochloridic acid, ethyl ester	$\text{C}_3\text{H}_5\text{ClO}_2$	0.13
2	11.705	Levomenthyl	$\text{C}_{10}\text{H}_{20}\text{O}$	0.74
3	14.509	Tridecane	$\text{C}_{13}\text{H}_{28}$	0.14
4	16.224	Tetradecane	$\text{C}_{14}\text{H}_{30}$	0.33
5	17.707	Pentadecane	$\text{C}_{15}\text{H}_{32}$	0.23
6	23.534	n-Hexadecanoic acid	$\text{C}_{16}\text{H}_{32}\text{O}_2$	37.56
7	24.314	Tetradecanoic acid, 2-hydroxy-1,3-propanediyl ester	$\text{C}_{31}\text{H}_{60}\text{O}_5$	0.17
8	24.647	Octadecanoic acid, 2-propenyl ester	$\text{C}_{21}\text{H}_{40}\text{O}_2$	0.40
9	24.902	Octadecanoic acid, 2-hydroxy-1,3-propanediyl ester	$\text{C}_{39}\text{H}_{76}\text{O}_5$	0.24
10	25.010	9-Octadecenoic acid, methyl ester	$\text{C}_{19}\text{H}_{36}\text{O}_2$	0.12
11	25.810	Oleic acid	$\text{C}_{18}\text{H}_{34}\text{O}_2$	31.05
12	26.063	Octadecanoic acid	$\text{C}_{18}\text{H}_{36}\text{O}_2$	14.10
13	26.305	Octadecane	$\text{C}_{18}\text{H}_{38}$	3.43
14	26.973	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	$\text{C}_{19}\text{H}_{38}\text{O}_4$	2.69
15	27.266	Octadecanoic acid, 2-propenyl ester	$\text{C}_{21}\text{H}_{40}\text{O}_2$	0.18
16	27.538	Glycidyl palmitate	$\text{C}_{19}\text{H}_{36}\text{O}_3$	1.77
17	28.497	Glycerol 1-palmitate	$\text{C}_{19}\text{H}_{38}\text{O}_4$	0.16
18	28.673	Heneicosane	$\text{C}_{21}\text{H}_{44}$	0.33
19	29.014	Oleoyl chloride	$\text{C}_{18}\text{H}_{33}\text{ClO}$	2.75
20	29.275	Octadecanoic acid, 2,3-dihydroxypropyl ester	$\text{C}_{21}\text{H}_{42}\text{O}_4$	0.78
21	29.374	1,2-Propanediol, 3-benzyloxy-1,2-diacetyl	$\text{C}_{14}\text{H}_{18}\text{O}_5$	0.22
22	29.532	Glycidyl oleate	$\text{C}_{21}\text{H}_{38}\text{O}_3$	1.21
23	29.726	Heneicosane	$\text{C}_{21}\text{H}_{44}$	0.79
24	30.025	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	$\text{C}_{19}\text{H}_{38}\text{O}_4$	0.33
25	30.712	Nonacosane	$\text{C}_{29}\text{H}_{60}$	0.17

4. Discussion

The GC–MS profile indicates that *Ixora brachiata* flower powder is rich in fatty acids and their derivatives. n-Hexadecanoic acid, the dominant compound, is reported to exhibit antioxidant, antibacterial, and anti-inflammatory properties. Oleic acid, another major constituent, is known for its cardioprotective, antimicrobial, and antioxidant activities. The presence of octadecanoic acid (stearic acid) contributes to antimicrobial and anti-inflammatory effects. Hydrocarbons such as octadecane, tridecane, and heneicosane are reported to possess antimicrobial and insecticidal properties. Ester compounds like glycidyl palmitate, glycidyl oleate, and glycerol esters enhance biological activity and may contribute to wound healing and anti-inflammatory effects. Overall, the phytochemical profile strongly supports the medicinal relevance of *Ixora brachiata* flowers.

Conclusion

The present study successfully identified twenty-five phytochemical compounds from *Ixora brachiata* flower powder using GC–MS analysis. The predominance of biologically active fatty acids, esters, and hydrocarbons confirms the plant's medicinal potential. These findings provide scientific evidence supporting traditional uses of *Ixora brachiata* and suggest its potential application in pharmaceutical and herbal formulations. Further biological and pharmacological studies are recommended.

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