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The Leaf Essential Oils of *Syzygium oblatum* and *Syzygium abortivum*: Chemical Composition, Antimicrobial Activity, and Molecular Docking Study

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Abstract

Background and Objectives: *Syzygium* (the family Myrtaceae) is a well-known genus in the field of food chemistry and medicinal purposes. The current study aims to provide a chemical analysis of essential oils from the fresh leaves of two Vietnamese *Syzygium* species *Syzygium oblatum* (Roxb.) Wall. ex Steudel and *S. abortivum* (Gagnep.) Merr. & L.M.Perry. **Methods:** Chemical compounds in essential oils were identified using GC-FID/MS (gas chromatography-flame ionization detection/mass spectrometry) analysis. The broth microdilution method was used for the antimicrobial assay. Docking stimulation aided experimental results. **Results:** (*E*)-Caryophyllene (27.89%), α-selinene (18.34%), β-selinene (17.48%), and α-pinene (5.20%) were identified to be the main compounds in *S. oblatum* leaf essential oil, whereas the leaf essential oil of *S. abortivum* was dominated by (*E*)-caryophyllene (19.56%), δ-cadinene (11.03%), germacrene D (10.34%), and γ-muurolene (5.50%). It noted that both studied oil samples with the MIC/IC_{50} values of 8-32 μg/mL/4.56-10.37 μg/mL were comparable to the standard drugs in antimicrobial experiments against the Gram-positive bacteria *Bacillus cereus* and *Enterococcus faecalis*, and yeast *Candida albicans*. Molecular docking results showed that the main compound (*E*)-caryophyllene primarily formed hydrophobic interactions with the microbial proteins *C. albicans* N-myristoyl transferase *B. cereus* patB1, and *E. faecalis* carbamate kinase with the binding affinities of −6.969, −6.342, and −5.530 kcal/mol, respectively **Conclusion:** It is advised to isolate the main chemicals and conduct *in vivo* antibacterial experiments for both essential oils and their main compounds.

Keywords
Syzygium oblatum, *Syzygium abortivum*, essential oil, antimicrobial, molecular docking

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Introduction

People have been searching for natural remedies to treat their illnesses since ancient times. The use of therapeutic plants was instinctive in the beginning. Everything was based on experience because, at the time, neither the causes of the ailments nor the types of plants and how they may be used as a therapy were sufficiently understood. Over time, the rationale for the use of particular medicinal plants to cure particular illnesses was uncovered.[1-4] As a result, the use of medicinal plants progressively departed from the empirical framework and was based on explanatory facts. Nowadays, aromatic and medicinal plants have been used for therapeutic, religious, cosmetic, nutritional, and beautification purposes since ancient times, and humanity of all civilizations and cultures are familiar with their usage.[1-4]

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The genus *Syzygium* belongs to the family Myrtaceae, which contains about 500 species. The plants of this genus are mainly distributed in tropical Asia.[5] Many are used as traditional remedies to cure conditions like fever, eczema, diarrhea, diabetes, and dysentery.[6] *Syzygium* species are edible and grown as ornamentals throughout the tropics, and some have even infiltrated some island settings.[5] Chromatographic studies exhibited the presence of the major chemical classes acylphloroglucinols, terpenoids, and phenolic compounds.[6] Research of biological activities delivered supportive evidence for the therapeutic effects of this genus, in which crude extracts and isolated compounds were reported to exert antioxidative, anti-inflammatory, antibacterial, anticancer, antidiarrheal, and hepatoprotective activities.[7]

Syzygium plants are also rich in essential oils. Especially, the clove (*S. aromaticum*) oil with more than 50% eugenol received much interest because of its wide uses in perfume, cosmetics, health care, medicine, flavoring, and food chemistry.[8] The leaf essential oil of *S. cunini* enriching in α-pinene (22.2%), *cis*-β-ocimene (10.2%), and (*E*)-caryophyllene (9.45%) is appropriate for treating inflammatory syndromes with the underlying mechanism of eosinophil migrated inhibition.[9] The isolated oil from *S. polyanthum* leaves was associated with the abundance of *cis*-4-decanal (43.489%), 1-decyl aldehyde (19.752%), and capryl aldehyde (14.092%), and strongly controlled the bacterium *B. subtilis* with the MIC value of 31.25 μg/mL.[10] The main constituents of *S. szemaoense* leaf essential oil *cis*-β-elemene (68.0%), as well as this essential oil suppressed the bacteria *E. faecalis* and *S. aureus* (MIC 128.0 μg/mL), and *C. albicans* (MIC 64.0 μg/mL).[11] Similarly, the leaf essential oils of *S. coriaceum* and *S. samarangense* showed anti-fungal activity against *C. albicans* with the same MIC value of 8.0 mg/mL.[12] So far, they exhibited anti-aging activity by inhibiting elastase and collagenase ezymes.[12]

Syzygium oblatum (Roxb.) Wall. ex Steudel and *Syzygium abortivum* (Gagnep.) Merr. & L.M.Perry can be found in tropical Asia regions.[13] A literature survey revealed that there have been reports of the isolation of acylphloroglucinols with ATP citrate lyase inhibitory effects from *S. oblatum*.[6] Phytochemical analysis for essential oils of these two species was not yet studied, to date. Therefore, the current research deals with chemical identification based on the GC-MS analysis. The obtained essential oils have been further subjected to antimicrobial examination. *In silico* approach has been also used to highlight the crucial interactions among the major compounds and bacterial proteins.

Materials and Methods

Plant Materials

The fresh leaves of two studied plants were collected from Binhchuan, Pu Huong Natural Reserve, Nghean, Vietnam (*S. oblatum*: 19°14′41′′N and 104°55′51′′E; *S. abortivum*: 19°18′8′′N and 104°54′9′′E) in December 2022. Botanical identification was confirmed by co-author Do Ngoc Dai. Two voucher specimens SOL-2022 (*S. oblatum*) and SAL-2022 (*S. abortivum*) have been deposited in Nghe An College of Economics.

Hydro-Distillation of Essential Oils

Essential oils were obtained by hydro-distilled procedures. In brief, 2.0 kg of the fresh leaves of each plant were chopped and subjected to hydro-distillation using a Clevenger-type apparatus for 3.0 h. For further analyses, essential oils have been made dry by Na_2SO_4 and kept in sealed glass vials at 3 °C. The obtained oils were yellow and pungent, in which the yields of 0.15 and 0.17%, w/v were assigned to *S. oblatum* and *S. abortivum*, respectively.

The GC-FID/MS Analyses

The GC-FID analysis was carried out using a Shimadzu GC2010 with the FID detector.[14] The HP5-MS column (30 × 0.25 mm, 0.25 m film thickness) was used. Operating conditions included: column temperature rises from 50 to 250 °C at 4 °C/min, and then held at 250 °C for 4 min; the helium (99.999%) was used as a carrier gas with a 1.0 mL/min flow rate; injection volume, 0.1 μL (split ratio of 1:20); and the injector and detector temperatures = 250 and 270 °C, respectively. The relative percentage of each component in essential oil was obtained by the normalized peak area (%).

The GC-MS analysis was carried out by a Shimadzu GC2010. The column was an HP5-MS fused silica capillary one (30 m × 0.25 mm i.d.×0.25 μm film thickness). The EI (electron ionization) mode happened at 70 eV. Helium was employed as a carrier gas at a flow rate of 1.0 mL/min. The injection volume was 0.1 μL (split ratio of 1:20). Injector and ion-source temperatures were established at 250 and 270 °C, respectively. The oven temperature program was the same as the one used for the GC. Mass spectra were taken at a scan interval of 0.5 s, in a mass range from 50 to 550 Da. Identifying constituents in essential oils was based on their RI (retention indices) on an HP-5MS capillary column, under the same operating conditions as those used in the GC-FID analysis, involving a homologous series of *n*-alkanes (C7-C30). Chemical structural identification was matched with the W09N08 library, Adams book,[15] and NIST Chemistry WebBook.[16]

Antimicrobial Assay

Microbial strains used in this study consist of three Gram-positive bacteria *Bacillus cereus* ATCC11778, *Staphylococcus aureus* ATCC29213, and *Enterococcus faecalis* ATCC51299, three Gram-negative bacteria *Escherichia coli* ATCC8739, *Pseudomonas aeruginosa* ATCC9027, and *Salmonella enterica* ATCC10708, and one yeast *Candida albicans* ATCC 60193. They were obtained from the Institute of Marine Biochemistry, VAST, Hanoi, Vietnam. The Mueller-Hinton

broth and Sabouraud dextrose broth were used as the mediums for bacteria and fungi, respectively. The experimental methods were identical to our previous publication (Supplemental material).[17,18]

Statistical Analysis

Data are processed using Microsoft Excel and represented as Mean ± SD (Standard Deviation). The difference was statistically meaningful with $P < .05$.

Molecular Docking

Based on the promising *in vitro* antimicrobial activity of *S. oblatum* and *S. abortivum* essential oils, it is hypothesized that the main compound, (*E*)-caryophyllene, plays a significant role in this activity. Molecular docking analysis was conducted to describe the antimicrobial mode of action through related biological targets. Three proteins *C. albicans* N-myristoyl transferase, *E. faecalis* carbamate kinase, and *B. cereus* patB1 were used as targets, and cyclohexamide and streptomycin were used as reference controls.[19-21] The crystal structures of these three proteins were obtained from the Protein Data Bank (https://www.rcsb.org/) with PDB IDs 1IYL, 2WE5, and 5V8E, respectively.[19-21] The structures of these proteins were then prepared by removing unnecessary molecules for docking and adding missing hydrogen atoms using AutoDockTools software. (*E*)-caryophyllene was drawn using Marvin JS software. The grid box of each protein target was determined based on previous literature reports and set up using the AutoDockTools software. AutoDock Vina 1.2.3 software was used to dock the ligands into the binding sites of the target proteins running on the Ubuntu operating system.[22] The docking procedure was validated by re-docking the co-crystallized ligands into the binding sites, and the RMSD values were calculated. The 2D and 3D visualizations of the ligand-protein interactions were generated using PyMOL and Discovery Studio Visualizer.

Results

Chemical Profile of Essential Oils

Hydro-distillation of *S. oblatum* fresh leaves resulted in a yellow essential oil with a yield of 0.15 w/v. A total of 43 compounds were identified, which accounted for 96.12% (Table 1 and Figure 1). The obtained essential oil was predominated by sesquiterpene hydrocarbons (81.24%). Meanwhile, monoterpene hydrocarbons, oxygenated sesquiterpenes, and oxygenated diterpene occurred with 7.37, 7.22, and 0.29%, respectively. (*E*)-Caryophyllene (27.89%), α-selinene (18.34%), β-selinene (17.48%), and α-pinene (5.20%) were the primary compounds. In addition, some compounds were recorded greater than 1.00%, consisting of conocephalenol (2.38%), α-humulene (2.23%), (*Z*)-β-farnesene (2.13%), α-copaene (2.00%), δ-cadinene (1.99%), 7-*epi*-α-selinene (1.95%), cedrol (1.30%), and β-bisabolene (1.05%).

The yellow essential oil of *S. abortivum* leaves was obtained with a yield of 0.17%, w/v. A list of 41 identified compounds was tabulated in Table 1 and Figure 2, which represented 94.51%. Sesquiterpene hydrocarbons (73.36%) and their oxygenated derivatives (21.15%) were the two main chemical classes, whereas monoterpene hydrocarbons and oxygenated diterpenes were completely absent. The major compounds in this essential oil sample included (*E*)-caryophyllene (19.56%), δ-cadinene (11.03%), germacrene D (10.34%), and γ-muurolene (5.50%). Some other compounds were found to reach exceeding 1.00%, such as caryophyllene oxide (4.95%), α-zingiberene (4.43%), γ-cadinene (4.26%), spathulenol (4.24%), *epi*-cedrol (3.59%), γ-amorphene (2.89%), α-humulene (2.22%), and α-cadinol (1.88%).

As can be seen, the percentage of (*E*)-caryophyllene in *S. oblatum* leaf essential oil is more than that of *S. abortivum* leaf essential oil by 10.55%. The remaining major compounds of *S. oblatum* leaf essential oil were insignificant or absent in *S. abortivum* leaf essential oil. In the same manner, δ-cadinene, germacrene D, and γ-muurolene were significant in *S. abortivum* essential oil, but they were much less or absent in the first oil sample. Various compounds have been only found in one species. For example, a series of monoterpene hydrocarbons α-pinene β-pinene, myrcene, limonene, (*Z*)-β-ocimene, and (*E*)-β-ocimene were unique in *S. oblatum* leaf essential oil, or various compounds, such as germacrene D, γ-muurolene, and α-zingiberene are significant compounds in *S. abortivum* essential oil, but they disappeared in the leaf essential oil of *S. oblatum* leaf essential oil.

Antimicrobial Activity

The studied essential oils have been further subjected to antimicrobial experiments. For Table 2, both two samples were comparable to the standard streptomycin (MIC/IC_{50} = 32 μg/mL/20.45-50.34 μg/mL in antimicrobial assay against three Gram-positive bacteria *B. cereus*, *S. aureus*, and *E. faecalis*. Regarding the Gram-negative bacteria, two essential oil samples inhibited the growth of the bacterium *P. aeruginosa* with the MIC/IC_{50} value of 64-128 μg/mL/21.44-44.92 μg/mL, but they did not show activity against two bacteria *E. coli* and *S. enterica*. In the last case, essential oils showed anticandidal activity against the yeast *C. albicans* with the same MIC value of 8 μg/mL and the IC_{50} values of 4.56-4.84 μg/mL, as compared with those of the standard cyclohexamide (MIC/IC_{50} = 32 μg/mL/10.46 μg/mL).

Molecular Docking Study

To validate the protocol before conducting the docking simulations, a re-docking approach was performed to determine its reliability by comparing it with the known binding positions of the co-crystallized ligand structures in the protein-ligand

Table 1. The Identified Compounds (%) in the Leaf Essential oOls of Two Myrtaceae Plants.

Rt	RI_E	RI_L	Constituents	*S. oblatum*	*S. abortivum*	Classification
9.88	940	932	α-Pinene	5.20	–	MH
11.24	985	974	β-Pinene	0.92	–	MH
11.48	993	988	Myrcene	0.32	–	MH
12.88	1035	1024	Limonene	0.37	–	MH
13.03	1039	1032	(*Z*)-β-Ocimene	0.17	–	MH
13.40	1050	1044	(*E*)-β-Ocimene	0.63	–	MH
14.94	1095	1086	Terpinolene	0.13	-	MH
24.08	1361	1345	α-Cubebene	–	0.61	SH
24.89	1385	1373	α-Ylangene	0.17	0.22	SH
25.04	1390	1374	α-Copaene	2.00	0.58	SH
25.48	1403	1387	β-Cubebene	–	0.32	SH
25.51	1404	1389	*cis*-β-Elemene	0.19	–	SH
26.22	1426	1411	α-*cis*-Bergamotene	0.34	–	SH
26.38	1431	1410	α-Cedrene	0.27	0.29	SH
26.61	1439	1417	(*E*)-Caryophyllene	27.89	19.56	SH
26.83	1446	1431	β-Gurjunene	0.54	0.55	SH
27.02	1452	1437	α-Guaiene	0.83	–	SH
27.17	1457	1439	Aromadendrene	–	1.28	SH
27.33	1461	1440	(*Z*)-β-Farnesene	2.13		SH
27.49	1467	1448	*cis*-Muurola-3,5-diene	–	0.14	SH
27.65	1472	1452	α-Humulene	2.23	2.22	SH
27.89	1479	1464	9-*epi*-(*E*)-Caryophyllene	0.15	0.71	SH
28.19	1489	1475	*trans*-Cadina-1(6),4-diene	0.27	0.29	SH
28.24	1491	1476	Conocephalenol	2.38	–	OS
28.27	1491	1478	γ-Muurolene	–	5.50	SH
28.38	1495	1483	α-Amorphene	0.49		SH
28.49	1498	1484	Germacrene D	–	10.34	SH
28.53	1500	1487	α-Zingiberene	–	4.43	SH
28.55	1500	1488	Selina-4,11-diene	0.52	–	SH
28.73	1506	1489	β-Selinene	17.48	1.38	SH
28.83	1510	1493	γ-Amorphene	–	2.89	SH
28.84	1510	1495	*trans*-Muurola-4(14),5-diene	0.71	–	SH
28.95	1514	1498	α-Muurolene	–	3.83	SH
28.97	1515	1500	α-Selinene	18.34		SH
29.10	1519	1505	β-Bisabolene	1.05		SH
29.18	1522	1509	β-Curcumene	0.38		SH
29.19	1522	1511	δ-Amorphene	–	0.64	SH
29.45	1531	1513	γ-Cadinene	0.57	4.26	SH
29.63	1537	1519	δ-Cadinene	1.99	11.03	SH
29.68	1538	1520	7-*epi*-α-Selinene	1.95		SH
29.78	1542	1528	Zonarene	–	0.32	SH
29.98	1548	1533	*trans*-Cadina-1,4-diene	0.17	0.41	SH
30.14	1554	1537	α-Cadinene	0.35	0.63	SH
30.35	1561	1544	α-Calacorene	0.23	0.48	SH
30.47	1565	1548	Elemol	–	0.20	OS
30.66	1571	1561	(*E*)-Nerolidol	0.16	–	OS
30.66	1571	1563	Salviadienol	–	0.92	OS
30.95	1581	1564	β-Calacorene	–	0.23	SH
31.30	1592	1570	Caryophyllenyl alcohol	0.19	–	OS
31.49	1599	1577	Spathulenol	–	4.24	OS
31.67	1605	1582	Caryophyllene oxide	0.49	4.95	OS
31.95	1615	1594	Salvial-4(14)-en-1-one	–	0.23	OS
32.11	1621	1599	Curzerenone	0.32	0.43	OS
32.30	1627	1600	Cedrol	1.30	–	OS
32.31	1628	1618	*epi*-Cedrol	–	3.59	OS
32.41	1631	1625	Torilenol	–	0.55	OS
32.87	1648	1627	1-*epi*-Cubenol	0.45	0.67	OS
33.21	1660	1638	*epi*-α-Cadinol	0.47	0.90	OS

(Continued)

Table 1. Continued

Rt	RI_E	RI_L	Constituents	*S. oblatum*	*S. abortivum*	Classification
33.22	1660	1640	*epi*-α-Muurolol	–	1.22	OS
33.27	1665	1644	α-Muurolol	–	0.92	OS
33.63	1674	1652	α-Cadinol	0.49	1.88	OS
33.72	1677	1658	*neo*-Intermedeol	0.97	–	OS
34.11	1691	1672	14-Hydroxy-9-*epi*-caryophyllene	–	0.45	OS
34.21	1695	1675	Cadalene	–	0.22	SH
44.84	2119	1942	Phytol	0.29		OD
Total				96.12	94.51	
Monoterpene hydrocarbons (MH)				7.37	–	
Sesquiterpene hydrocarbons (SH)				81.24	73.36	
Oxygenated sesquiterpenes (OS)				7.22	21.15	
Oxygenated diterpene (OD)				0.29	–	

Abbreviations: Rt, Retention time; RI_E, Experimental retention indices; RI_L, Literature retention indices.

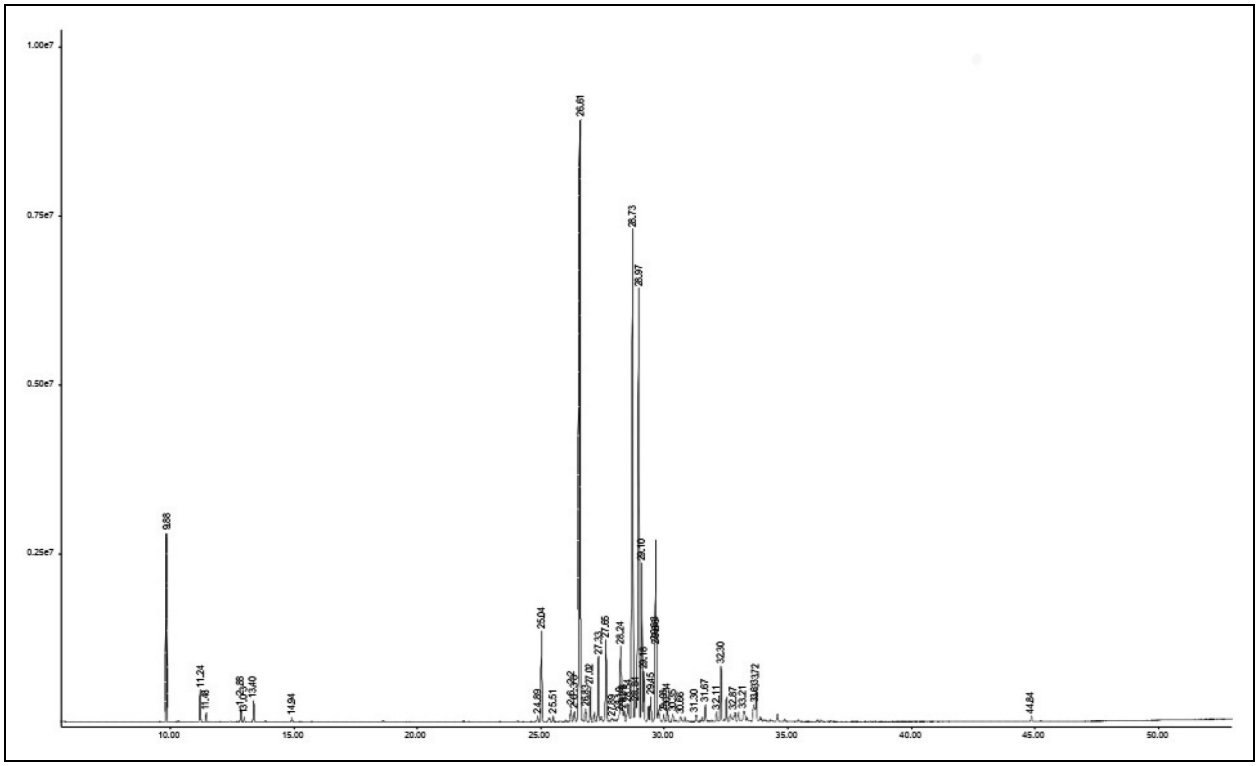

Figure 1. The GC chromatogram of essential oil of *Syzygium oblatum* leaves.

complexes. The results, as shown in Figure 3, with the calculated RMSD value of 1.041 Å (< 2 Å), indicated that the protocol was highly reliable.[14,23] Subsequently, the results of the docking simulation of (*E*)-caryophyllene with the selected target proteins are presented in Figure 4 and Table 3. It was found that (*E*)-caryophyllene interacted with *C. albicans* N-myristoyl transferase with the ΔG (binding energy) value of −6.969 kcal/mol, followed by interactions with *E. faecalis* carbamate kinase (ΔG = −5.53 kcal/mol) and *B. cereus* patB1 (ΔG = −6.342 kcal/mol). The comparison with the two control compounds is analyzed. The interaction analysis of (*E*)-caryophyllene with the studied proteins showed that the compound primarily formed hydrophobic interactions with the amino acid residues in the selected proteins due to its hydrocarbon nature (Figure 4). Specifically, (*E*)-caryophyllene formed pi-alkyl interactions with Phe117, Tyr354, Phe339, His227, and Phe240, and pi-sigma interactions with residue Tyr225. In contrast, this molecule only formed alkyl interactions with two proteins *E. faecalis* carbamate kinase and *B. cereus* patB1. (*E*)-Caryophyllene interacted with *E. faecalis* carbamate kinase at amino acid residues Lys209 and Val206, and with *B. cereus* patB1 at residues Met195, Leu210, and Ala233.

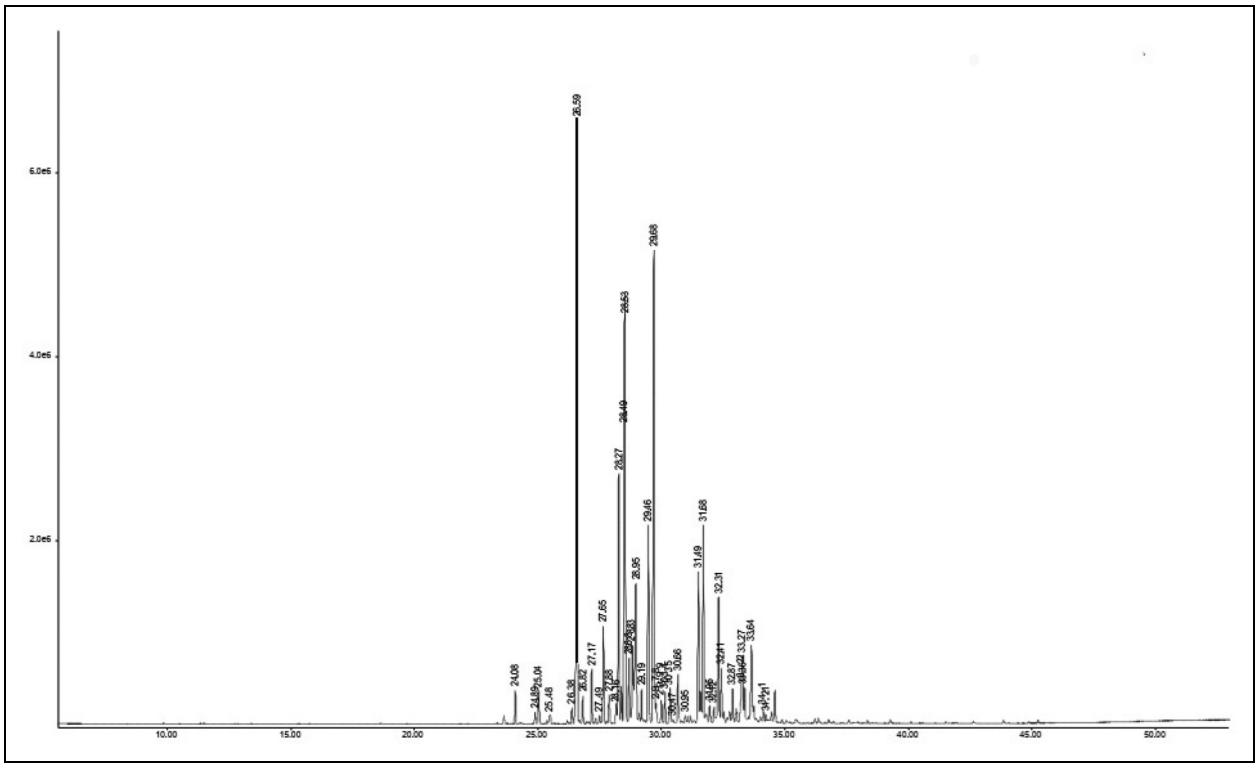

Figure 2. The GC chromatogram of essential oil of *Syzygium abortivum* leaves.

Table 2. Antimicrobial Activity of the Studied Essential Oils.

		Minimum inhibitory concentration (MIC: μg/mL)			
Microbial strains		*S. oblatum*	*S. abortivum*	Streptomycin	Cyclohexamide
Gram (+)	*B. cereus*	16	32	32	
	S. aureus	64	32	32	
	E. faecalis	16	8	32	
Gram (–)	*E. coli*	–	–	256	
	P. aeruginosa	128	64	64	
	S. enterica	–	–	256	
Yeast	*C. albicans*	8	8		32
Microbial strains		Half maximal inhibitory concentration (IC_{50}: μg/mL)			
Gram (+)	*B. cereus*	10.37	6.96	20.45	
	S. aureus	11.05	22.31	45.24	
	E. faecalis	4.82	8.76	50.34	
Gram (–)	*E. coli*	–	–	9.45	
	P. aeruginosa	21.44	44.92	41.46	
	S. enterica	–	–	45.67	
Yeast	*C. albicans*	4.56	4.84		10.46

"-": Inactive.

Discussion

(*E*)-Caryophyllene is one of the major compounds found in the genus *Syzygium*. As an example, it was found to reach 18.21, 16.0, and 12.72%, respectively, in the leaf essential oil of Indian *S. caryophyllatum*, Brazilian *S. cumini*, and German *S. aqueum*.[5,24,25] It is also recognized that (*E*)-caryophyllene is a naturally occurring bicyclic sesquiterpene that is widely present in essential oils derived from a variety of fruits, species, and medicinal plants. It is classified as a phytocannabinoid and is accepted for use as a food additive, flavoring agent, and taste enhancer by the US Food and Drug Administration and European agencies.[26] Thereby, the appropriate methods to isolate and enrich this sesquiterpene hydrocarbon from the current studied species are expected.

Table 3. Binding Energies and Hydrophobic Interactions of the major (E)-Caryophyllene in Essential Oils and Target Proteins.

Compounds	Target proteins	Binding energy (ΔG, kcal/mol)	Hydrophobic interactions
(*E*)-Caryophyllene	N-myristoyl transferase (PDB ID: 1IYL)	−6.969	Phe117, Tyr354, Tyr225, Phe339, His227, and Phe240
	Carbamate kinase (PDB ID: 2WE5)	−5.530	Lys209, and Val206
	PatB1 (PDB ID: 5V8E)	−6.342	Met195, Leu210, and Ala233
Cycloheximide	N-myristoyl transferase (PDB ID: 1IYL)	−7.777	Leu415, Tyr354, and Leu394
Streptomycin	Carbamate kinase (PDB ID: 2WE5)	−5.875	–
	PatB1 (PDB ID: 5V8E)	−8.707	–

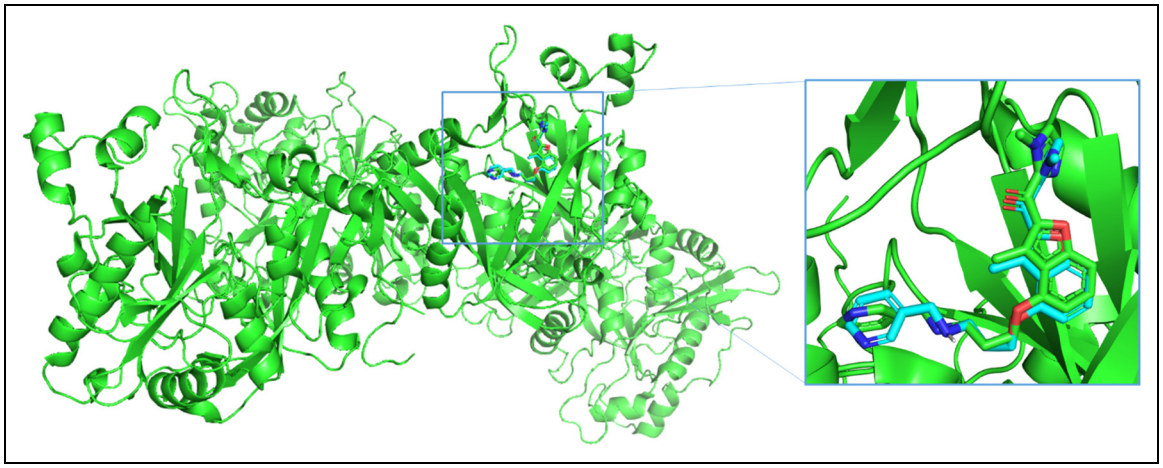

Figure 3. The outcome of re-docking the R64 representative ligand and superimposing their binding positions at the 1IYL protein's active pocket.

It noted that *Syzygium* essential oils exhibited higher activity against the Gram-positive bacteria than the Gram-negative bacteria. This is deduced from the great role of the membrane of bacteria, in which the Gram-positive bacteria are known as monoderms because they have a single, thick peptidoglycan cell wall enclosing them.[27] The Gram-negative bacteria are called diderms because they have an outside membrane containing lipopolysaccharides enclosing the cell while having a much weaker peptidoglycan cell wall.[27] It matches well with previous records, *Syzygium* essential oils are excellent agents for treating microbial strains.

Various records indicated the appropriate uses of *Syzygium* essential oils for antimicrobial treatments. For instance, the leaf essential oils from four Vietnamese species *S. formosum*, *S. syzygioides*, *S. megacarpum*, and *S. chantaranothaianum* with MIC values of 16-128 μg/mL were comparable to the standard streptomycin against the Gram-positive bacteria *S. aureus* and *B. cereus*, and Gram-negative bacterium *P. aeruginosa*.[28] The clove oil showed both antibacterial and antibiofilm against *B. substilis* due to its effects on the protein structures of older biofilms.[29]

(*E*)-Caryophyllene is a well-known natural product that exhibits various pharmacological activities, such as anticancer, and antiinflammation, especially antimicrobial activities. For instance, this metabolite inhibited *S. mutans* with a MIC value of 0.32% by penetrating the biofilm, which constituted a protective barrier against external substances, acting as an ion exchange resin.[30] In another report, (*E*)-caryophyllene was comparable to the standard compound kanamycin to inhibit the proliferation of the bacteria *S. aureus*, *E. coli*, *P. aeruginosa*, *A. niger*, and *Rhizopus oryzae*.[31] In this study, the molecular docking method has been implemented to get good fits in the interactions and binding energies between the main compound (*E*)-caryophyllene, and the target proteins *C. albicans* N-myristoyl transferase, *E. faecalis* carbamate kinase, and *B. cereus* patB1.

Conclusions

The current research first describes the chemical analysis of essential oils from the leaves of two Vietnamese Myrtaceae plants *S. oblatum* and *S. abortivum*. Generally, sesquiterpene hydrocarbons and their oxygenated derivatives were the main chemical classes. (*E*)-Caryophyllene was found to reach the highest percentage in both two species. The studied essential oils have shown good antimicrobial activity, especially strongly inhibiting the growth of the Gram-positive bacteria *B. cereus* and *E. faecalis*, and yeast *C. albicans*. The *in silico* studies were also conducted to investigate the inhibitory potential of (*E*)-caryophyllene against the microbial targets *C. albicans* N-myristoyl transferase, *E. faecalis* carbamate kinase, and *B. cereus* patB1. Hydrophobic

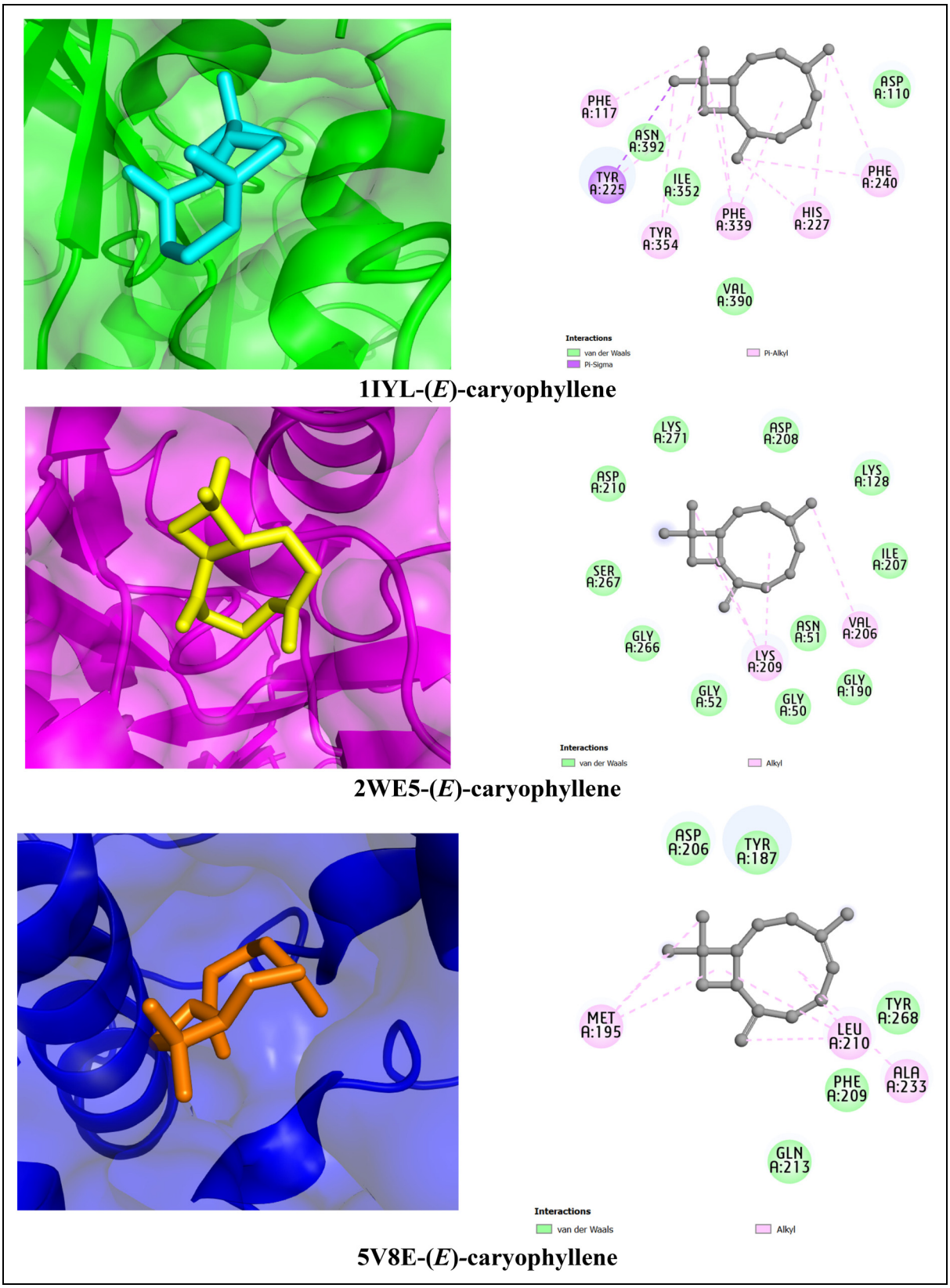

Figure 4. Molecular interactions among target proteins and (*E*)-caryophyllene.

interactions such as alkyl, pi-alkyl, and pi-sigma primarily contributed to their binding affinities.

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Supplemental Material

Supplemental material for this article is available online.

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