ISSN 1859 - 4735

# JOURNAL OF MEDICINAL MATERIALS

No. 2 - Vol. 30
3/2025

NATIONAL INSTITUTE OF MEDICINAL MATERIALS

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# *SARCANDRA GLABRA* ESSENTIAL OILS: IDENTIFICATION OF CHEMICAL COMPONENTS AND THEIR ANTIMICROBIAL ACTIVITIES USING *IN VITRO* AND *IN SILICO* STUDIES

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Received March 05th, 2025 Accepted March 29th, 2025

**Summary**

***Sarcandra glabra* Essential Oils: Identification of Chemical Components and their Antimicrobial Activities Using *in vitro* and *in silico* Studies**

*Sarcandra glabra* is a medicinal plant known for its diverse biological activities, including antimicrobial effects. This study presents the first investigation into the chemical composition and antimicrobial properties of essential oils (EOs) from leaves and fruits of *S. glabra* collected in Vietnam. GC-MS analysis identified 49 compounds in the leaf EO (97.16% of total composition) and 45 in the fruit EO (96.95%). Chloranthalactone B was a major component in both oils, accounting for 26.04% in the leaf EO and 7.05% in the fruit EO. Other predominant compounds included $\beta$-(*E*)-ocimene (7.49% in leaf, 35.82% in fruit), $\beta$-cyclogermacrane (9.29% in leaf), and $\alpha$-phellandrene (21.67% in fruit). The variation in chemical composition between the two EOs corresponded to differences in their antimicrobial activities. The leaf EO exhibited strong effects, particularly against *S. aureus* (MIC = 16 µg/mL), while the fruit EO was less effective and showed no inhibition against *E. coli* and *P. aeruginosa*. Due to its significant presence in both EOs, chloranthalactone B was further evaluated for its antimicrobial activity, revealing selective effects against *S. aureus* (MIC = 32 µg/mL), *E. faecalis* (MIC = 64 µg/mL), and *C. albicans* (MIC = 64 µg/mL). To further understand its antimicrobial mechanism, molecular docking analysis was performed. The results showed strong interactions between chloranthalactone B and microbial target proteins. Notably, it exhibited high binding affinity with 1IYL (-7.755 kcal/mol) through hydrogen bonding with key residues, as well as effective interactions with 1JIJ (-7.156 kcal/mol) and 2WE5 (-6.412 kcal/mol). These findings suggest that chloranthalactone B plays a key role in the antimicrobial activity of *S. glabra* EOs and highlights its potential as a natural agent against antibiotic-resistant pathogens.

**Keywords**: *Sarcandra glabra; Essential oil; Antimicrobial activity;Chloranthalactone B; Molecular docking.*

## 1. Introduction

*Sarcandra glabra* (Thunb.) Nakai belongs to the Chloranthaceae family and is widely distributed in China, Japan, Korea, and Southeast Asia [1],[2],[3]. It is highly valued in traditional medicine. Traditionally, it has been used to treat traumatic fractures, joint swelling and pain, sore throats, abscesses, bleeding, and other ailments. In modern clinical practice, it has also been applied to treat upper respiratory tract infections, pneumonia, gastritis, viral myocarditis, tumors, and thrombocytopenia, with significant therapeutic effects [1],[2]. In recent decades, research has focused on the pharmacology and phytochemistry of *S. glabra*. Studies have shown that it possesses diverse pharmacological activities, such as anti-inflammatory, antibacterial, antiviral, anti-tumor, antioxidant, and anti-thrombocytopenic effects [2],[3]. So far, researchers have identified nearly 400 compounds from this species, including terpenoids, coumarins, lignans, flavonoids, sterols, anthraquinones, organic acids, and organic esters, many of which exhibit unique structures and significant pharmacological activities [1],[2],[3],[4]. Despite extensive studies on its chemical composition and biological effects, research on its essential oil is still limited. Yang R. et al. (2007) identified 29 compounds in the volatile oil from *S. glabra* stems, accounting for 75.88% of the total oil content. Similarly, 64 compounds were detected in the volatile oil from its leaves, representing 87.98% of the total oil content [5]. Additionally, Wong K. C. et al. (2009) reported that sesquiterpenoids were the most abundant chemical class, making up 80% of the

leaf essential oil. The oil contained a remarkably high level (51.7%) of a novel sesquiterpenoid, identified as 3$\alpha$-acetoxy-8,12-epoxyeudesma-4,7,11-triene [6]. However, its essential oil's biological activities remain unexplored. This study examines the chemical composition of *S. glabra* essential oils from Vietnam and their antimicrobial activities using *in vitro* and *in silico* studies. We aim for this study to serve as a helpful guide for the future research and application of *S. glabra*, particularly its essential oils.

## 2. Materials and methods

### *2.1. Plant materials*

The leaves and fruits of *S. glabra* were collected at Quan Ba district, Ha Giang province, Vietnam in December 2023 and identified by Msc. Bui Van Huong of the Vietnam National Museum of Nature, Vietnam Academy of Science and Technology (VAST). A voucher specimen (LAB212-12.2023) was deposited at the Department of Chemistry, Vinh University, Vietnam.

### *2.2. General experiment procedures*

GC-MS analysis was performed on an Agilent Technologies 7890B GC System linked to a 5977B MSD model working in EI mode. All NMR spectra were acquired on a Bruker 600 MHz (Bruker, Massachusetts, United States). ESIMS data were acquired on Waters micromass ZQ mass spectrometer (Waters Corp., United States). Column chromatography (CC) was performed on silica-gel (Kieselgel 60, 230-400 mesh, Merck, Germany). Prep-HPLC was performed on an Agilent 218 purification system using a ZORBAX SBC18 column (250 mm × 9.4 mm × 5 μm).

### *2.3. Extraction of essential oils and isolation of chloranthalactone B*

Fresh leaves and ripe fruits of *S. glabra* were washed, cut, and crushed (for fruits). Each 200 g sample was extracted by hydrodistillation using a Clevenger-type apparatus for 3.5 hours or until no further oil was obtained. The yields were 0.2 mL for leaves and 0.5 mL for fruits. The essential oils were dried with anhydrous sodium sulfate and stored at 4°C in the dark for further use. The procedure was repeated three times.

A 300 mg of the leaf essential oil was chromatographed on a *silica gel* CC eluting with gradient solvents of hexane/acetone (from 100/1 to 5/1, v/v) to give twenty-six fractions (SREO.1–SREO.26). Fraction SREO.16 (32 mg) was purified by a prep-HPLC using 80% MeCN in water (v/v) to yield chloranthalactone B (25 mg).

Chloranthalactone B (compound **1**): Colorless crystal; positive ESI-MS *m/z* 245 $[M + H]^+$; $^1$H-NMR (600 MHz, $CDCl_3$, $\delta_H$) 1.72 (1H,td, $J$ = 7.8, 3.6 Hz, H-1), 0.90–0.93 (1H, m, H-2a), 0.84–0.86 (1H, m, H-2b), 2.00 (1H, m, H-3), 3.38–3.41 (1H, m, H-5), 2.54 (1H, dd, $J$ = 18.0, 12.1 Hz, H-6a), 2.09–2.15 (1H, m, H-6b), 4.18 (1H, s, H-9), 1.90 (3H,s, H-13), 0.65 (3H, s, H-14), 5.04 (1H, br s, H-15a), 4.70 (1H, br s, H-15b); $^{13}$C-NMR (150 MHz, $CDCl_3$, $\delta_C$) 23.9 (C-1), 16.9 (C-2), 23.0 (C-3), 150.0 (C-4), 50.6 (C-5), 21.3 (C-6), 152.3 (C-7), 87.9 (C-8), 64.5 (C-9), 41.2 (C-10), 129.1 (C-11), 170.4 (C-12), 9.00 (C-13),16.8 (C-14), 106.8 (C-15).

### *2.4. GC-MS analysis*

The chemical components of *S. glabra* essential oils were analyzed using a GC-MS instrument (Agilent Technologies) equipped with an HP-5MS UI (30 m × 0.25 mm × 0.25 μm). Helium was used as the transferor gas at a constant flow rate of 1.0 mL/min (pressure 8.23 psi). The essential oil samples (1.0 μL) were injected separately by splitting at a split ratio of 40:1. The column was programmed from 60°C (with 1 min hold), then gradually increased to 240ºC at 4°C/min and finally continued for 4 min at 240°C. The mass spectrometer was activated in the EI mode at 70 Ev and the mass range was 50-550 m/z. The volatile compounds in oil were identified by comparing their mass spectra and retention indices (RIs) with those reported in published literature (NIST 17 and Adams book [7]. Besides, chloranthalactone B, a main compound that is identified by GC-MS analysis, was isolated and determined by ESI-MS and NMR spectra.

### *2.5. In vitro antimicrobial assay*

The antimicrobial activity of *S. glabra* essential oils and chloranthalactone B was evaluated against some microorganisms, including two strains of Gram-positive bacteria (*Enterococcus faecalis* ATCC 299212 and *Staphylococcus aureus* ATCC 25923), two strains of Gram-negative bacteria (*Escherichia coli* ATCC 25922 and *Pseudomonas aeruginosa* ATCC 27853), and a strain of yeast (*Candida albicans* ATCC 10231). They were obtained from the Institute of Marine Biochemistry, VAST, Hanoi, Vietnam. The bacteria were cultured in Mueller-Hinton broth, whereas the yeast was

grown in Sabouraud broth. The minimum inhibitory concentration (MIC) values of samples were determined using the broth microdilution method, as outlined in a previous publication [8].

*2.6. Molecular docking study*

Molecular docking studies were conducted following the protocol outlined in the report by Hieu et al. [9]. To gain better insights into the binding mechanisms and potential inhibitory activity of the major components identified in the essential oil of *Sarcandra glabra* against microbial strain-related targets, we applied molecular docking using AutoDock Vina v1.2.3 [10],[11]. Protein structures were retrieved from the RCSB Protein Data Bank (https://www.rcsb.org/). The proteins were then prepared by removing water molecules, metal atoms, co-crystallized ligands, and other non-covalently bound molecules. After adding Kollman charges, polar hydrogens, and merging non-polar hydrogens, the target file was saved in pdbqt format using the AutoDockTools software. The structures of the major compounds in the essential oil were prepared by downloading *.sdf (3D) files from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/) and optimizing their energy using the MMFF94s force field in the Avogadro software [12],[13]. The final pdbqt ligand files were generated using AutoDock Tools v1.5.6. The grid box, defining the docking search space, was resized to best fit the active binding site as accurately as possible. Docking results were presented as binding free energy values (ΔG, kcal/mol), and protein-ligand interactions were analyzed and visualized as 2D interaction diagrams using the Discovery Studio Visualizer software.

## 3. Results and discussion

*3.1. Chemical composition of essential oils*

Compound **1** was obtained as a colorless crystal. Its mass spectrum, generated by ESI-MS, gave a molecular ion at *m/z* 245 $[M + H]^+$, which was consistent with a molecular formula of $C_{15}H_6O_3$. The $^1$H-NMR spectrum of compound **1** displayed characteristic resonances for two methyl groups at $\delta_H$ 0.65 (3H, s, H-14) and 1.90 (3H, s, H-13). Signals indicative of a cyclopropane ring were observed at $\delta_H$ 1.72 (1H, td, $J$ = 7.8, 3.6 Hz, H-1), 0.90–0.93 (1H, m, H-2a), 0.84–0.86 (1H, m, H-2b), and 2.00 (1H, m, H-3). Additionally, terminal vinyl protons resonated at $\delta_H$ 5.04 (1H, br s, H-15a) and 4.70 (1H, br s, H-15b). The $^{13}$C-NMR and DEPT spectra revealed 15 carbon signals, including key resonances characteristic of a five-membered *α,β*-unsaturated lactone system, specifically at $\delta_C$ 152.3 (C-7), 87.9 (C-8), 129.1 (C-11), and 170.4 (C-12). An oxygenated carbon appeared at $\delta_C$ 64.5 (C-9), while the two methyl carbons resonated at $\delta_C$ 9.00 (C-13) and 16.8 (C-14). These spectroscopic features strongly suggested that compound **1** belonged to the lindenane sesquiterpene class. In the HMBC spectrum, the proton signal at $\delta_H$ 4.18 (H-9) exhibited a key correlation with $\delta_C$ 87.9 (C-8), confirming the presence of an oxygenated quaternary carbon. Additionally, correlations between the vinyl protons ($\delta_H$ 5.04, 4.70; H-15) and the carbon resonances at $\delta_C$ 150.0 (C-4), 129.1 (C-11), and 170.4 (C-12) further supported the *α,β*-unsaturated lactone moiety. The COSY spectrum demonstrated strong scalar couplings between H-1, H-2, and H-3, thereby establishing the connectivity of the cyclopropane ring. Based on the comprehensive analysis of the spectroscopic data and comparison with previously reported literature [14], compound **1** was unambiguously identified as chloranthalactone B (**Fig. 1**).

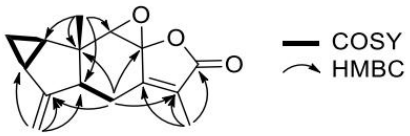



**Fig. 1.** The key HMBC and COSY correlations of chloranthalactone B

The essential oil of *S. glabra* is a light yellow liquid with a pleasant aroma and a lower density than water. The results of GC-MS analysis (**Table 1**) showed that there were fifty-five known compounds in both oils.

**Table 1.** Chemical compositions of *S. glabra* essential oils

| No. | RT (min) | RI (exp.) | RI (lit.) | Compounds | Formula | Area % | | Identification method |
|---|---|---|---|---|---|---|---|---|
| | | | | | | Leaf | Fruit | |
| 1 | 5.279 | 927 | 925 | Tricyclene | $C_{10}H_{16}$ | 0.05 | - | MS, RI |
| 2 | 5.358 | 931 | 929 | *α*-Thujene | $C_{10}H_{16}$ | - | 0.22 | MS, RI |
| 3 | 5.542 | 939 | 937 | *α*-Pinene | $C_{10}H_{16}$ | 3.18 | 1.84 | MS, RI |
| 4 | 5.902 | 954 | 952 | Camphene | $C_{10}H_{16}$ | 3.14 | 1.16 | MS, RI |
| 5 | 6.509 | 978 | 974 | Sabinene | $C_{10}H_{16}$ | 1.48 | 1.1 | MS, RI |

| No. | RT (min) | RI (exp.) | RI (lit.) | Compounds | Formula | Area % | | Identification method |
|---|---|---|---|---|---|---|---|---|
| | | | | | | Leaf | Fruit | |
| 6 | 6.606 | 981 | 979 | *β*-Pinene | $C_{10}H_{16}$ | 0.94 | 0.4 | MS, RI |
| 7 | 6.955 | 993 | 991 | *β*-Myrcene | $C_{10}H_{16}$ | **8.66** | 1.85 | MS, RI |
| 8 | 7.338 | 1007 | 1005 | *α*-Phellandrene | $C_{10}H_{16}$ | 1.95 | **21.67** | MS, RI |
| 9 | 7.659 | 1020 | 1017 | *α*-Terpinene | $C_{10}H_{16}$ | - | 0.2 | MS, RI |
| 10 | 7.882 | 1028 | 1025 | *p*-Cymene | $C_{10}H_{14}$ | 0.1 | 3.79 | MS, RI |
| 11 | 8.02 | 1033 | 1030 | *α*-Limonene | $C_{10}H_{16}$ | 1.03 | 4 | MS, RI |
| 12 | 8.099 | 1036 | 1032 | 1,8-Cineole | $C_{10}H_{18}O$ | - | 0.09 | MS, RI |
| 13 | 8.26 | 1041 | 1038 | *β*-(*Z*)-Ocimene | $C_{10}H_{16}$ | 0.13 | 0.73 | MS, RI |
| 14 | 8.597 | 1053 | 1049 | *β*-(*E*)-Ocimene | $C_{10}H_{16}$ | **7.49** | **35.82** | MS, RI |
| 15 | 8.912 | 1063 | 1060 | *γ*-Terpinene | $C_{10}H_{16}$ | 0.06 | 0.12 | MS, RI |
| 16 | 9.833 | 1091 | 1088 | Terpinolene | $C_{10}H_{16}$ | 0.11 | 0.13 | MS, RI |
| 17 | 10.073 | 1097 | 1093 | *α*-Naginatene | $C_{10}H_{14}O$ | - | 0.05 | MS, RI |
| 18 | 10.165 | 1100 | 1099 | *β*-Linalool | $C_{10}H_{18}O$ | 0.11 | 0.83 | MS, RI |
| 19 | 11.098 | 1132 | 1131 | (4*E*,6Z)-allo-Ocimene | $C_{10}H_{16}$ | - | 0.19 | MS, RI |
| 20 | 15.195 | 1256 | 1252 | Isopentyl hexanoate | $C_{11}H_{22}O_2$ | 0.08 | - | MS, RI |
| 21 | 16.305 | 1288 | 1285 | Bornyl acetate | $C_{12}H_{20}O_2$ | 1.47 | 0.44 | MS, RI |
| 22 | 17.999 | 1342 | 1338 | *δ*-Elemene | $C_{15}H_{24}$ | **8.58** | 1.7 | MS, RI |
| 23 | 18.348 | 1353 | 1350 | *α*-Terpinyl acetate | $C_{12}H_{20}O_2$ | 0.28 | - | MS, RI |
| 24 | 18.92 | 1370 | 1368 | Cyclosativene | $C_{15}H_{24}$ | - | 0.06 | MS, RI |
| 25 | 19.218 | 1379 | 1376 | *α*-Copaene | $C_{15}H_{24}$ | 0.09 | 0.08 | MS, RI |
| 26 | 19.75 | 1395 | 1391 | *β*-Elemene | $C_{15}H_{24}$ | **6.37** | 1.24 | MS, RI |
| 27 | 20.299 | 1413 | 1409 | *α*-Gurjunene | $C_{15}H_{24}$ | 0.07 | - | MS, RI |
| 28 | 20.597 | 1423 | 1419 | *β*-Caryophyllene | $C_{15}H_{24}$ | 0.37 | 0.12 | MS, RI |
| 29 | 21.031 | 1438 | 1433 | *γ*-Elemene | $C_{15}H_{24}$ | **5.32** | 2.29 | MS, RI |
| 30 | 21.203 | 1443 | 1440 | Aromadendrene | $C_{15}H_{24}$ | 0.23 | - | MS, RI |
| 31 | 21.552 | 1455 | 1451 | *α*-Cubebene | $C_{15}H_{24}$ | 0.07 | 0.06 | MS, RI |
| 32 | 21.644 | 1458 | 1454 | *α*-Caryophyllene | $C_{15}H_{24}$ | 0.12 | 0.06 | MS, RI |
| 33 | 21.873 | 1465 | 1461 | Alloaromadendrene | $C_{15}H_{24}$ | 0.13 | - | MS, RI |
| 34 | 22.37 | 1481 | 1477 | *γ*-Muurolene | $C_{15}H_{24}$ | 0.2 | - | MS, RI |
| 35 | 22.491 | 1485 | 1481 | Germacrene D | $C_{15}H_{24}$ | 0.24 | 0.18 | MS, RI |
| 36 | 22.645 | 1489 | 1486 | *β*-Eudesmene | $C_{15}H_{24}$ | 0.22 | 0.05 | MS, RI |
| 37 | 22.817 | 1495 | 1493 | *δ*-Selinene | $C_{15}H_{24}$ | 0.12 | 0.1 | MS, RI |
| 38 | 22.994 | 1500 | 1495 | *β*-Cyclogermacrane | $C_{15}H_{24}$ | **9.29** | 2.71 | MS, RI |
| 39 | 23.275 | 1510 | 1508 | *α*-Farnesene | $C_{15}H_{24}$ | 0.66 | 0.15 | MS, RI |
| 40 | 23.509 | 1519 | 1518 | *β*-Cadinene | $C_{15}H_{24}$ | 0.3 | 0.83 | MS, RI |
| 41 | 23.744 | 1527 | 1524 | *δ*-Cadinene | $C_{15}H_{24}$ | 0.37 | 0.34 | MS, RI |
| 42 | 24.522 | 1554 | 1549 | Elemol | $C_{15}H_{26}O$ | 4.58 | 1.07 | MS, RI |
| 43 | 24.745 | 1561 | 1557 | Germacrene B | $C_{15}H_{24}$ | 0.27 | 0.1 | MS, RI |
| 44 | 24.9 | 1567 | 1564 | Nerolidol | $C_{15}H_{26}O$ | 0.53 | 0.34 | MS, RI |
| 45 | 25.34 | 1581 | 1577 | Spathulenol | $C_{15}H_{24}O$ | 0.77 | 2.14 | MS, RI |
| 46 | 25.529 | 1588 | 1580 | Globulol | $C_{15}H_{26}O$ | 0.32 | 0.39 | MS, RI |
| 47 | 25.912 | 1600 | 1596 | Guaiol | $C_{15}H_{26}O$ | 0.07 | - | MS, RI |
| 48 | 26.788 | 1633 | 1631 | Longifolenaldehyde | $C_{15}H_{24}O$ | 0.06 | - | MS, RI |
| 49 | 26.874 | 1636 | 1631 | *γ*-Eudesmol | $C_{15}H_{26}O$ | 0.17 | 0.17 | MS, RI |
| 50 | 27.051 | 1642 | 1638 | Isospathulenol | $C_{15}H_{24}O$ | 0.12 | 0.26 | MS, RI |
| 51 | 27.16 | 1646 | 1642 | Cubenol | $C_{15}H_{26}O$ | 0.24 | 0.23 | MS, RI |
| 52 | 27.394 | 1655 | 1649 | *β*-Eudesmol | $C_{15}H_{26}O$ | 0.33 | 0.18 | MS, RI |
| 53 | 27.497 | 1658 | 1653 | *α*-Eudesmol | $C_{15}H_{26}O$ | 0.56 | 0.42 | MS, RI |
| 54 | 27.864 | 1671 | 1667 | Bulnesol | $C_{15}H_{26}O$ | 0.09 | - | MS, RI |
| **55** | **36.121** | **1994** | - | **Chloranthalactone B** | $\mathbf{C_{15}H_6O_3}$ | **26.04** | **7.05** | **Co-GC, NMR** |
| | | | | Total | | 97.16 | 96.95 | |

*RT (min): Retention time (min); RI (exp.): Retention indices on HP-5MS UI column; RI (lit.): Retention indices from the literature; Co-GC: Co-injection with the authentic compound; NMR: Nuclear magnetic resonance.*

In the leaf essential oil, 49 constituents were identified, accounting for 97.16% of the total composition. The predominant compounds (≥ 5%) included chloranthalactone B (26.04%), *β*-cyclogermacrane (9.29%), *β*-myrcene (8.66%), *δ*-elemene (8.58%), *β*-(*E*)-ocimene (7.49%), *β*-elemene (6.37%), and *γ*-elemene (5.32%), indicating a chemical profile primarily composed of sesquiterpenes and monoterpenes. Additionally, several notable constituents (≥ 2%) were detected, including elemol (4.58%), *α*-pinene (3.18%), and camphene (3.14%), highlighting the presence of oxygenated monoterpenes. Notably, these findings deviated from previously reported compositions. In contrast, Malaysian essential oil comprised 40 constituents, representing 92.00% of the total composition. The predominant components were 3*α*-acetoxy-8,12-epoxyeudesma-4,7,11-triene (51.7%), bicyclogermacrene (7.4%), and (*E*)-nerolidol (6.9%), suggesting a chemical profile rich in oxygenated sesquiterpenes [6]. These results highlight significant variations in the chemical profiles of the two essential oils. These observed differences may be attributed to environmental, geographical, or genetic factors.

In the fruit essential oil, 45 constituents were identified, accounting for 96.95% of the total composition. The predominant compounds included *β*-(*E*)-ocimene (35.82%), *α*-phellandrene (21.67%), and chloranthalactone B (7.05%). Additionally, several noteworthy constituents were detected, such as *α*-limonene (4%), *p*-cymene (3.79%), *β*-cyclogermacrane (2.71%), *γ*-elemene (2.29%), and spathulenol (2.14%). To the best of our knowledge, published data on the chemical composition of fruit essential oil are currently unavailable, precluding direct comparisons with the results obtained in this study. Given its high *β*-(*E*)-ocimene content, fruit essential oil presents potential applications in the pharmaceutical and cosmetic industries.

*3.2. Antimicrobial activity*

Both studied essential oils and one pure compound (chloranthalactone B) have been subjected to antimicrobial activity, and the result is shown in **Table 2.**

**Table 2.** Antimicrobial activity of *S. glabra* essential oils and chloranthalactone B

| Microorganisms | Minimum inhibitory concentration (μg/mL) | | | |
|---|---|---|---|---|
| | Leaf EO | Fruit EO | Chloranthalactone B | Positive control |
| *E. faecalis* ATCC 299212 | 64 | 128 | 64 | 64 |
| *S. aureus* ATCC 25923 | 16 | 64 | 32 | 32 |
| *E. coli* ATCC 25922 | 64 | - | - | 256 |
| *P. aeruginosa* ATCC 27853 | 128 | - | - | 128 |
| *C. albicans* ATCC 10231 | 32 | 32 | 64 | 32 |

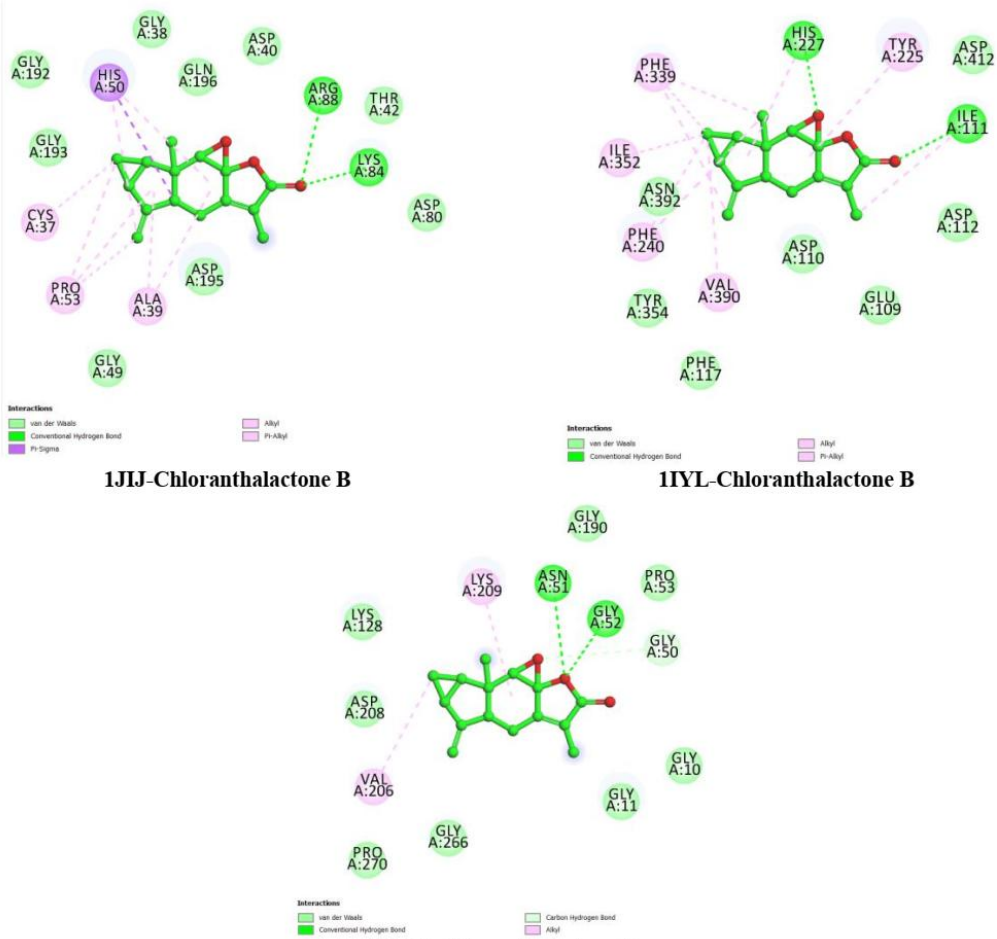
*The positive controls for bacteria and yeast were streptomycin and cycloheximide, respectively; "-" inactive in the current experiment.*

The antimicrobial properties of *S. glabra* EOs extracted from leaves and fruits, along with the bioactive compound chloranthalactone B, were evaluated against a panel of bacterial and fungal strains, including *E. faecalis*, *S. aureus*, *E. coli*, *P. aeruginosa*, and *C. albicans*. The minimum inhibitory concentration (MIC) values were determined and compared with positive controls (streptomycin for bacteria and cycloheximide for yeast). The results indicated that *S. glabra* leaf EO exhibited broad-spectrum antimicrobial activity, with MIC values ranging from 16 to 128 μg/mL. Among the tested microorganisms, *S. aureus* was the most susceptible (MIC = 16 μg/mL), followed by *C. albicans* (MIC = 32 μg/mL), *E. faecalis* (MIC = 64 μg/mL), and *E. coli* (MIC = 64 μg/mL). In contrast, *P. aeruginosa* displayed higher resistance, with a MIC of 128 μg/mL. The fruit EO demonstrated weaker antimicrobial activity, showing no inhibition against *E. coli* and *P. aeruginosa*. Its most notable effects were observed against *S. aureus* (MIC = 64 μg/mL) and *C. albicans* (MIC = 32 μg/mL), while *E. faecalis* exhibited moderate susceptibility (MIC = 128 μg/mL). Chloranthalactone B displayed selective antimicrobial activity, effectively inhibiting *S. aureus* (MIC = 32 μg/mL), *E. faecalis* (MIC = 64 μg/mL), and *C. albicans* (MIC = 64 μg/mL), but was inactive against *E. coli* and *P. aeruginosa*. To date, the antimicrobial properties of *Sarcandra* species have not been extensively investigated. The antimicrobial potential of *S. glabra* EOs may be attributed to the presence of monoterpenoids, which are known for their strong antibacterial

properties [15]. The sensitivity of bacteria to terpenoids is influenced by the composition, charge of the outer structures, and membrane permeability of the bacterial cell. Monoterpenes are believed to alter bacterial membrane permeability, increasing membrane fluidity and inducing changes in membrane protein topology, ultimately disrupting the respiratory process [16]. Additionally, the lipophilicity, hydrophobicity, and presence of hydroxyl groups in terpenes are suggested to play a crucial role in their antibacterial mechanism [17].

*3.3. Molecular docking*

Based on the promising *in vitro* antimicrobial activity of *S. glabra* essential oils and chloranthalactone B, we further conducted molecular docking simulations to evaluate the inhibitory potential and interactions between the studied proteins involved in antibacterial and antifungal mechanisms and the key components of the essential oils. The selected protein targets for molecular docking include *C. albicans N*-myristoyltransferase (PDB ID 1IYL), *E. faecalis* carbamate kinase (PDB ID 2WE5), and *S. aureus* TyrRS (PDB ID 1JIJ), chosen based on their biological significance and potential application in drug development [18],[19],[21]. These proteins are essential for the survival and pathogenicity of these microorganisms and significantly differ from similar human proteins, which enhance selectivity and reduce the risk of side effects [18]. For example, *N*-myristoyltransferase is crucial for *C. albicans* growth, while TyrRS is involved in tRNA synthesis in *S. aureus*, particularly important in antibiotic-resistant strains [18]. Therefore, these targets were used in the current docking simulation study. The compounds *α*-pinene, *α*-phellandrene, *β*-cyclogermacrane, *β*-(*E*)-ocimene, *β*-elemene, *β*-myrcene, camphene, and chloranthalactone B were docked into the active sites of 1IYL, 2WE5, and 1JIJ. The molecular docking results in **Table 3** indicate that the key compounds in *S. glabra* essential oils can bind to various protein receptors with differing binding affinities. Specifically, for the target protein 1IYL, the main compounds exhibit binding affinities ranging from -5.068 kcal/mol to -7.755 kcal/mol. For the target 2WE5, the binding affinities fall between -4.079 kcal/mol and -7.755 kcal/mol, while for 1JIJ, they range from -4.492 kcal/mol to -7.156 kcal/mol. Notably, chloranthalactone B demonstrates the highest binding affinity for all three target proteins among the studied compounds, suggesting strong biological potential in inhibiting microbial protein activity. Furthermore, *in vitro* antimicrobial activity assays have confirmed its effectiveness against tested microbial strains, highlighting the need for further research into its mechanism of action and interactions with key protein targets. Regarding interaction types, these compounds primarily engage in pi-alkyl, pi-sigma, and conventional hydrogen bonding, which contribute to the stabilization of their binding to target proteins. Remarkably, chloranthalactone B exhibits the strongest binding affinity with receptor 1IYL (-7.755 kcal/mol), forming hydrogen bonds with two crucial residues, His227 and Ile111 (**Fig. 2**). These amino acids play essential roles in the catalytic activity of the enzyme, implying that such interactions could lead to functional inhibition of the target protein. Additionally, chloranthalactone B establishes alkyl and Pi-alkyl interactions with residues Phe339, Tyr225, Ile352, Phe240, Val390, and Ile111 (**Fig. 2**). Similarly, in its interaction with 1JIJ (-7.156 kcal/mol), chloranthalactone B forms hydrogen bonds with Arg88 and Lys84, alongside alkyl and pi-alkyl interactions with Cys37, Pro53, and Ala39, as well as pi-sigma interaction with His50, further enhancing its binding stability. Moreover, against 2WE5 (-6.412 kcal/mol), it exhibits strong interactions through hydrogen bonding with Asn51 and Gly52, coupled with alkyl and pi-alkyl interactions involving Lys209 and Val206 (**Fig. 2**). Overall, the strong binding capacity of key compounds, particularly chloranthalactone B, with multiple microbial receptors mediated through hydrogen bonding and pi-alkyl interactions demonstrates their high potential for inhibiting target proteins, thereby contributing to the antimicrobial effects of *S. glabra* essential oil. This finding offers valuable insights for the development of natural antimicrobial agents, especially in response to the growing concern of antibiotic resistance.




**1JIJ-Chloranthalactone B** **1IYL-Chloranthalactone B**

**2WE5-Chloranthalactone B**

**Fig. 2.** Interaction results of chloranthalactone B with studied target proteins

**Table 3.** Binding affinities of main compounds with proteins *C. albicans N*-myristoyltransferase (PDB ID: 1IYL), *E. faecalis* carbamate kinase (PDB ID: 2WE5), *S. aureus* TyrRS (PDB ID: 1JIJ)

| No. | Compounds | ID Protein | Binding affinity (kcal/mol) | Binding/ Interaction types | Amino acid residue interactions |
|---|---|---|---|---|---|
| 1 | $\alpha$-Pinene | 1IYL | -5.682 | Pi-alkyl | His227, Phe115, Phe339, Phe240 |
| | | 2WE5 | -4.284 | Alkyl | Lys209 |
| | | 1JIJ | -4.705 | Alkyl, Pi-alkyl | His50, Pro53, Cys37 |
| 2 | $\alpha$-Phellandrene | 1IYL | -6.419 | Pi-sigma | Tyr225 |
| | | | | Alkyl, Pi-alkyl | Leu394, His227, Tyr354, Val449 |
| | | 2WE5 | -5.325 | Alkyl, Pi-alkyl | Ala264, Met268, Cys235, Val234, Tyr238 |
| | | 1JIJ | -5.575 | Alkyl | Ile200, Cys37, Leu70 |
| 3 | $\beta$-Cyclogermacrane | 1IYL | -7.171 | Pi-sigma | His227 |
| | | | | Pi-alkyl | Tyr225, Phe339, Tyr354 |
| | | 2WE5 | -5.372 | Alkyl | Lys209 |
| | | 1JIJ | -5.792 | Alkyl | Pro53 |
| 4 | $\beta$-(*E*)-Ocimene | 1IYL | -6.192 | Pi-sigma | Tyr225 |
| | | | | Alkyl, Pi-alkyl | Tyr354, Tyr335, |

| No. | Compounds | ID Protein | Binding affinity (kcal/mol) | Binding/ Interaction types | Amino acid residue interactions |
|---|---|---|---|---|---|
| | | | | | Val449, Leu415, Leu394, His227 |
| | | 2WE5 | -4.819 | Pi-sigma | Tyr238 |
| | | | | Alkyl, Pi-alkyl | Met268, Val234, Val231, Ala264 |
| | | 1JIJ | -4.536 | Alkyl, Pi-alkyl | Ala39, Tyr36, Leu70 |
| 5 | *β*-Elemene | 1IYL | -6.878 | Pi-sigma | Tyr225 |
| | | | | Pi-alkyl | Tyr354 |
| | | 2WE5 | -5.016 | Alkyl | Val206 |
| | | 1JIJ | -5.772 | - | - |
| 6 | *β*-Myrcene | 1IYL | -5.855 | Pi-sigma | Tyr225 |
| | | | | Alkyl, Pi-alkyl | Leu394, Cys393, His227, Tyr354 |
| | | 2WE5 | -4.682 | Alkyl, Pi-alkyl | Met268, Tyr238, Phe263, Val234, Ala264, Val231 |
| | | 1JIJ | -4.77 | Alkyl, Pi-alkyl | Cys37, Tyr36, Leu70 |
| 7 | Camphene | 1IYL | -5.068 | Pi-alkyl | His227, Phe240 |
| | | 2WE5 | -4.079 | Alkyl | Lys209 |
| | | 1JIJ | -4.492 | Pi-sigma | His50 |
| | | | | Alkyl, Pi-alkyl | Phe54, Ala39, Pro53, Cys37 |
| 8 | Chloranthalactone B | 1IYL | -7.755 | Convertional hydrogen bond | His227, Ile111 |
| | | | | Alkyl, Pi-alkyl | Val390, Phe240, Phe339, Ile352, Tyr225 |
| | | 2WE5 | -6.412 | Convertional hydrogen bond | Asn51, Gly52 |
| | | | | Alkyl | Lys209, Val206 |
| | | 1JIJ | -7.156 | Convertional hydrogen bond | Arg88, Lys84 |
| | | | | Alkyl and pi-alkyl | Cys37, Pro53, Ala39 |
| | | | | Pi-sigma | His50 |
| 9 | *δ*-Elemene | 1IYL | -7.096 | Pi-sigma | Tyr225 |
| | | | | Alkyl, Pi-alkyl | Tyr354, Leu415 |
| | | 2WE5 | -4.869 | Alkyl | Val206 |
| | | 1JIJ | -5.259 | - | - |
| 10 | Elemol | 1IYL | -6.633 | Pi-alkyl | His227, Tyr225 |
| | | 2WE5 | -5.611 | Convertional hydrogen bond | Gly52 |
| | | | | Alkyl | Val206 |
| | | 1JIJ | -6.512 | Convertional hydrogen bond | Tyr170 |
| | | | | Pi-alkyl | His50 |
| 11 | *γ*-Elemene | 1IYL | -7.29 | Pi-sigma | Tyr225 |
| | | | | Pi-alkyl | Tyr354 |
| | | 1C14 | -6.754 | Pi-sigma | Tyr146 |
| | | 2WE5 | -5.017 | Alkyl | Val206 |
| | | 1JIJ | -6.08 | Alkyl, Pi-alkyl | Ala39, Pro53, His50, Phe54 |
| | | 5V8E | -4.148 | Pi-alkyl | His201 |
| 12 | *p*-Cymene | 1IYL | -6.803 | Pi-sigma | Tyr225 |
| | | | | Alkyl, Pi-alkyl | Tyr335, Val449, Leu394 |
| | | | | Pi-Pi-T shaped | Tyr354 |
| | | 2WE5 | -5.399 | Pi-sigma | Tyr238 |
| | | | | Alkyl, Pi-alkyl | Val231, Cys235, Met268 |
| | | 1JIJ | -5.805 | Alkyl | Cys200 |

## 4. Conclusion

This study provides the first report on the chemical composition and antimicrobial activity of *Sarcandra glabra* essential oils from leaves and fruits collected in Vietnam, along with the bioactive compound chloranthalactone B. GC-MS analysis identified 49 constituents in leaf EO and 45 in fruit EO, with major components including chloranthalactone B, $\beta$-(*E*)-ocimene, and $\beta$-cyclogermacrane. The leaf EO exhibited broad-spectrum antimicrobial activity, with *S. aureus* being the most susceptible. In contrast, the fruit EO demonstrated weaker activity and was ineffective against *E. coli* and *P. aeruginosa*. Chloranthalactone B showed selective antimicrobial effects, particularly against *S. aureus*, *E. faecalis*, and *C. albicans*. Molecular docking studies confirmed strong interactions between key compounds and microbial target proteins, suggesting their potential as natural antimicrobial agents against antibiotic-resistant pathogens.

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