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Metabolomic Profile of Ethanol Extract from Qust Al Hindi (*Saussurea lappa*) Roots Through GC-MS Analysis

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ABSTRACT: *Saussurea lappa,* a member of the Compositae family, is a medicinal plant that has been widely used in traditional medicine systems across various regions, particularly Persia and India. Traditionally, the plant has been used to treat various conditions, including asthma, cough, bloating, rhinitis, urticaria, epilepsy, headaches, leukoderma, allergies, and chronic skin diseases. This study aimed to identify and characterize the secondary metabolites present in the ethanol extract of *S. lappa* roots (Qust al-Hindi) using a gas chromatography–mass spectrometry (GC-MS)-based metabolomic approach. The roots were extracted using the Soxhlet method with 96% ethanol as the extraction solvent, and the resulting extract was subsequently analyzed by GC-MS. A total of 57 compounds were detected, of which eight exhibited the highest relative peak-area percentages: Aromadendrene oxide-(2); 2-(4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-2-yl)prop-2-en-1-ol; 2(3H)-benzofuranone, 6-ethenylhexahydro-3,6-dimethyl-7-(1-methylethenyl)-[3S-(3α,3aα,6α,7β,7aβ)]; 5,8-dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydrophenanthren-2(3H)-one; azuleno[4,5-b]furan-2(3H)-one, 3a,4,6a,7,8,9a,9b-octahydro-6-methyl-3,9-bis(methylene)-[3aS-(3aα,6aα,9aα,9bβ)]; acetic acid, 2-(2-acetoxy-2,5,5,8a-tetramethyldecalin-1-yl); propanoic acid, 2-methyl-, (dodecahydro-6a-hydroxy-9a-methyl-3-methylene-2,9-dioxoazuleno[4,5-b]furan-6-yl)methyl ester; and cyclopentanolcarboxylic acid, 2-(2,2-dimethyl-1,3-dioxol-4-yl)-4-methylene-5,5-dimethyl-methyl ester, (S,R,R or S,S,S). The identified compounds were predominantly classified as terpenoids, a group of natural products associated with diverse pharmacological activities, including anticancer, antimicrobial, antibiotic, antifeedant, hormonal, immunostimulant, anti-inflammatory, antihepatotoxic, anticonvulsant, analgesic, muscle-relaxant, sedative, hepatoprotective, antidepressant, antioxidant, and antidiabetic effects.

KEYWORDS: GC-MS; metabolomics; *Saussurea lappa*; soxhlet extraction.

1. INTRODUCTION

Qust al-Hindi (*Saussurea lappa*), a medicinal plant belonging to the Compositae (Asteraceae) family, has been extensively utilized in various traditional medicine systems across Persia and India. This perennial herb thrives in the Himalayan region at altitudes ranging from 2,500 to 3,500 meters, encompassing areas of India, Pakistan, and China. Traditionally, the dried root of *S. lappa* has been employed to manage a wide spectrum of ailments, including respiratory disorders such as asthma and cough, gastrointestinal issues like bloating, common colds, dermatological conditions such as hives, chronic skin diseases, and leukoderma, as well as neurological disorders including epilepsy and headaches (Salam, Syarif & Muflihunna, 2023; Sukmawati, Musfiroh & Fristiohady, 2022).

The pharmacological potential of *S. lappa* is largely attributed to its diverse secondary metabolites, including flavonoids, alkaloids, phenols, steroids, and terpenoids. These bioactive compounds have been reported to exhibit a wide range of biological activities, such as antioxidant, anticancer, anti-inflammatory, and antimicrobial effects. Previous studies have confirmed the presence of alkaloids, flavonoids, and terpenoids in the root, which contribute to its antioxidant capacity (Rahayu, Sukmawati & Rahman, 2024). Additionally, phytochemical analyses have identified other constituents, including glycosides, coumarins, quinones, and tannins, further supporting the plant's therapeutic potential (Sukmawati, Musfiroh & Fristiohady, 2022; Berghuis, Farida & Ilmiawati, 2023). Despite these findings, comprehensive profiling of all active compounds within the root extract remains limited.

In this context, a metabolomics approach offers a powerful tool for systematically studying the chemical composition of medicinal plants. Metabolomics involves the global analysis of metabolites within a biological system, enabling the identification and characterization of both primary and secondary metabolites (Meshram et al., 2024). Among the analytical techniques available, Gas Chromatography-Mass Spectrometry (GC-MS) is particularly effective for metabolomic profiling, allowing for the sensitive and accurate detection of volatile and semi-volatile compounds in complex plant matrices (Juswardi, Putriani & Harmida, 2023).

Building on this background, the present study was designed to investigate the metabolomic profile of secondary metabolites in the ethanol extract of *S. lappa* root using GC-MS. This analysis aims to provide a comprehensive understanding of the plant's bioactive compounds, which may serve as a foundation for future pharmacological and therapeutic research.

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2. EXPERIMENTAL SECTION

2.1. Tools and Materials

Soxhlet extractor, rotary vacuum evaporator, water bath, Gas Chromatography-Mass Spectrometry (GC-MS, Thermo Scientific Trace 1310), blender, porcelain plate, aluminum foil, tissue, filter paper, and general laboratory glassware. Qust al-Hindi root (*Saussurea lappa*), 96% ethanol, concentrated sulfuric acid (H_2SO_4), concentrated hydrochloric acid (HCl), anhydrous acetic acid ($C_4H_6O_3$), 2N sulfuric acid, magnesium powder (Mg), Mayer reagent, Wagner reagent.

2.2. Sample collection and processing

The roots of *Saussurea lappa* were first cleaned, dried, and cut into small pieces before being ground into a fine powder. A total of 40 g of the powdered root was subjected to extraction using the Soxhlet apparatus with 200 mL of 96% ethanol at 60°C for 3 hours. The resulting liquid extract was concentrated using a rotary vacuum evaporator at 60°C for 30 minutes and subsequently thickened in a water bath at 70°C. The yield of the extract was determined by calculating the weight of the condensed extract obtained

2.3. Phytochemical Screening

2.3.1. Alkaloids

To 1 mL of ethanol extract, 2 mL of 2N sulfuric acid was added, and the mixture was divided into two test tubes. Each tube was then treated with Mayer and Wagner reagents. A positive result was indicated by the formation of white or yellow precipitate with Mayer reagent, or red to brown precipitate with Wagner reagent (Triwahyuono & Hidajati, 2020; Putri & Mahfur, 2023).

2.3.2. Flavonoids

For flavonoid detection, 1 mL of ethanol extract was mixed with 0.5 mg of magnesium powder (Mg) and 1 mL of concentrated hydrochloric acid. A color change to red indicated a positive result (Rahayu, Sukmawati & Rahman, 2024).

2.3.3. Saponins

To detect saponin, 1 mL of ethanol extract was added to 5 mL of hot distilled water and vigorously shaken for 1 minute. Subsequently, 3 drops of concentrated HCl were added. The presence of saponins was confirmed if the foam remained stable for approximately 7 minutes (Sabandar et al., 2020; Wardani, Erwin & Hayani, 2024).

2.3.4. Terpenoids/Steroids

To detect terpenoids and steroids, 1 mL of ethanol extract was mixed with 10 drops of anhydrous acetic acid ($C_4H_6O_3$) and 2 drops of concentrated H_2SO_4. The appearance of purple or orange rings indicated the presence of terpenoids, while green or blue rings indicated steroids (Triwahyuono & Hidajati, 2020).

2.4 GC-MS analysis

One microliter (1 µL) of ethanol extract was injected into the GC-MS system (Thermo Scientific Trace 1310) in a splitless mode for 2 minutes. The injector temperature was maintained at 275 °C, with a split flow rate of 30 mL/min and a purge flow of 5 mL/min. The gas saver system was activated at 5 mL/min, 1.5 minutes after injection. Separation was performed using a TG-5MS capillary column (30 m × 0.25 mm). The column temperature was initially set at 60°C, then gradually increased to 300 °C over 30 minutes and held until the end of the run. Helium was used as the carrier gas at a flow rate of 1.5 mL/min. The interface temperature was set at 280°C and the ion source temperature at 225°C, with a scanned mass range of 40–450 m/z. The resulting spectra were analyzed and compared with NIST library data to identify the compounds present.

3. RESULTS AND DISCUSSION

In this study, the extraction method used is soxhlettasi. From the 40 g of simplicia powder extracted, 2.38 g of thick extract was obtained with a percentage yield of 5.95%. The phytochemical screening test can be seen in **Table 1**.

Table 1. Results of Phytochemical Screening Tests of Ethanol Extracts from the Roots of *Saussurea lappa*

Compound Identified	Results	Description

Alkaloids	Mayer: yellow deposits are formed Wagner: brown deposits are formed	+ alkaloids
Flavanoids	Concentrated Mg + HCl powder: turns red	+ flavanoids
Saponins	Distilled water + concentrated HCl: no stable foam formation	- saponins
Terpenoids/ Steroids	$C_4H_6O_3$ + H_2SO_4 : formed purple ring	+ terpenoids

GC-MS analysis of ethanol extracts from *S. lappa* root identified a total of 57 compounds. Of these, eight compounds showed the highest percentage of area. The results can be seen in **Table 2**, which shows 57 compounds, of which eight compounds had Rt values ranging from 20.54 to 28.05 with the highest relative abundance of % area 1.57 to 40.24. The results of gas chromatography showed eight compounds with the largest relative abundance marked with red circles. can be seen in **Figure 1**.

Table 2. Compounds Identified by GC-MS Ethanol Extract of *Saussurea lappa* Root

No.	*Retention time* (min)	Area (%)	Molecular Formula	Molecular Weight	Compound Name	Pharmacological Effect
1.	20.54	1.57	$C_{15}H_{24}O$	220	Aromadendrene oxide-(2)	Oxygenated sesquiterpene compounds are naturally present as chemical components of essential oils that have anti-cancer activity (Pavithra, Mehta & Verma, 2018).
2.	22.06	1.39	$C_{15}H_{24}O$	220	2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalen-2-yl)-prop-2-en-1-ol	Sesquiterpenoids are antifeedants, hormones, antimicrobials, antibiotics, and toxins, (Hotmian et al., 2021)
3.	22.59	5.17	$C_{15}H_{22}O_2$	234	2(3H)-Benzofuranone, 6-ethenylhexahydro-3,6-dimethyl-7-(1-methylethenyl)-, [3S-(3a,3aa,6a,7ß,7aß)]-	The lactone sesquiterpenoid group is known to have antimicrobial, immunostimulant, antiinflammatory, and antihepatotoxic properties (Amara et al., 2017).
4.	24.44	19.07	$C_{15}H_{22}O_3$	250	5,8-Dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydro-2(3H)-phenanthrenone	The lactone sesquiterpenoid group is known to have antimicrobial, immunostimulant, antiinflammatory, and antihepatotoxic properties (Amara et al., 2017).
5.	24.59	40.24	$C_{15}H_{22}O_3$	250	5,8-Dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydro-2(3H)-phenanthrenon	The lactone sesquiterpenoid group is known to have antimicrobial, immunostimulant, antiinflammatory, and antihepatotoxic properties (Amara et al., 2017).
6.	25.07	4.00	$C_{15}H_{18}O_2$	230	Azuleno[4,5-b]furan-2(3H)-one, 3a,4,6a,7,8,9,9a,9b-octahydro-6-methyl-3,9-bis(methylene)-, [3aS-(3aa,6aa,9aa,9bß)]-	The lactone sesquiterpenoid group is known to have antimicrobial, immunostimulant, antiinflammatory, and antihepatotoxic properties (Amara et al., 2017).
7.	26.72	3.57	$C_{18}H_{30}O_4$	310	Acetic acid, 2-(2-acetoxy-2,5,5,8a-tetramethyldecalin-1-yl)-	Lactone sesquiterpenoids, which have antimicrobial, anticonvulsant, analgesic, myorerelaxant, sedative, hepatoprotective, and antidepressant properties (Taher et al., 2024).
8.	27.15	5.54	$C_{19}H_{26}O_6$	350	Propanoic acid, 2-methyl-, (dodecahydro-6a-hydroxy-9a-methyl-3-methylene-2,9-dioxoazuleno[4,5-b]furan-6-yl)methyl ester, [3aS-(3aa,6ß,6aa,9aß,9ba)]-	The lactone sesquiterpenoid group is known to have antimicrobial, immunostimulant, antiinflammatory, and antihepatotoxic properties (Amara et al., 2017).
9.	28.05	4.15	$C_{13}H_{20}O_4$	240	Cyclopentanecarboxylic acid, 2-(2,2-dimethyl-1,3-dioxolan-4-yl)-4-methylene-	Contains dioxolane groups and esters that have been shown to have antioxidant and antidiabetic properties (Konidala et al., 2020)

	5,5-dimethyl-, methyl ester, (S,R,R or S,S,S)

The compound with the highest concentration was 5,8-Dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydro-2(3H)-phenanthrenone, which emerged as the top two with an area percentage of 19.07% and 40.24%. Despite having the same compound name, the difference in retention time indicates the possibility of stereoisomers, which are compounds with the same structure but different spatial orientation, so that the interaction with the stationary phase of the GC column is slightly different, resulting in different retention times. So that both are counted as one compound in the calculation of the total number of identified compounds (Athaayaa et al., 2025). These compounds belong to the group of lactone sesquiterpenoids.

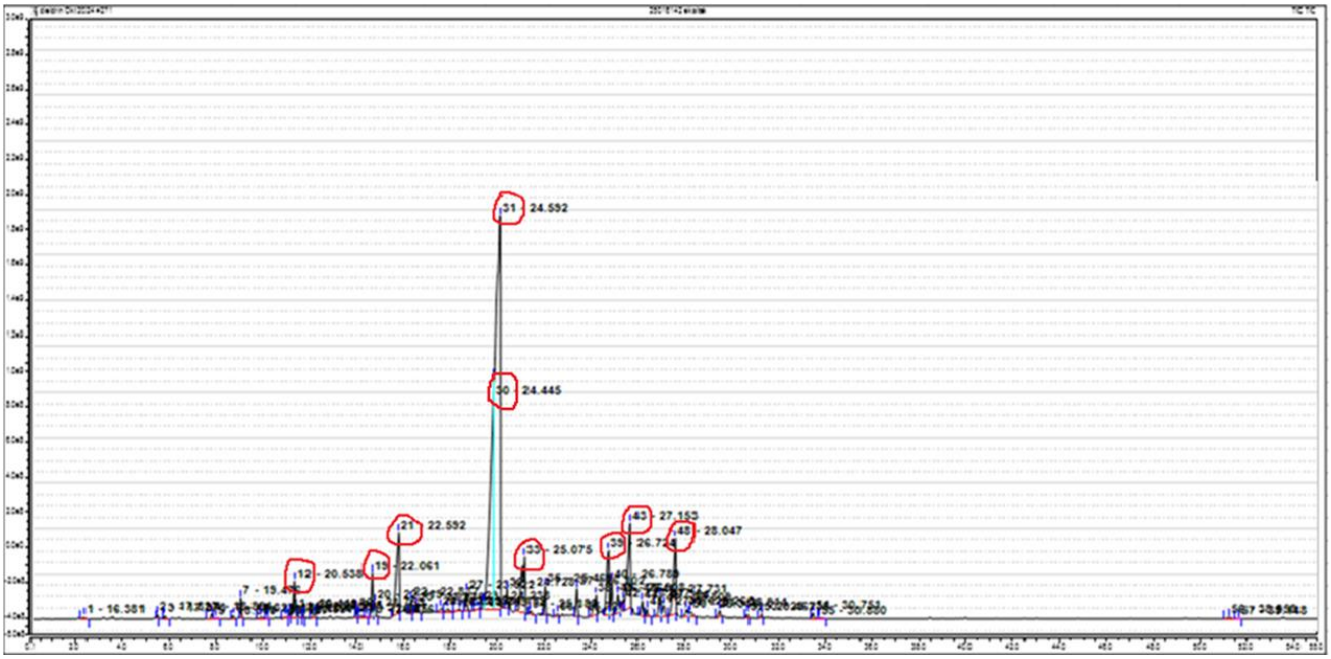


Figure 1. GC-MS Measurement Results on Ethanol Extracts of *S. lappa* Plant Roots

Five of the eight compounds with the highest abundance are 2(3H)-Benzofuranone, 6-ethenylhexahydro-3,,6-dimethyl-7-(1-methylethenyl)-, [3S-(3a,3aa,6a,7ß,7aß)]-, 5,8-Dihydroxy-4a-methyl-4,4a,4b,5,6,7,8,8a,9,10-decahydro-2(3H)-phenanthrenone, Azuleno[4,5-b]furan-2(3H)-one, 3a,4,6a,7,8,9,9a,9b-octahydro-6-methyl-3,9-bis(methylene)-, [3aS-(3aa,6aa,9aa,9bß)]-, Acetic acid, 2-(2-acetoxy-2,5,5,8a-tetramethyldecalin-1-yl)-, and Propanoic acid, 2-methyl-, (dodecahydro-6a-hydroxy-9a-methyl-3-methylene-2,9-dioxoazuleno[4,5-b]furan-, all belong to the group of sesquiterpenoid lactones (Amara et al., 2017). These compounds are known to have extensive biological activities, including antimicrobial, immunostimulant, anti-inflammatory, and antihepatotoxic (Salam, Syarif & Muflihunna, 2023).

Aromadendrene oxide-(2), with an area percentage of 1.57%, is an oxygenated sesquiterpene naturally found in essential oils and has anticancer activity (Pavithra, Mehta & Verma, 2018). 2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalen-2-yl)-prop-2-en-1-ol (1.39%) also belongs to the group of sesquiterpenoids (Hotmian et al., 2021) and has antioxidant, antiviral, immunomodulatory, antiparasitic, antiseptic, and expectorant activity (Sukmawati, Musfiroh & Fristiohady, 2022). Two compounds with the same molecular formula and molecular weight but different names and retention times are likely to be structural isomers, i.e. compounds that have the same number of atoms but different atomic arrangements (Athaayaa et al., 2025).

Cyclopentanecarboxylic acid, 2-(2,2-dimethyl-1,3-dioxolan-4-yl)-4-methylene-5,5-dimethyl-, methyl ester, (S,R,R or S,S,S) with an area percentage of 4.15% belongs to the ester group with a dioxolane group. This group of esters with dioxolane groups has been shown to have antioxidant and antidiabetic properties (Konidala et al., 2020).

Although phytochemical screening showed the presence of flavonoids, alkaloids, and terpenoids in the GC-MS analysis, only terpenoid compounds were present. This may be due to the limitations of GC-MS in detecting all types of compounds, or because the flavonoids and alkaloids present may be non-volatile or semi-volatile, so they are not optimally detected by this method. In addition, some of the peaks detected may be new compounds that have not yet been listed in the NIST data library, so only the peaks are visible without the identification of the compound name (Pertala, Tutik & Nofita, 2023).

Overall, the eight main compounds identified in the ethanol extract of *S. lappa* root all belong to the terpenoid group. This corresponds to the characteristics of terpenoids, which have an isoprene unit carbon framework (C_{5H8}), both open and cyclic, with various functional groups (Azalia et al., 2023). The presence of these compounds supports the

pharmacological potential of *S. lappa* as an anticancer, antimicrobial, anti-inflammatory, antioxidant, and antidiabetic agent, which is in line with its traditional use.

4. CONCLUSION

The ethanol extract of the root of Qust al-Hindi (*S. lappa*) was found to contain a total of 57 compounds. Among these, eight compounds exhibited the highest relative abundance based on peak area and were identified as secondary metabolites belonging to the terpenoid group. Of these eight major compounds, five were classified as lactone sesquiterpenoids, while the remaining three consisted of an oxygenated sesquiterpene, a sesquiterpenoid, and an ester derivative. These findings highlight the predominance of terpenoid-based bioactive compounds in the root extract, which may contribute to its reported pharmacological activities.

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Ethical Approval: Not applicable

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