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# Phytochemical Profiling of *Ixora brachiata* (Roxb.) Flower Powder by Gas Chromatography–Mass Spectrometry (GC–MS) Analysis

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**Abstract**
*Ixora brachiata* (Roxb.), a member of the Rubiaceae family, is an important medicinal plant distributed in the Western Ghats of India. Although the plant has been traditionally utilized in indigenous medicine, detailed information regarding the phytochemical composition of its flowers remains limited. The present investigation aimed to characterize the phytochemical constituents present in the flower powder of *Ixora brachiata* using Gas Chromatography–Mass Spectrometry (GC–MS). The chromatographic analysis revealed twenty-five phytochemical constituents with varying retention times and relative peak areas. Among the detected compounds, n-hexadecanoic acid (37.56%) was the predominant constituent, followed by oleic acid (31.05%), octadecanoic acid (14.10%), octadecane (3.43%), oleoyl chloride (2.75%), hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester (2.69%), glycidyl palmitate (1.77%), glycidyl oleate (1.21%), heneicosane, levomenthol and several minor fatty acids, esters, hydrocarbons, and glycerides. Most of the identified compounds have been previously reported to possess antimicrobial, antioxidant, anti-inflammatory, hypocholesterolemic, anticancer, insecticidal, and wound-healing activities. The predominance of long-chain fatty acids and their esters indicates that the flowers of *I. brachiata* constitute a rich source of bioactive metabolites with considerable pharmaceutical and nutraceutical importance. The findings provide the first comprehensive GC–MS-based phytochemical profile of *I. brachiata* flower powder and establish a scientific basis for its traditional medicinal use. The study further supports the exploration of this species for isolation of biologically active compounds and development of plant-based therapeutic formulations.

**Keywords:** *Ixora brachiata*, GC–MS, phytochemical profiling, fatty acids, palmitic acid, oleic acid, medicinal plants, bioactive compounds.

## 1. Introduction

Medicinal plants have been utilized as primary healthcare resources since ancient civilizations and continue to serve as invaluable reservoirs of biologically active secondary metabolites. Approximately eighty percent of the world's population relies on herbal medicines for primary healthcare, particularly in developing countries. Plants synthesize a wide range of phytochemicals, including alkaloids, flavonoids, terpenoids, phenolics, tannins, glycosides, steroids, fatty acids, volatile oils, and other specialized metabolites that contribute significantly to their therapeutic properties. These phytoconstituents exhibit diverse pharmacological activities such as antioxidant, antimicrobial, anti-inflammatory, anticancer, antidiabetic, antiviral, hepatoprotective, cardioprotective, and immunomodulatory effects. Consequently, medicinal plants remain indispensable resources for pharmaceutical industries, drug discovery programs, nutraceutical development, and evidence-based herbal medicine.

The genus *Ixora* belongs to the family Rubiaceae and comprises more than 500 species distributed throughout tropical and subtropical regions of Asia, Africa, and Australia. Several species of *Ixora* have long been recognized in traditional medicine for treating skin diseases, wounds, ulcers, dysentery, fever, inflammation, diarrhoea, hypertension, and gastrointestinal disorders. Different plant parts including leaves, flowers, bark, stems, and roots are employed in indigenous systems of medicine due to their richness in phenolic compounds, flavonoids, anthocyanins, triterpenoids, tannins, and other bioactive metabolites. Previous phytochemical investigations on different *Ixora* species have demonstrated remarkable antioxidant, antimicrobial, anti-

inflammatory, hepatoprotective, cytotoxic, and antidiabetic activities, thereby emphasizing their medicinal significance.

*Ixora brachiata* (Roxb.) is an evergreen shrub or small tree naturally distributed in the Western Ghats, especially in Maharashtra, Goa, Karnataka, Kerala, and adjoining regions. Despite its ecological importance and traditional medicinal applications, comparatively little information is available regarding the phytochemical composition of its flowers. Comprehensive chemical characterization is essential to understand the therapeutic potential of this species and to identify bioactive compounds responsible for its medicinal properties. Modern analytical techniques such as Gas Chromatography–Mass Spectrometry (GC–MS) have become indispensable tools for qualitative and semi-quantitative analysis of volatile and semi-volatile phytochemicals. GC–MS combines excellent chromatographic separation with precise mass spectral identification, allowing rapid characterization of complex mixtures of natural products through comparison with established spectral libraries.

In the present study, GC–MS analysis was employed to identify the phytochemical constituents present in the flower powder of *Ixora brachiata*. The chromatogram revealed twenty-five compounds, among which long-chain fatty acids and their derivatives constituted the major phytochemical group. The dominant compounds included n-hexadecanoic acid, oleic acid, octadecanoic acid, glycidyl esters, fatty acid glycerides, hydrocarbons, and aliphatic alcohol derivatives. Many of these compounds are well documented for their antioxidant, antimicrobial, anti-inflammatory, hypocholesterolemic, anticancer, pesticidal, and wound-healing properties, highlighting the medicinal importance of the species.

The present investigation was therefore undertaken to characterize the phytochemical profile of *Ixora brachiata* flower powder using GC–MS analysis and to provide scientific evidence supporting its medicinal value. The results generated from this study may contribute to future pharmacological investigations, isolation of novel bioactive compounds, standardization of herbal formulations, and conservation of this valuable medicinal species.

## 2. Materials and Methods

### 2.1 Collection of Plant Material

Fresh flowers of *Ixora brachiata* (Roxb.) were collected during the flowering season from healthy and disease-free plants. The collected flowers were thoroughly cleaned to remove adhering dust and foreign materials and subsequently shade-dried at room temperature until a constant weight was obtained. The dried flowers were finely powdered using a mechanical grinder and stored in airtight containers until further analysis.

### 2.2 Preparation of Sample

The dried flower powder of *Ixora brachiata* was processed for phytochemical analysis. The prepared sample was subjected to Gas Chromatography–Mass Spectrometry (GC–MS) analysis for identification of volatile and semi-volatile phytochemical constituents. According to the analytical report, the sample analyzed was "sample 01_Ixora brachiata_flower powder" (Sample ID: 1567) with an injection volume of 1.00 µL.

### 2.3 GC–MS Analysis

Gas Chromatography–Mass Spectrometry analysis was carried out using the prepared flower powder sample. The chromatographic separation generated a Total Ion Chromatogram (TIC), and the individual compounds were identified by comparing their mass spectra with the NIST 14 Mass Spectral Library. Each detected compound was characterized based on its retention time, molecular ion fragmentation pattern, and similarity index obtained from the spectral library.

The chromatogram showed 25 detectable phytochemical constituents, indicating the presence of several biologically important fatty acids, fatty acid esters, hydrocarbons, alcohols, glycerides, and related metabolites.

### 2.4 Identification of Phytochemicals

The identification of phytochemical constituents was performed using the National Institute of Standards and Technology (NIST14) spectral database. The mass spectrum of each chromatographic peak was compared with the reference spectra available in the library, and compounds showing high similarity indices were considered for identification. Retention time, molecular formula, molecular weight, and percentage peak area were used for qualitative characterization of the phytochemical profile.

### 2.5 Data Analysis

The relative abundance of each compound was estimated from its percentage peak area obtained from the Total Ion Chromatogram. The identified compounds were arranged according to increasing retention time and interpreted based on available phytochemical and pharmacological literature to understand their possible biological significance.

## 3. Results

### 3.1 GC–MS Analysis of *Ixora brachiata* Flower Powder

Gas Chromatography–Mass Spectrometry (GC–MS) analysis of *Ixora brachiata* flower powder revealed a chemically diverse phytochemical profile. The Total Ion Chromatogram (TIC) showed 25 distinct chromatographic peaks, indicating the presence of twenty-five volatile and semi-volatile phytoconstituents. The compounds were identified by matching their mass spectra with those available in the NIST14 Mass Spectral Library. The identified constituents comprised predominantly fatty acids, fatty acid esters, glycerides, hydrocarbons, alcohols, and related lipid derivatives. The occurrence of these compounds suggests that the flowers of *I. brachiata* are rich in lipid-derived bioactive metabolites possessing potential pharmacological importance.

Among the identified compounds, n-Hexadecanoic acid was the major constituent with a relative peak area of 37.56%, followed by Oleic acid (31.05%) and Octadecanoic acid (14.10%). Together, these three compounds constituted more than 82% of the total detected phytochemical composition, indicating that saturated and unsaturated long-chain fatty acids represent the dominant chemical class in the flower powder. Other compounds detected in moderate concentrations included Octadecane (3.43%), Oleoyl chloride (2.75%), Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester (2.69%), Glycidyl palmitate (1.77%), and Glycidyl oleate (1.21%). Several minor constituents such as Levomenthol, Tridecane, Tetradecane, Pentadecane, Heneicosane, Nonacosane, glycerides, and fatty acid esters were also identified in lower proportions.

The predominance of fatty acids and their esters demonstrates that *I. brachiata* flowers possess an abundant lipid fraction. Such compounds are widely recognized in phytochemical investigations because of their reported antioxidant,

antimicrobial, anti-inflammatory, hypolipidemic, anticancer, insecticidal, and wound-healing properties. The overall chromatographic profile therefore indicates that *I. brachiata* flowers constitute a promising source of biologically active phytochemicals deserving further pharmacological evaluation.

**Table 1:** GC–MS Profile of *Ixora brachiata* Flower Powder

| S. No. | RT (min) | Compound Identified | Area (%) |
|---|---|---|---|
| 1 | 1.408 | Carbonochloridic acid, ethyl ester | 0.1269 |
| 2 | 11.705 | Levomenthol | 0.7352 |
| 3 | 14.509 | Tridecane | 0.1403 |
| 4 | 16.224 | Tetradecane | 0.3283 |
| 5 | 17.707 | Pentadecane | 0.2256 |
| 6 | 23.534 | n-Hexadecanoic acid | 37.5622 |
| 7 | 24.314 | Tetradecanoic acid, 2-hydroxy-1,3-propanediyl ester | 0.1655 |
| 8 | 24.647 | Octadecanoic acid, 2-propenyl ester | 0.4001 |
| 9 | 24.902 | Octadecanoic acid, 2-hydroxy-1,3-propanediyl ester | 0.2375 |
| 10 | 25.010 | 9-Octadecenoic acid, methyl ester | 0.1213 |
| 11 | 25.810 | Oleic acid | 31.0451 |
| 12 | 26.063 | Octadecanoic acid | 14.0995 |
| 13 | 26.305 | Octadecane | 3.4317 |
| 14 | 26.973 | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 2.6867 |
| 15 | 27.266 | Octadecanoic acid, 2-propenyl ester | 0.1793 |
| 16 | 27.538 | Glycidyl palmitate | 1.7685 |
| 17 | 28.497 | Glycerol 1-palmitate | 0.1581 |
| 18 | 28.673 | Heneicosane | 0.3332 |
| 19 | 29.014 | Oleoyl chloride | 2.7523 |
| 20 | 29.275 | Octadecanoic acid, 2,3-dihydroxypropyl ester | 0.7840 |
| 21 | 29.374 | 1,2-Propanediol, 3-benzyloxy-1,2-diacetyl | 0.2236 |
| 22 | 29.532 | Glycidyl oleate | 1.2084 |
| 23 | 29.726 | Heneicosane | 0.7860 |
| 24 | 30.025 | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 0.3296 |
| 25 | 30.712 | Nonacosane | 0.1713 |

**Source:** GC–MS peak report.

### 3.2 Major Phytochemical Classes Identified

The detected compounds can be grouped into the following phytochemical classes:

**Table 2:** Major Phytochemical Classes

| Phytochemical class | Representative compounds |
|---|---|
| Fatty acids | n-Hexadecanoic acid, Oleic acid, Octadecanoic acid |
| Fatty acid esters | Octadecanoic acid esters, Methyl oleate |
| Fatty acid glycerides | Glycidyl palmitate, Glycidyl oleate, Glycerol 1-palmitate |
| Hydrocarbons | Tridecane, Tetradecane, Pentadecane, Octadecane, Heneicosane, Nonacosane |
| Terpenoid alcohol | Levomenthol |
| Acid chloride | Oleoyl chloride |

These results indicate that fatty acids and their derivatives are the dominant phytochemical group detected in the analyzed flower powder.

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