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CHEMICAL COMPOSITION AND *IN VITRO*/*IN SILICO* ENZYME INHIBITORY ACTIVITIES OF THE LEAF ESSENTIAL OIL OF *ACTINODAPHNE PILOSA* (LOUR.) MERR. FROM QUANG TRI PROVINCE

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Summary

The GC-MS analysis identified 49 components, accounting for 94.98% of the total content. The most abundant chemical class was sesquiterpene hydrocarbons (67.88%), followed by monoterpene hydrocarbons (20.03%), oxygenated sesquiterpenes (6.86%), and oxygenated monoterpenes (0.21%). The major compounds identified were germacrene D (16.73%), *β*-caryophyllene (11.80%), *δ*-elemene (11.02%), bicyclogermacrene (10.98%), and *β*-(*E*)-ocimene (5.59%). The study confirmed that the *A. pilosa* leaf essential oil possesses significant inhibitory activity against *α*-amylase (IC_{50} = 78.02 ± 2.64 µg/mL) and moderate activity against tyrosinase (IC_{50} = 631.82 ± 52.18 µg/mL). Notably, its effect on *α*-amylase was more potent than the standard acarbose (IC_{50} = 95.71 ± 3.43 µg/mL), while its tyrosinase inhibition was significantly weaker than kojic acid (IC_{50} = 72.90 ± 2.67 µg/mL). Molecular docking further supported these results, showing that *β*-caryophyllene (-7.57 kcal/mol), germacrene D (-7.24 kcal/mol), *δ*-elemene (-6.75 kcal/mol), and bicyclogermacrene (-7.00 kcal/mol) share key binding interactions with the positive control mini-montbretin A, thereby rationalizing their *α*-amylase inhibitory activity. These findings, representing the first reported enzyme inhibitory activity of this essential oil, suggest its potential for antidiabetic applications.

Keywords: *Actinodaphne pilosa; Essential oil; Enzyme inhibition; Phytochemical profile.*

1. Introduction

The genus *Actinodaphne* Nees, also known as *Actinomorphe* Kuntze, belongs to the Lauraceae family and includes approximately 125 species found across tropical and subtropical Asia to the South West Pacific [1]. In traditional medicine, a number of *Actinodaphne* species have found application in treating various diseases in some parts of the world. For example, a decoction from *A. angustifolia* leaves is used to treat kidney stones, while the seed oil of *A. hookeri* is applied for rheumatic pain [2]. The bark of *A. obovata* is used for treating fractures, and *A. lancifolia* is particularly useful for treating arthritis, edema, overexertion, and stomachaches [2],[3]. The genus *Actinodaphne* is known to produce various compounds, including alkaloids, lignans, lactonic compounds, and essential oils [4],[5],[6],[7],[8],[9],[10].

Actinodaphne pilosa (Lour.) Merr. is a tree or shrub, 4-12 m tall, with young parts covered in a rusty, hair-like growth. The leaves are obovate or elliptic, pinninerved, and arranged alternately or in clusters. Flowers are in 5-flowered clusters on a peduncle. Male flowers have 9 hairy, fertile stamens, while female flowers have a hairy ovary. The fruit is a small, round berry seated on a subflat disc [11]. In Chinese traditional medicine, the leaves and bark of *A. pilosa* have been used medicinally to treat skin infections, coughs, rheumatism, and swelling [11]. In Vietnamese traditional medicine, a decoction from *A. pilosa* is used to treat stomachache [12]. To date, studies on this species remain very limited and have primarily focused on its essential oils [13],[14]. Notably, the *A. pilosa* essential oils from Pù Hoạt Nature Reserve, Vietnam, were found to have broad antimicrobial and excellent mosquito larvicidal activity. This oil effectively inhibited the growth of several bacteria and fungi and was highly lethal to larvae of *Aedes aegypti*, *A. albopictus*, and *Culex quinquefasciatus* [13]. This study was conducted to analyze the volatile organic compounds of the leaf essential oil of *A. pilosa* growing wild in Quang Tri province, Vietnam, and to evaluate its inhibitory effects on *α*-amylase and tyrosinase. The findings from this work are expected to provide insight into the oil's

potential as an antidiabetic agent and its possible use in nutraceutical applications.

2. Materials and methods

2.1. Plant materials

Fresh leaves of *Actinodaphne pilosa* (Lauraceae family) were collected from Thuong Trach commune, Quang Tri province, Vietnam (17°29'13.1N, 106°21'2.73E; Elevation: 671 m) in March 2024. For scientific identification, a representative voucher specimen was carefully prepared and identified by MSc. Bui Van Huong (Vietnam National Museum of Nature, Vietnam Academy of Science and Technology). This voucher specimen (APL-05.03.2024) was subsequently deposited at the Department of Chemistry, Vinh University, Vietnam. The remaining fresh leaf material was immediately processed for essential oil extraction and subsequent phytochemical and bioactivity investigations.

2.2. Extraction of essential oil

The essential oil from the fresh leaves of *A. pilosa* was obtained via a hydrodistillation method utilizing a Clevenger-type apparatus. This experimental process was performed in triplicate, three runs (3.5 h each), until no further oil distilled. Following collection, the leaf essential oil was dried over anhydrous Na_2SO_4 and stored at 4°C in the dark for subsequent analysis.

2.3. Gas chromatography-mass spectrometry (GC-MS) analysis

Using a GC-MS (Agilent Technologies) instrument combined with an HP-5MS UI column (30 m × 0.25 mm × 0.25 μm), the chemical components in the essential oil of *A. pilosa* were analyzed. Helium was used as the carrier gas, maintained at a constant flow rate of 1.0 mL/min. A 1.0 μL essential oil sample (1% in dichloromethane, v/v) was injected into the system with a split ratio of 10:1. The column oven temperature program was as follows: an initial temperature of 50°C was held for 3 minutes, then the temperature was increased to 180°C at a rate of 3°C/min. Subsequently, it was ramped up to 240°C at a rate of 5°C/min, and finally held at this temperature for 5 minutes. The mass spectrometer was operated in EI mode at 70 eV with a mass range of 45-500 m/z. Volatile compounds were identified by comparing their mass spectra and retention indices (RIs) with published data (from the NIST 17 library and Adams' book [15]).

2.4. Inhibition of α-amylase

The *α*-amylase inhibitory assay was performed using a modified version of previously established protocols [16],[17]. A diluted essential oil sample of *A. pilosa* leaves was combined with 10 mL of an *α*-amylase solution (0.14 U/mL) in phosphate buffer (pH 6.9) and incubated for 15 minutes at 37°C. The reaction was initiated by adding 10 mL of starch solution (0.25%), followed by a second 15-minute incubation at the same temperature. A blank sample was prepared identically but without the addition of *α*-amylase. The reaction was terminated by adding 50 mL of 1 M HCl, after which 100 mL of a KI_3 solution was added. Absorbance was then measured at 595 nm using a spectrophotometer. The percentage of enzyme inhibition was calculated using the following formula: Percentage of inhibition (%) = [1 - (X/Y)] × 100 (%). Where X and Y represent the absorbance of the sample and blank, respectively. Acarbose was used as a reference standard, and the activity of the *A. pilosa* leaf oil was estimated by its IC_{50} value (μg/mL).

2.5. Inhibition of tyrosinase

The tyrosinase inhibitory assay was performed based on a modified version of a previously established protocol [18]. A sample (100 μL) of either *A. pilosa* leaf essential oil or kojic acid was combined with 40 μL of tyrosinase (0.5 g/L) and 100 μL of phosphate buffer (pH 7.4). Following a 15-minute pre-incubation at room temperature, the reaction was initiated with 40 μL of L-DOPA (0.5 mM). After the mixture had reacted for another 15 minutes at room temperature, the change in absorbance was measured at 490 nm. Kojic acid was used as a reference standard, and the activity of the *A. pilosa* leaf oil was estimated by its IC_{50} value (μg/mL).

2.6. Docking calculations

Molecular docking simulations were performed using the AutoDock Vina v1.2.3 program to predict the binding modes and interaction energies between the major compounds identified from the essential oil of *Actinodaphne pilosa* and the *α*-amylase enzyme [19]. The three-dimensional structures of the major constituents were retrieved from the PubChem database, protonated at pH 7.4, and geometry-optimized using the MMFF94 force field in Avogadro software [20]. The optimized structures were then converted to PDBQT format with Gasteiger charges applied using AutoDockTools v1.5.6 software. The target protein, *α*-amylase (PDB ID: 5E0F), was obtained from the

RCSB Protein Data Bank and preprocessed by removing crystallographic water molecules and unnecessary ligands, adding polar hydrogens, and saving in PDBQT format using AutoDockTools v1.5.6 software. The docking grid box was centered on the co-crystallized ligand mini-montbretin A to cover the entire active site, with parameters set according to a previously reported study [18]. The docking protocol was validated by re-docking the native ligand, and was accepted when the RMSD value was ≤ 2.0 Å.. Docking results were ranked based on binding free energy values (ΔG, kcal/mol), and the best binding poses of each ligand-enzyme complex were further analyzed using Discovery Studio Visualizer to generate 2D and 3D interaction profiles.

3. Results and discussion

3.1. Chemical composition of the essential oil

The essential oil from the *A. pilosa* leaves was a light-yellow liquid, with a yield of 0.07% (w/w) based on fresh weight. The GC-MS analysis (**Fig. S1**) of this leaf essential oil identified 49 volatile components, which constituted 94.98% of the total oil content (**Table 1**). Sesquiterpene hydrocarbons (67.88%) and monoterpene hydrocarbons (20.03%) were identified as the primary group constituents in the essential oil of *A. pilosa* leaves, comprising 67.88% and 20.03%, respectively. The major compounds of the investigated essential oil were germacrene D (16.73%), *β*-caryophyllene (11.80%), *δ*-elemene (11.02%), bicyclogermacrene (10.98%), and *β*-(*E*)-ocimene (5.59%). Other components that were also found in significant quantities in the *A. pilosa* leaf oil were *β*-(*Z*)-ocimene (4.71%), *α*-pinene (3.90%), *β*-elemene (3.42%), *δ*-cadinene (2.77%), *α*-caryophyllene (2.19%), *α*-copaene (1.87%), and neo-allo-ocimene (1.84%).

Table 1. Chemical compositions of the essential oil of *A. pilosa* leaves

No.	RT (min)	Name	RI (exp.)	RI (lit.)	Type	Area %
1	6.183	*α*-Thujene	928	929	MH	0.21
2	6.395	*α*-Pinene	935	937	MH	3.90
3	6.864	Camphene	950	952	MH	0.36
4	7.699	Sabinene	974	974	MH	0.54
5	7.802	*β*-Pinene	977	979	MH	0.40
6	8.317	*β*-Myrcene	991	991	MH	0.61
7	8.804	*α*-Phellandrene	1003	1005	MH	0.50
8	9.021	3-Carene	1010	1011	MH	0.20
9	9.742	*α*-Limonene	1029	1030	MH	0.42
10	9.845	Eucalyptol	1032	1032	OM	0.21
11	10.148	*β*-(*Z*)-Ocimene	1040	1038	MH	4.71
12	10.566	*β*-(*E*)-Ocimene	1050	1049	MH	5.59
13	10.972	*γ*-Terpinene	1060	1060	MH	0.12
14	12.202	Terpinolene	1088	1088	MH	0.63
15	13.988	Neo-allo-ocimene	1130	1131	MH	1.84
16	23.126	*δ*-Elemene	1337	1338	SH	11.02
17	23.635	*α*-Cubebene	1349	1351	SH	0.17
18	24.734	*α*-Copaene	1374	1376	SH	1.87
19	25.134	*β*-Bourbonene	1383	1384	SH	0.28
20	25.357	*β*-Cubebene	1388	1389	SH	1.48
21	25.449	*β*-Elemene	1390	1391	SH	3.42
22	26.565	*β*-Caryophyllene	1417	1419	SH	11.80
23	26.942	*β*-Copaene	1426	1432	SH	1.19
24	27.332	Aromandendrene	1436	1440	SH	0.12
25	27.549	Isogermacrene D	1442	1447	SH	0.87
26	27.927	*α*-Caryophyllene	1451	1454	SH	2.19
27	28.184	*β*-(*E*)-Farnesene	1457	1457	SH	0.79
28	28.270	Cadina-1(6),4-diene	1459	1461	SH	0.80
29	28.934	*γ*-Muurolene	1475	1477	SH	0.81
30	29.111	Germacrene D	1479	1481	SH	16.73
31	29.489	Bicyclosesquiphellandrene	1488	1489	SH	0.15
32	29.723	Bicyclogermacrene	1494	1495	SH	10.98
33	29.861	*α*-Muurolene	1497	1499	SH	0.14
34	30.227	*β*-Bisabolene	1506	1509	SH	0.17

No.	RT (min)	Name	RI (exp.)	RI (lit.)	Type	Area %
35	30.439	Cubebol	1512	1515	OS	0.28
36	30.782	δ-Cadinene	1521	1524	SH	2.77
37	31.097	Cubenene	1529	1532	SH	0.13
38	32.418	Ledol	1564	1565	OS	0.21
39	32.830	Spathulenol	1574	1576	OS	0.80
40	33.054	β-Caryophyllene oxide	1580	1581	OS	1.21
41	33.363	Viridiflorol	1587	1591	OS	0.38
42	33.786	Cedrol	1598	1600	OS	0.25
43	34.473	Epicedrol	1617	1618	OS	0.37
44	34.765	Epicubenol	1625	1627	OS	0.27
45	35.125	Isospathulenol	1635	1638	OS	0.24
46	35.274	*t*-Cadinol	1639	1640	OS	0.65
47	35.428	δ-Cadinol	1643	1645	OS	0.20
48	35.726	α-Cadinol	1651	1653	OS	0.56
49	38.518	Guaiol acetate	1728	1727	OS	1.44
		Monoterpene hydrocarbons (MH)				20.03
		Oxygenated monoterpenes (OM)				0.21
		Sesquiterpene hydrocarbons (SH)				67.88
		Oxygenated sesquiterpenes (OS)				6.86
		Total				**94.98**

RT (min): Retention time; RI (Exp.): Retention indices on HP-5MS UI column; RI (Lit.): Retention indices from the literature.

Based on a review of previous reports, the major components in the *A. pilosa* leaf essential oils from the Pù Hoạt Nature Reserve were α-pinene (6.0-7.2%), β-(*Z*)-ocimene (10.1-14.3%), β-(*E*)-ocimene (6.5-10.4%), β-caryophyllene (9.0-14.9%), germacrene D (12.0-16.2%), bicyclogermacrene (syn. β-cyclogermacrane) (11.0-15.9%), and spathulenol (1.0-6.2%) [13]. In contrast, the major components identified in the essential oil of *A. pilosa* leaves from Guangdong, China, were viridiflorene (ledene, 12.7%), γ-muurolene (12.3%), germacrene D (11.6%), β-caryophyllene (10.7%), and globulol (5.9%) [14]. The most consistently present major components in *A. pilosa* leaf essential oils, as observed in both the present and previous reports, are β-caryophyllene and germacrene D. Additionally, the chemical composition and content of the *A. pilosa* leaf essential oils showed some variation across studies, which may be attributed to environmental, geographical, or temporal factors.

3.2. In vitro enzyme inhibitory activity

The leaf essential oil of *A. pilosa* growing wild in Quang Tri province, Vietnam, was evaluated for its inhibitory effect on enzymes, and the results are presented in **Table 2**.

Table 2. Half maximal inhibitory concentrations (IC_{50}, µg/mL) of the *A. pilosa* leaf essential oil on the enzymes

Samples	IC_{50} (µg/mL)	
	α-Amylase	**Tyrosinase**
A. pilosa leaf essential oil	78.02 ± 2.64	631.82 ± 52.18
Acarbose*	95.71 ± 3.43	–
Kojic acid*	–	72.90 ± 2.67

** The reference standards (acarbose and kojic acid) for the inhibition of α-amylase and tyrosinase, respectively; –: Not tested.*

Based on the results shown in **Table 2**, the *A. pilosa* leaf essential oil demonstrated inhibitory activity against both α-amylase and tyrosinase enzymes. The oil exhibited a more potent effect on α-amylase, with an IC_{50} value of 78.02 ± 2.64 µg/mL. This value indicates a stronger inhibitory capacity compared to the standard acarbose (IC_{50} = 95.71 ± 3.43 µg/mL). In contrast, the *A. pilosa* leaf essential oil showed a significantly weaker inhibitory effect on tyrosinase, with an IC_{50} value of 631.82 ± 52.18 µg/mL. This activity was notably less potent than that of the positive control, kojic acid, which had an IC_{50} of 72.90 ± 2.67 µg/mL. Overall, the findings suggest that the *A. pilosa* leaf essential oil exhibits a strong inhibitory

effect on α-amylase but is less effective against tyrosinase.

The inhibitory activity of the *A. pilosa* leaf essential oil against α-amylase and tyrosinase can be attributed to the presence of several major compounds. For example, prior research has shown that the essential oils of *Piper nigrum* and *P. lolot* exhibit notable α-amylase inhibitory activity [21],[22]. These oils are rich in major components such as β-caryophyllene and (*E*)-β-ocimene [21],[22]. Literature studies also show that caryophyllene, a major component of the essential oil, inhibits both tyrosinase activity (by suppressing melanogenesis) and α-amylase activity, which is linked to diabetes [23],[24]. Additionally, the observed anti-enzyme properties may also be due to additive or synergistic interactions between the different components of the essential oil. To the best of our knowledge, this is the first record of the anti-α-amylase and anti-tyrosinase activities of the *A. pilosa* essential oil. The findings of this study suggest that the *A. pilosa* leaf essential oil has significant potential for use in the development of diabetes treatments, although further studies are needed.

3.3. Molecular docking

To ensure the reliability of the docking protocol, a re-docking validation was first performed by re-docking the co-crystallized ligand into the active site of the target enzyme. The reproduced binding pose was highly consistent with the crystallographic orientation, with an RMSD value of 1.728 Å below 2.0 Å, confirming that the docking parameters and scoring function were appropriate for predicting ligand–protein interactions. Subsequently, docking simulations were conducted on the major phytochemicals identified in the essential oil of *A. pilosa*, since compounds with higher abundance are more likely to contribute significantly to its overall biological activity. The results, as shown in Table S1 and Fig. S2, were compared with mini-montbretin A (-10.58 kcal/mol), a known inhibitor used as a positive control [25]. Among the phytochemicals, sesquiterpenes such as β-caryophyllene (–7.57 kcal/mol) and germacrene D (–7.24 kcal/mol) displayed the most favorable affinities, stabilized by hydrophobic interactions with Tyr62, Trp58, Trp59, Gln63, Asp197, Leu165, and Leu162 (Fig. S2). δ-Elemene (–6.75 kcal/mol) and bicyclogermacrene (–7.00 kcal/mol) showed slightly weaker yet still relevant interactions involving Asp300 and His299. In contrast, (*E*)-β-ocimene exhibited the lowest affinity (–4.97 kcal/mol), suggesting a limited contribution to enzyme inhibition. Notably, the major constituents of *A. pilosa* leaf essential oil also exhibit several key amino acid interactions similar to those observed with the positive control, mini-montbretin A. Mini-montbretin A interacted with Lys200, Tyr151, Ile235, His305, Trp59, Asp300, Trp58, Leu165, Thr163, His299, Tyr62, and Leu162. Remarkably, β-caryophyllene and germacrene D showed the highest overlap, engaging Tyr62, Trp58, Trp59, Leu165, Leu162, and Thr163; δ-elemene displayed common interactions with Asp300, His299, Tyr62, Trp58, and Trp59; whereas bicyclogermacrene maintained interactions with Tyr62, Trp58, Trp59, Leu165, and Asp300. Even (*E*)-β-ocimene, despite its weaker affinity, still engaged Tyr62, Trp59, and His299, which are also involved in mini-montbretin A binding (Fig. S2). These findings suggest that the sesquiterpenes in *A. pilosa* leaf essential oil may partially mimic the binding pattern of mini-montbretin A, thereby contributing to its potential α-amylase inhibitory activity.

4. Conclusion

This study provides the first report on the enzyme inhibitory activities of the *A. pilosa* leaf essential oil. The GC-MS analysis showed the oil is rich in sesquiterpene hydrocarbons (67.88%) and monoterpene hydrocarbons (20.03%), with germacrene D (16.73%), β-caryophyllene (11.80%), δ-elemene (11.02%), bicyclogermacrene (10.98%), and β-(*E*)-ocimene (5.59%) as major components. The oil exhibited strong inhibitory activity against α-amylase (IC_{50} = 78.02 ± 2.64 μg/mL), surpassing the standard drug acarbose (IC_{50} = 95.71 ± 3.43 μg/mL), suggesting its promise for developing antidiabetic products. In particular, molecular docking revealed that β-caryophyllene, germacrene D, δ-elemene, and bicyclogermacrene also exhibit similar interactions with crucial binding residues as observed with the positive control, mini-montbretin A, offering a molecular basis for their α-amylase inhibitory effect. The medicinal potential of this plant warrants further investigation. Future research should focus on *in vivo* evaluation of the essential oil's biological activities, as well as the isolation and characterization of its active constituents.

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