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## Rhizome essential oil of *Meistera verrucosa* from Ha Giang Province, Vietnam: Chemical composition, antioxidant activities, and molecular docking study

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### Abstract

This work aimed to determine the chemical composition and antioxidant activity of rhizome essential oil (EO) of *Meistera verrucosa* growing wild in Ha Giang Province, Vietnam. The EO was isolated using hydrodistillation, then the chemical composition was analyzed by Gas chromatography-mass spectroscopy (GC-MS). In addition, the antioxidant activities were determined by the DPPH scavenging method and ferric reducing antioxidant power (FRAP) assay. The results showed that  $\alpha$ -pinene,  $\beta$ -pinene, and (*E*)- $\beta$ -ocimene were major components in the EO, accounting for 39.6%, 20.7%, and 12.2%, respectively. The EO showed antioxidant activity, the IC<sub>50</sub> value of DPPH scavenging activity, and the EC<sub>50</sub> value of FRAP assay were 91.01 mg/mL and 17.50 mg/mL, respectively. Furthermore, to evaluate the inhibitory interaction potential of Keap1, docking analysis indicated that  $\alpha$ -pinene has the strongest affinity among the major compounds surveyed. The key interactions observed in the complexes of the major compounds with Keap1 are predominantly hydrophobic interactions ( $\pi$ - $\sigma$  and  $\pi$ -alkyl), which significantly contribute to their binding affinities. These results provide more information on the volatile compounds of the EO from the rhizomes of *M. verrucosa* and first reveal its antioxidant power.

### Keywords

*Meistera verrucosa*, Essential oil, Phytochemical composition, Antioxidant activity, Molecular docking.

## INTRODUCTION

Essential oils (EOs), isolated from plants and having various important bioactivities, are valuable natural products used in the pharmaceutical, food, and fragrance industries, thus garnered increasing attention in recent years<sup>1-7</sup>. The genus *Meistera* Giseke is an aromatic member of the family Zingiberaceae, with about 45 species distributed in several regions of the world<sup>8</sup>. Most species of *Meistera* are characterized by large clump-forming herbs with compact flowering heads, a fertile bract supporting a single trumpet-shaped, spreading

or exposed flower, a semilunar anther crest, and mostly echinate fruits<sup>9</sup>. Some species of *Meistera* are used as food and local medicines in Vietnam<sup>10</sup>.

To date, there are some studies about the phytochemical and biological activities of the genus *Meistera* in literature. For example, according to Tee *et al.*<sup>11</sup>, the fruits of *M. chinensis* contained major compounds of saponins, terpenoids, steroids, alkaloids, phenolics, tannins, and flavonoids. In another study, the chemical compositions of the EOs from *M. cristatissima* leaves and rhizomes were also determined, showing that  $\alpha$ -pinene (19.8%) and spathulenol (14.6%) are corresponding major compounds<sup>12</sup>. Similarly, the main chemical compositions in the EOs of *M. tomrey* pseudostems and leaves included  $\beta$ -pinene (6.6-14.2%), 1,8-cineole (13.5-16.7%),  $\alpha$ -pinene (4.6-6.9%), and borneol (4.2-4.6%)<sup>13</sup>. The volatile compounds of the EOs of the rhizomes, flowers, leaves, and roots of *M. verrucosa* from Tuyen Quang Province, Vietnam, and their antimicrobial activities were also investigated<sup>14</sup>. However, there have been limited reports on the antioxidant activity of this species. In the present study, we analyzed the chemical components of the rhizomes EO of this species from Ha Giang Province, Vietnam, and first determined its antioxidant properties. Furthermore, a molecular docking approach was utilized to evaluate the interaction modes and binding affinities between the major components of the EO and the target protein, correlating with the intracellular antioxidant mechanism.

## MATERIALS AND METHODS

### Plant material

Fresh rhizomes of *Meistera verrucosa* (S.Q.Tong) Škorničk. & M.F.Newman were collected from Quan Ba District, Ha Giang Province (23°01'30.15"N, 104°57'48.23"E), Vietnam in August 2022. This plant was identified by Assoc. Prof. Dr. Nguyen Hoang Tuan. The voucher specimen has been deposited at the Natural Products Laboratory, Department of Chemistry, Vinh University, Nghe An Province, Vietnam, under voucher no. HC-30MV/2022.

### Chemicals

Ascorbic acid (99%), 2,2-di(4-tert-octylphenyl)-1-picrylhydrazyl (DPPH), 2,4,6-tris(2-pyridyl)-s-triazine (TPTZ), and dimethyl sulfoxide (DMSO) were purchased from Sigma-Aldrich (St. Louis, MO, USA). Sodium sulfate and dichloromethane were purchased from Merck (Darmstadt, Germany). All other chemicals were of analytical grade.

### Extraction of the essential oil

Fresh rhizomes of *M. verrucosa* were hydrodistilled in the Clevenger apparatus at 100°C using an electric stove (Sanaky SNK2102HG, Vietnam) until no more EO was produced (about 3.5 h). Obtained EO was dried over anhydrous sodium sulfate and stored at 4°C in a refrigerator for further analysis. The experiments were conducted in triplicate<sup>15-17</sup>.

### Gas chromatography-mass spectrometry (GC-MS) analysis

The chemical compositions of the EO of *M. verrucosa* rhizomes were analyzed via GC-MS system. The instrument used was GC 7890B coupled with MSD 5977B (Agilent Technologies, USA). The GC column was an HP-5MS UI column (30 m  $\times$  0.25 mm, 0.25  $\mu$ m film thickness, Agilent Technologies, USA). The parameters for GC-MS system in this study were similar to those in the previous study, with some minor modifications<sup>18</sup>. The EI mode was used for the detection of the volatile composition, and helium was used as the carrier gas at a flow rate of 1.0 mL/min. A diluted sample in CH<sub>2</sub>Cl<sub>2</sub> (1:100 v/v) was injected in a split mode of 25:1. The oven temperature began at 60°C, maintained for 1 min, gradually increased to 240°C at a rate of 4°C/min, and eventually reached an isothermal end (240°C) for 4 min. The temperatures of the injector and MS Quad were correspondingly set at 300°C and 150°C, while the MS source was fixed at 230°C. The mass spectra were recorded at 70 eV with a mass scan ranging from m/z 50 to 550 (2.0 scan/s). Collected data were analyzed by the MassHunter Workstation Software (Version B.08.00), and mass spectra and retention indices

were compared with published data (NIST 17 and Adams<sup>19</sup>) to identify the EO constituents.

### Antioxidant activity test

#### DPPH free radical scavenging activity

Scavenging activities of the rhizome EO of *M. verrucosa* against DPPH were determined based on the previous reports<sup>20,21</sup>. Briefly, the EO was dissolved in DMSO at given concentrations, after which they were mixed with the 3 mM DPPH solution, followed by a 30-minute incubator. Ascorbic acid (0-100 µg/mL) was used as a positive control, while the sample was replaced by DMSO in the negative control (NC). The mixture was spectrophotometrically measured at 517 nm. The DPPH scavenging activity (%) was calculated using the following equation:

$$\text{DPPH Scavenging Activity (\%)} = \frac{A(\text{NC}) - A(\text{t})}{A(\text{NC})} \times 100 (\%)$$

Where A(NC) denoted the absorbance of the negative control and A(t) represented the absorbance of the tested sample.

#### Ferric reducing antioxidant power (FRAP) assay

The ferric-reducing power of the rhizome EO of *M. verrucosa* was determined according to the previous reports<sup>21,22</sup>. Briefly, add 10 mM TPTZ solution, 300 mM acetate buffer, and 20 mM ferric chloride solution to create a fresh working FRAP solution. This solution (240 µL) was then mixed with the EO sample (10 µL) and incubated for 15 min in the dark. The absorbance was then spectroscopically measured at 593 nm. The reducing power was expressed as EC<sub>50</sub> (mg/mL), the concentration at which the absorbance of the reaction was 0.5<sup>23</sup>.

#### Molecular docking

To determine the binding sites of the major compounds from the rhizome EO of *M. verrucosa*, molecular docking software was used, and the protein associated with oxidation was the crystal structure of the target protein Kelch-like ECH-associated protein (Keap1) (PDB ID: 4L7B) with a resolution of 2.02 Å, which was downloaded from the RCSB Protein Data Bank<sup>24</sup>. The preparation of the protein structure for molecular docking included

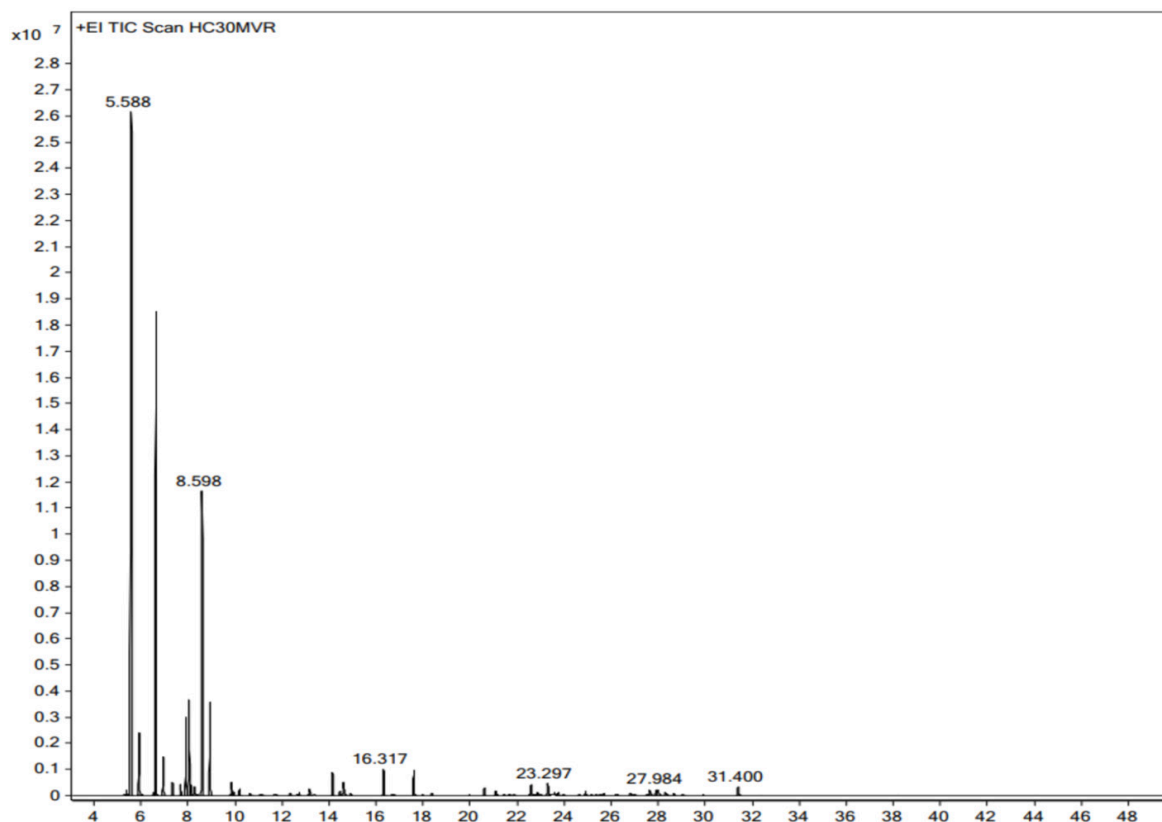
removing water molecules and ligands, followed by macromolecule energy minimization using Chimera v1.16.51 software. The chemical structures of the major compounds α-pinene, β-pinene, and (*E*)-β-ocimene were generated in Marvin Sketch and then energy optimized using Avogadro v1.2.0 software with the MMFF94s force field<sup>25</sup>. The energy-minimized chemical structures of the ligands were then converted to PDBQT format using AutoDockTools v1.5.6 software. The AutoDock Vina v1.2.3 program was selected for molecular docking simulation<sup>26</sup>. A grid box was chosen to cover the binding site of the co-crystallized ligand (1S,2R)-{[(1S)-1-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)methyl]-3,4-dihydroisoquinolin-2(1H)-yl]carbonyl}cyclohexanecarboxylic acid (1VV), specifically, with the center of the box at x = -2.6 Å, y = 3.3 Å, z = -27.4 Å, and box dimensions of 22x22x22. All parameters during the docking experiments were set to default, except for the exhaustiveness value, which was set to 400. The docking protocol was validated through re-docking. Additionally, Discovery Studio Visualizer and PyMOL software were used to visualize the binding modes of receptor-ligand interactions.

## RESULTS AND DISCUSSION

### Identification of chemical composition

The chemical composition of the EO of *M. verrucosa* rhizomes was determined by using GC-MS analysis (Fig. 1), the results of which are presented in Table 1.

A total of 37 compounds were detected, accounting for 97.6% of the EO content. Monoterpene hydrocarbons were the predominant class of compounds in the analyzed EO sample, comprising the highest proportion of up to 89.1%. On the other hand, other subgroups, including oxygenated monoterpenes, sesquiterpene hydrocarbons, and oxygenated sesquiterpenes, accounted for lower proportions of 5.5, 2.4 and 0.6%, respectively. The major compounds α-pinene, β-pinene, and (*E*)-β-ocimene were identified with high percentages, making up 39.6, 20.7 and 12.2%, respectively. Additionally, several other components were



**Figure 1.** The GC chromatogram of the rhizome EO of *M. verrucosa*

**Table 1.** Chemical composition of the rhizome EO of *M. verrucosa*

No.	RT (min)	Compounds	RI <sup>a</sup>	RI <sup>b</sup>	Percentage (%)	
					In this study	In reference <sup>14</sup>
1	5.387	$\alpha$ -Thujene	932	929	0.2	-
-	-	$\beta$ -Thujene	-	-	-	2.2
2	5.588	<b><math>\alpha</math>-Pinene</b>	941	937	39.6	-
-	-	Cyclofenchene	-	-	-	42.8
3	5.920	Camphene	955	952	2.2	1.1
4	6.526	Sabinene	978	974	0.1	-
5	6.635	<b><math>\beta</math>-Pinene</b>	982	979	20.7	19.7
6	6.944	$\beta$ -Myrcene	993	991	1.3	2.4
7	7.339	$\alpha$ -Phellandrene	1007	1005	0.6	0.4
8	7.682	$\alpha$ -Terpinene	1020	1017	0.4	0.2
9	7.911	<i>p</i> -Cymene	1029	1025	2.9	0.3
10	8.037	Limonene	1033	1030	4.4	1.8
11	8.117	Eucalyptol	1036	1032	0.4	-
12	8.271	( <i>Z</i> )- $\beta$ -Ocimene	1042	1038	0.3	-
13	8.598	<b>(<i>E</i>)-<math>\beta</math>-Ocimene</b>	1053	1049	12.2	22.9
14	8.929	$\gamma$ -Terpinene	1064	1060	3.6	0.7
15	9.845	Terpinolene	1091	1088	0.6	0.3

Table 1 *cont.*

No.	RT (min)	Compounds	RI <sup>a</sup>	RI <sup>b</sup>	Percentage (%)	
					In this study	In reference <sup>14</sup>
16	10.183	Linalool	1100	1099	0.3	0.5
17	10.640	Fenchol	1116	1113	0.1	-
18	12.345	Borneol	1170	1166	0.1	-
19	12.729	Terpinen-4-ol	1181	1177	0.2	0.1
20	13.164	$\alpha$ -Terpineol	1193	1189	0.3	0.1
21	14.148	Fenchyl acetate	1224	1223	1.0	-
22	14.611	Thymol methyl ether	1238	1235	0.6	-
23	14.915	Carvacrol methyl ether	1248	1244	0.1	-
24	16.317	Bornyl acetate	1289	1285	1.2	0.3
25	17.598	Myrtenyl acetate	1329	1327	1.1	0.2
26	18.359	$\alpha$ -Terpinyl acetate	1353	1350	0.1	-
27	20.602	$\alpha$ -Santalene	1423	1420	0.3	0.5
28	21.089	$\alpha$ -Bergamotene	1440	1435	0.2	-
29	21.449	<i>epi</i> - $\beta$ -Santalene	1451	1448	0.1	-
30	21.655	Humulene	1458	1454	0.1	-
31	21.850	$\beta$ -Santalene	1464	1462	0.1	-
32	22.594	Aristolochene	1488	1487	0.6	-
33	22.863	Valencene	1496	1492	0.2	-
34	23.297	$\beta$ -Bisabolene	1511	1509	0.6	-
35	23.750	$\beta$ -Sesquiphellandrene	1527	1524	0.2	0.4
36	24.900	Nerolidol	1567	1564	0.2	-
37	31.400	Ambrial	1803	1809	0.4	-
		Total (%)			97.6	96.9
		Monoterpene hydrocarbons			89.1	95.3
		Oxygenated monoterpenes			5.5	0.7
		Sesquiterpene hydrocarbons			2.4	0.9
		Oxygenated sesquiterpenes			0.6	-

RT: Retention time (min); RI<sup>a</sup>: Retention Indices on HP-5MS UI column; RI<sup>b</sup>: Retention Indices in literature

also majored in the rhizome EO, exceeding 2%, including camphene (2.2%), *p*-cymene (2.9%), limonene (4.4%), and  $\gamma$ -terpinene (3.6%). These findings contradict a recently published study showing that  $\alpha$ -pinene was not identified in the rhizome EO of *M. verrucosa* from Tuyen Quang, Vietnam, but cyclofenchene was detected as the predominant compound, constituting the highest percentage at 42.8%. This variation in compound composition could be attributed to differences in the growth origin of the plant studied. However,  $\beta$ -pinene and (*E*)- $\beta$ -ocimene yielded results consistent with previous reports<sup>14</sup>. Moreover,

$\alpha$ -pinene and  $\beta$ -pinene were also detected in the rhizome EO of *M. caudata* at levels of 27.6 and 21.3%, respectively<sup>27</sup>. Additionally,  $\alpha$ -pinene, at a concentration of 19.8%, was identified in the leaf EO of *M. cristatissima*. Furthermore, the EO extracted from the fresh leaves of *M. sudaie* from Vietnam, was reported to contain major compounds,  $\beta$ -pinene (27.4%) and  $\alpha$ -pinene (21.2%)<sup>28</sup>.

#### Evaluation of antioxidant activity

Antioxidant compounds could stabilize free radicals, thus maintaining the physiological

functions of the body<sup>29</sup>. There have been several reports on the antimicrobial effects of the EOs from *M. verrucosa*, but it seems that the antioxidant activity of those EOs has still been limited. In this study, the antioxidant power of the EO of *M. verrucosa* rhizomes was first examined by DPPH and FRAP assays.

For DPPH scavenging activity, the EO showed moderate and concentration-dependent activity (Table 2), with the IC<sub>50</sub> value of 91.01 mg/mL. This power was much lower than the positive control, ascorbic acid, showing the IC<sub>50</sub> value of 0.014 mg/mL.

As for ferric reducing power, the EO also showed concentration-dependent reducing activity (Fig. 2), with an EC<sub>50</sub> of 17.5 mg/mL. This reducing activity was also weaker than the positive control, as the EC<sub>50</sub> values of ascorbic acid were approximately 0.07 mg/mL.

The EO also showed a lower antioxidant than *M. chinensis* fruit extract, IC<sub>50</sub> DPPH of 47.62 mg/mL<sup>11</sup>. To date, there has been little information about the antioxidant activity of *Meistera* plants compared with other species in the Zingiberaceae family such as the *Alpinia* genus. Indeed, this EO showed higher antioxidant activities than those of the rhizome EO of *Alpinia nelumboides*, whose highest percentage of scavenging activity was merely 17.4% and EC<sub>50</sub> of reducing power was 23.0 mg/mL<sup>21</sup>.

The gap in antioxidant activities of different EOs may be correlated with the variations of the major bioactive compounds, such as  $\alpha$ -pinene and  $\beta$ -pinene, in the EO's chemical compositions. Specifically, the percentage of these monoterpenes in the EO of *M. verrucosa* was 39.63 and 20.73%, much higher than those in *Alpinia nelumboides*'s EO, just 4.1-6.0%. These results confirm the strong positive correlation between the levels of  $\alpha$ -pinene and  $\beta$ -pinene and the antioxidant activity of the EOs. A previous study also showed that increasing  $\alpha$ -pinene led to a corresponding rise in DPPH and FRAP activities<sup>30</sup>.

### Molecular docking

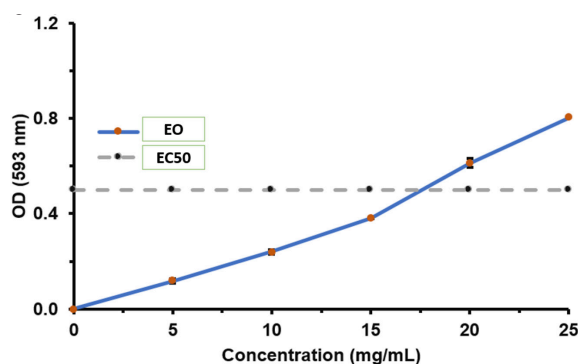
Keap1 (Kelch-like ECH-associated protein 1) plays a crucial role in the body's antioxidant

system by binding to Nrf2 and keeping it inactive<sup>31</sup>. When the body experiences oxidative stress, Nrf2 is released, moves into the cell nucleus, and activates antioxidant genes to protect the cell from free radicals and other harmful agents<sup>32</sup>. Inhibiting Keap1 can effectively activate the natural antioxidant system, presenting potential in treating oxidative stress-related diseases such as Parkinson's, Alzheimer's, cancer, and other pathologies<sup>33-35</sup>. Therefore, in this study, the Keap1 protein (PDB ID: 4L7B) was selected to dock the major compounds discovered in the rhizome EO of *M. verrucosa* into its active site. Before proceeding, a re-docking method was performed to verify the protocol by calculating the RMSD value to observe the ability to estimate the position of the co-crystallized ligand before and after re-docking into the protein's active site<sup>36</sup>. As a result, the obtained RMSD value was 0.755 Å, indicating that the positional deviation of the re-docked ligand was minor compared to the original co-crystallized ligand, leading to a high reliability of the docking protocol (Fig. 3).

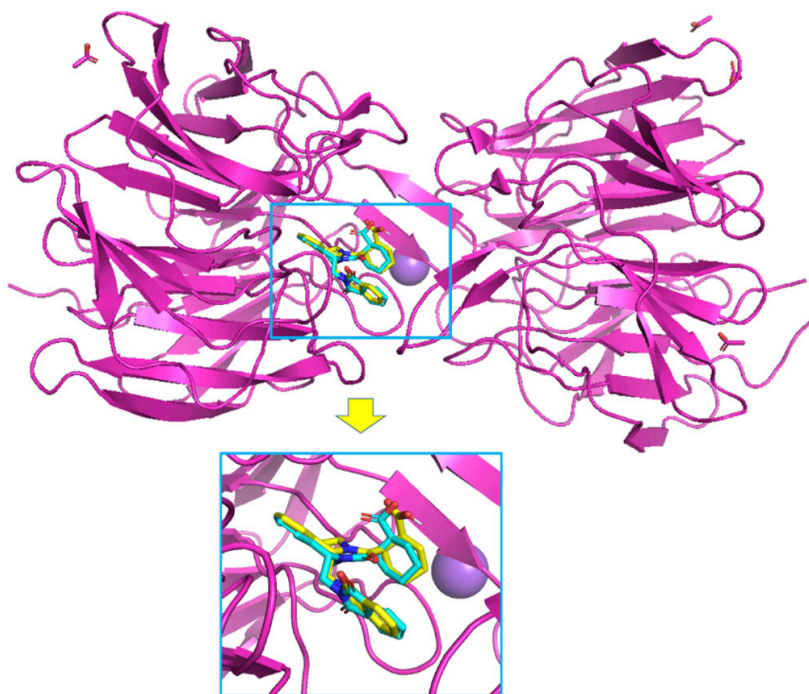
Next, the major compounds were evaluated for

**Table 2.** DPPH scavenging activity of the rhizome EO of *M. verrucosa*

Concentration (mg/mL)	% Scavenging activity	IC <sub>50</sub> (mg/mL)
0	0.00 ± 3.17	91.01 ±
25	13.72 ± 3.09	2.45
50	28.07 ± 4.34	
75	46.72 ± 0.94	
100	51.20 ± 2.08	



**Figure 2.** Ferric reducing activity of the rhizome EO of *M. verrucosa*



**Figure 3.** The re-docking results of the co-crystallized ligand 1VV within the binding site pocket with Keap1 protein (PDB ID: 4L7B)

**Table 3.** Binding affinity and hydrophobic interactions (pi-alkyl and pi-sigma) within the binding site of major compounds observed in complex with Keap1

Compound	Binding affinity (kcal/mol)	Pi-alkyl interaction	Pi-sigma interaction
$\alpha$ -Pinene	-5.390	Phe577, Tyr334	Tyr572
$\beta$ -Pinene	-5.336	Tyr572, Tyr334	Tyr572, Tyr334
( <i>E</i> )- $\beta$ -Ocimene	-5.093	Tyr572, Tyr334	-

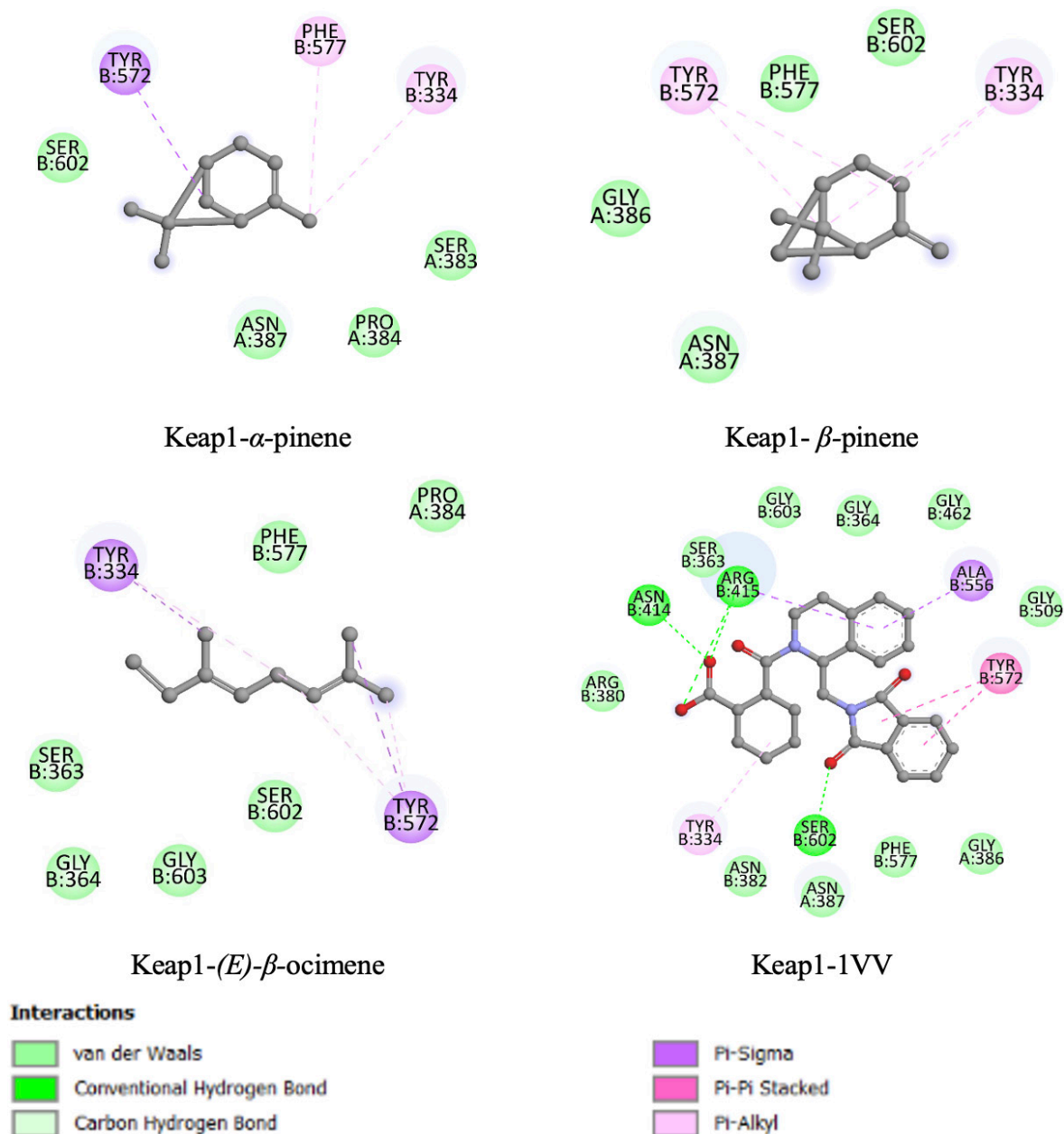
their binding affinity to the Keap1 protein, as shown in Table 3 and Fig. 4.  $\alpha$ -Pinene exhibited the strongest binding affinity at -5.390 kcal/mol, followed by  $\beta$ -pinene and (*E*)- $\beta$ -ocimene with affinities of -5.336 kcal/mol and -5.093 kcal/mol, respectively. The interactions of these compounds with the amino acid residues in the active site of the Keap1 protein are depicted in Fig. 4. It can be seen that the main interactions are hydrophobic, such as pi-alkyl and pi-sigma interactions, which primarily contribute to the binding capability with the studied protein. Specifically, the residue Tyr334 forms pi-alkyl interactions with all three compounds while forming a pi-sigma interaction with  $\alpha$ -pinene. The residue Tyr572 establishes pi-alkyl interactions with  $\beta$ -pinene and (*E*)- $\beta$ -ocimene and a pi-sigma interaction with  $\alpha$ -pinene.

Additionally, the residue Phe577 forms a pi-alkyl interaction with  $\alpha$ -pinene. Notably, the two residues Tyr572 and Tyr334 are also observed in similar interactions as the inhibitor 1VV when complexed with Keap1 (Fig. 4). These findings could serve as a basis for directing the major components in *M. verrucosa* to develop antioxidant fragrance products.

## CONCLUSION

This study further provides information on volatile compounds and newly reports the antioxidant activities of the rhizome EO of *M. verrucosa*. The major compounds of the EO were  $\alpha$ -pinene,  $\beta$ -pinene, and (*E*)- $\beta$ -ocimene, accounting for 39.63%, 20.73%, and 12.22%, respectively. Other components, including camphene, *p*-cymene, limonene, and  $\gamma$ -terpinene,





**Figure 4.** 2D interaction of the major compounds in the rhizome EO of *M. verrucosa* within the active site pocket of Keap1 protein (PDB ID: 4L7B)

were also predominant at lower proportions. The EO displayed moderate antioxidant activities; the  $IC_{50}$  of DPPH scavenging activity was 91.01 mg/mL, and the  $EC_{50}$  of ferric reducing power was 17.50 mg/mL. These results confirm the positive correlation of major volatile compounds with the EO's antioxidant activities. Among the main chemicals studied, docking studies revealed that

$\alpha$ -pinene has the highest affinity with the Keap1 protein. Pi-sigma and pi-alkyl interactions are the main interactions seen in the complexes of the major compounds with Keap1, and they play a crucial role in their binding affinities. More pharmaceutical effects of *M. verrucosa*'s EO should be further explored for their new potential applications.

**COMPETING INTERESTS**

No potential conflict of interest was reported by the authors.

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