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Chemical Composition, Antioxidant Activity, and *In Silico* Pharmacokinetics of Essential Oils from Four *Ocimum basilicum* Cultivars in Iraq

Reham A. Al-Anssari[1,*], Anwar H. Ali[1], Ola Adel Al-Saad[1]

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Abstract: Basil *(Ocimum basilicum*) is acknowledged for its vast medicinal properties, primarily due to antioxidant-rich essential oils. While these oils exhibit diverse therapeutic properties, comparative studies on chemical profiles, antioxidant activities, and pharmacokinetics across different basil cultivars remain limited. This study intended to identify the chemical constituents, antioxidant potential, and *in silico* pharmacokinetic and toxicity profiles of essential oils extracted from four distinct *Ocimum basilicum* cultivars: cinnamon, purple, green, and citriodorum. The main goal was to evaluate their therapeutic potential, focusing on antioxidant activity and their suitability for pharmaceutical applications. Essential oils were obtained from the fresh leaves of each Basil cultivar using steam distillation. Gas Chromatography-Mass spectrometry technique (GC-MS) was used to establish the chemical composition of these oils. The antioxidant potential of the Basil oils was assessed using the 2,2-Diphenyl-1-picrylhydrazyl (DPPH) assay. Molecular docking studies investigated the interaction of Basil oils' key components with the human antioxidant enzyme peroxiredoxin 5 (Prx5). Finally, *in silico* studies evaluated the identified compounds' pharmacokinetic and toxicity properties. GC-Mass analysis results showed 38 volatiles were identified across cultivars, with Cinnamon basil showed to possess the highest constituent diversity and antioxidant activity (96.67% inhibition), while molecular docking showed that key compounds such as Phytol exhibited the highest binding affinity at -5.4440 kcal/mol, surpassing Cedrelanol at -4.9524 kcal/mol and *cis*-β-farnesene at -4.7075 kcal/mol, which is consistent with experimental findings on antioxidants. The ADME analysis indicated that both phytol and Cedrelanol have the potential for good absorption in the gut and can penetrate the blood-brain barrier. Although these compounds are generally categorized as low-risk (Class IV), phytol (51%) and Cedrelanol (76%) raised concerns regarding potential carcinogenicity, while fenchone (50%) and humulene (69%) presented risks for immunotoxicity. This study demonstrates the significant antioxidant potential and favourable pharmacokinetic profiles of *Ocimum basilicum* oils, particularly cinnamon basil. These findings highlight the potential of cinnamon basil essential oils as novel sources for antioxidant therapies and nutraceuticals, particularly in diseases linked to oxidative stress. In addition to therapeutic potential, the strong antioxidant properties also support their application in food preservation and pharmaceutical formulations. *In vivo* studies are needed to validate their efficacy, conduct safety evaluations—especially regarding potential carcinogenicity and immunotoxicity—and to assess the synergistic effects of these compounds in multi-compound formulations aimed at enhancing therapeutic outcomes.

Keywords: ADME properties; Antioxidant activity; DPPH assay; Essential oils; Molecular docking; *Ocimum basilicum*

Introduction

Oxidative stress, defined as an imbalance between the production of reactive oxygen species (ROS) and the body's antioxidant defense mechanisms, has been widely implicated in the pathogenesis of numerous chronic diseases. Including cardiovascular disorders, neurodegenerative diseases, diabetes, and various forms of cancer [1,2]. Oxidative damage to proteins, lipids, and DNA can disrupt normal cellular function, leading to inflammation, apoptosis, and disease progression [1,2]. As scientists and healthcare professionals continue to uncover the role oxidative stress plays in the development of chronic diseases, there's growing interest in finding effective antioxidants-especially from natural sources. Among these, plant-based essential oils have gained attention for their richness in phenolic and terpenoid compounds, which can help neutralize reactive oxygen species and support the body's antioxidant defenses. Among these, *Ocimum basilicum* (basil), which has long been valued in traditional medicine and is now recognized for its diverse range of bioactive compounds that may offer real therapeutic potential.

Ocimum basilicum, generally known as basil, is a useful aromatic herb widely used in food applications and traditional medicine. In traditional Iraqi medicine, basil leaves have been widely used not only in culinary preparations but also for addressing a variety of health conditions, including digestive disorders, acne, fungal infections, headaches, and the common cold. Beyond Iraq, the medicinal applications of basil are well recognized throughout the Middle East, where it is traditionally valued for its anti-inflammatory, antimicrobial, and antioxidant properties [3, 4]. These traditional uses are supported by modern phytochemical studies, as *Ocimum basilicum* is known to contain a wide range of bioactive compounds with demonstrated antimicrobial, anti-inflammatory, and antioxidant activities [5, 18]. The medicinal benefits of basil are mainly assigned to its volatile oils' contents, which consist of a complex mixture of phenolic compounds, terpenoids, and flavonoids [18,19,5]. Among these, antioxidant activity has been the most extensively studied, with evidence suggesting that basil oil's bioactive constituents can neutralize free radicals and protect cells from

1 Department of Pharmacognosy and Medicinal Plants, College of Pharmacy, University of Basra, Basra, Iraq.
*Corresponding author: reham.taha@uobasrah.edu.iq

oxidative damage [18, 19, 5]. With the increasing interest in the role of oxidative stress in diseases such as cancer, cardiovascular diseases, and neurodegenerative conditions, the antioxidant potential of basil oil has attracted considerable attention.

Basil is cultivated in several varieties, each with a unique chemical composition and therapeutic properties. The most commonly studied cultivars include sweet basil (*O. basilicum* cv. green), cinnamon basil (*O. basilicum* cv. cinnamon), lemon basil (*O. basilicum* cv. citriodorum), and purple basil (*O. basilicum* cv. purple) [20,6]. These varieties differ significantly in the concentrations of key components such as methyl chavicol, methyl eugenol, linalool, and anethole [20, 21,7].

Cinnamon basil (cv cinnamon) is known to contain high levels of methyl cinnamate, eugenol, and linalool, giving it a distinctive spicy aroma and notable pharmacological potential. Methyl cinnamate has been associated with anti-inflammatory and antioxidant activities, while eugenol is a well-established phenolic compound with strong radical scavenging abilities [8,20].

Purple basil (cv. purple) is known for its vibrant anthocyanin pigmentation and its relatively high content of methyl eugenol, linalool, and other phenolic compounds [9]. These contribute to its strong antioxidant potential and anti-inflammatory properties.

Lemon basil (cv. citriodorum) stands out for its high citral (a mixture of geranial and neral) and limonene content, compounds that give it a citrus-like aroma and contribute to its antimicrobial and antioxidant activity, and is used widely in flavoring and fragrance industries [20,10].

Sweet basil (cv. green) is the most familiar and widely used basil variety, both in cooking and in herbal remedies. Its essential oil is rich in linalool, a compound known for its calming scent, antioxidant, and antimicrobial properties. Another common component is methyl chavicol, which adds to its fragrance [11].

Although various studies have investigated individual basil cultivars' chemical composition and antioxidant activity, comprehensive studies comparing multiple cultivars are limited. Additionally, while studies have highlighted the potential of basil oils in combating oxidative stress, the underlying mechanisms and the bioactivity of specific volatile components remain underexplored.

Molecular docking studies, which allow for the exploration of ligand-receptor interactions, have developed as a valuable tool in evaluating the potential therapeutic targets of plant-derived compounds [22,12]. In this context, human peroxiredoxin 5 (Prx5), an enzyme involved in cellular antioxidant defence mechanisms, has been recognized as a potential target for antioxidants [23,13].

However, the precise mechanism of interaction between basil's volatile components and Prx5 has not been fully investigated. Moreover, evaluating the pharmacokinetic properties of these components using ADME (Absorption, Distribution, Metabolism, Excretion) analysis is essential in understanding their potential as therapeutic agents.

The well-established medicinal properties of basil (*Ocimum basilicum*), largely attributed to its antioxidant-rich essential oils, necessitate a comprehensive investigation. While these oils possess diverse therapeutic potential, comparative analyses focusing on the chemical composition, antioxidant activity, and pharmacokinetic profiles across different basil cultivars remain limited, particularly for those cultivated in Iraq. This study compares the volatile oil composition, antioxidant activity, molecular docking interactions, and pharmacokinetic properties of four *Ocimum basilicum* cultivars: *O. basilicum* cv. cinnamon, cv. green, cv. purple, and cv. citriodorum. We hypothesize that different cultivars will exhibit varying antioxidant potential due to differences in their chemical profiles. In addition, we aim to explore the binding affinities of key volatile components to Prx5 and assess their safety and bioavailability using toxicity and ADME predictions. The results of this study will provide important insights into the promising therapeutic role of basil oils and contribute to the advancement of new natural products for clinical use.

Materials and Methods

Collection of plant samples: Plant samples for this study were collected from field collection and controlled cultivation and were identified by Prof. Dr. Abbas K. Obaid / Department of Horticulture and Garden Landscape, College of Agriculture, University of Basrah, Basrah, Iraq. Sweet basil (*Ocimum basilicum* cv. green L.) (**Figure 1**) was gathered from the Zariji area, located northeast of Basra city. In contrast, the other cultivars—lemon basil (*Ocimum basilicum* cv. citriodorum), cinnamon basil (*Ocimum basilicum* cv. cinnamon), and purple basil (*Ocimum basilicum* cv. purple) (**Figure 1**)—were cultivated in a controlled greenhouse. Mature leaves were harvested early morning in March 2019. After collection, the leaves were thoroughly washed and air-dried in the shade at room temperature, with periodic flipping, according to the procedure described by Tarakemeh [14]. Once dried, the plant material was ground and stored in airtight containers.

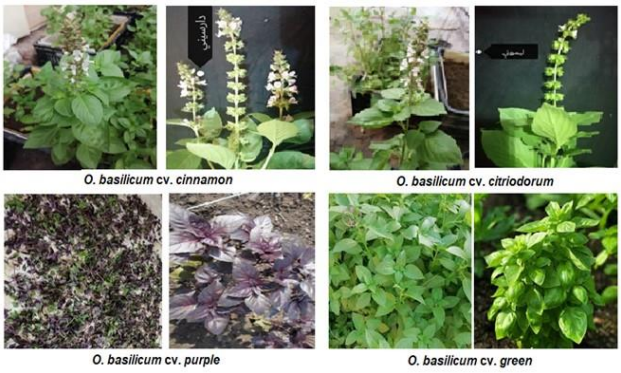

Figure (1): *Ocimum basilicum* Varieties Under Cultivation.

Essential Oils extraction*:* Essential oils were extracted from the selected plant species using steam distillation with a Clevenger apparatus. A total of 25 grams of each plant sample was weighed and placed in a 500 mL volumetric flask, to which 250 mL of distilled water was added. The mixture was then heated to 80 –100°C for 4 hours. After the extraction, the essential oils were isolated and carefully separated from the aqueous phase. The obtained oils were transferred to sealed, dark glass containers and stored at 4°C till further analysis [15].

Isolation and Identification of Essential Oils: Volatile oils' chemical composition was analysed using Gas Chromatography-Mass Spectrometry (GC-MS):

GC-MS System: Agilent Technologies 7890B GC system coupled to an Agilent Technologies 5977A MSD with EI Signal detector (available at Basra Oil Company/Nahran Omar Laboratories).

Analytical Column: HP-5ms 5% phenyl, 95% methyl siloxane (30 m length x 250 µ diameter x 0.25 µ film thickness)

- **Injection Type:** split
- **Injection Volume:** 1 µ
- **Injector Temperature:** 290°C
- **Carrier Gas:** Helium
- **Carrier Gas Flow Rate:** 1 mL/min
- **Oven Program:**
- **Initial Temperature:** 40°C hold for 5 min
- **Ramp:** 8°C/min to 300°C for 20 min
- **Ion Source Temperature:** 230°C
- **Scan Range:** 44-750 m/z
- **Scan Speed:** 1562 (N2)
- **Spectral Library:** NIST 2005

Antioxidant Activity Assay: DPPH (2,2-Diphenyl-1-picrylhydrazyl) assay was used to assess the antioxidant activity of the isolated essential oils, as described by Zheng Chen and coworkers [24]. Five concentrations of each plant extract (3, 6, 12, 25, and 50 µ/mL) were prepared by diluting the original extract with methanol. Each dilution added 1 mL of DPPH solution (prepared by dissolving 0.004 mg of DPPH in 100 mL of methanol). Samples were incubated away from light at room temperature. After 30 30-minute incubation period, the absorbance was measured at 517 nm using a spectrophotometer. The analyses were performed in 3 replications. Initially, the solution appeared purple, and as the extract reacted with the free radicals, the purple colour faded, indicating the scavenging activity. A blank control was prepared by adding 1 mL of methanol to 1 mL of DPPH solution, and its absorbance was measured as a baseline. Then, the following formula was used to calculate the percentage of antioxidants:

$$\textbf{Antioxidant Activity}\ \% = \frac{\textbf{A control} - \textbf{A sample}}{\textbf{A control}} * \textbf{100}\%$$

where:

- $A_{control}$ the absorbance of the control, and
- A_{sample} the absorbance of the sample.

Molecular docking studies: *In silico* molecular docking investigations were conducted to evaluate the interactions between the key natural components within the essential oils and the human antioxidant protein, peroxiredoxin 5 (Prx5). The X-ray crystallographic structure of Prx5 (PDB ID: 1HD2) [25] was retrieved from the RCSB Protein Data Bank and prepared for docking using the Molecular Operating Environment (MOE) 2022 software [9]. The protein structure was refined by removing water molecules, adding hydrogen atoms, correcting missing residues, and optimizing its geometry using the Amber EHT force field. The chemical structures of the components of volatile oils and ascorbic acid (used as a reference ligand) were obtained from PubChem and imported into MOE for docking analysis. The ligands were prepared by adding hydrogens, assigning partial charges, and performing energy minimization using the Amber EHT force field. A ligand database was created for docking studies. To validate the docking process, the natural ligand, benzoic acid, must be re-docked into the active site of Prx5 to verify the accuracy of the docking protocol. Subsequently, the selected compounds from the essential oils were docked into the protein's active site using the Triangle Matcher placement method and evaluated using the London dG scoring function.

ADME and toxicity analysis: Swiss ADME web tool (http://www.swissadme.ch/) [27] was used for in silico investigation of the pharmacokinetics and drug-likeness properties of the four selected compounds. Additionally, the oral toxicity of these compounds was assessed using the ProTox-II web server (tox.charite.de/protox_II/) [28]. The SMILES code for each compound was generated through Swiss ADME and then input into the ProTox-II tool to predict various toxicity parameters.

Statistical analysis: Statistical analysis of the *in vitro* antioxidant activity was performed using Microsoft Excel 2021 to calculate the IC_{50} values (i.e., the concentration of essential oil required to reduce 50% of DPPH radical activity). Concentration-response curves were used. These curves were plotted by the percentage antioxidant activity (on the Y axis) against essential oil concentrations (on the X axis). Then, IC_{50} values were determined by fitting the trendline to the data and using the supplied equation to determine the 50% inhibition concentration for each essential oil. The trendline followed logarithmic fitting with an R^2 value ranging between 0.8047 - 0.9558.

Results

Isolation and Identification of Essential Oils:

GC-MS analysis identified a total of 38 volatile components across the four basil cultivars (*O. basilicum* cv. cinnamon, cv. purple, cv. green, and cv. citriodorum) (the detailed GC-MS profile of essential oils is provided in **Supplementary Table 1**). The chromatogram's x-axis plots retention time, directly visualizing the Gas Chromatography (GC) separation of compounds based on their unique elution profiles. Subsequent Mass Spectrometry (MS) then identifies these separated compounds via their characteristic mass spectra.

The number and concentration of volatile components varied among the cultivars. *O. basilicum* cv. cinnamon exhibited the highest number of identified compounds (22), with methyl eugenol (20.81%), methyl chavicol (19.64%), and anethole (10.64%) being the dominant components. In *O. basilicum* cv. citriodorum, methyl chavicol (47.01%) was the predominant component, followed by methyl eugenol (16.25%) and eucalyptol (5.97%). *O. basilicum* cv. purple contained methyl chavicol (23.10%), linalool (7.32%), and beta-ocimene (7.32%), while *O. basilicum* cv. green showed a higher proportion of methyl chavicol (32.72%) and caryophyllene (9.22%) (GC-MS chromatograms are available in **supplementary Figure 1**).

Antioxidant Activity Assay: The antioxidant potential of the volatile oils was evaluated using the DPPH assay (**Table 1 and Figure 2**). *O. basilicum* cv. Cinnamon exhibited the greatest antioxidant activity, with a 96.67% inhibition at 50 µ/mL, closely followed by vitamin E (95.17%). The antioxidant activities of the other cultivars were lower: cv. green (81.61%), cv. citriodorum (77.01%), and cv. purple (75.86%). The IC_{50} values, calculated for each cultivar, were lowest for *O. basilicum* cv. cinnamon (2.16 µ/mL), indicating the highest efficiency in scavenging free radicals. *O. basilicum* cv. purple had the highest IC_{50} value (2.483 µ/mL).

Table (1): antioxidant activity and IC_{50} values of volatile oil extracts and vitamin E.

	DPPH inhibition %					IC_{50}
Conc. µg/mL	**3**	**6**	**12**	**25**	**50**	
Vitamin E	70.11	73.56	74.71	75.9	95.2	2.148
Cinnamon	60.56	70.22	82.76	90.8	96.7	2.16
Lemon	57.93	66.67	71.26	77	81.6	2.42
Purple	62.07	64.37	69.77	71.3	75.9	2.483
Sweet basil	60.2	64.37	77.01	80.5	88.5	2.415

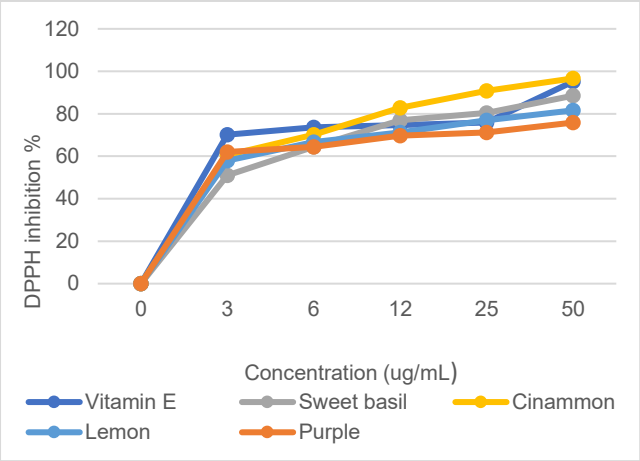

Figure (2): Concentrations' - DPPH radical scavenging activity correlation curve of Vitamin E, *O. basilicum* cv. Cinnamon, *O. basilicum* cv. Citriodorum, *O. basilicum cv.* purple and *O. basilicum cv.* Green volatile oils.

Molecular docking studies:. The docking results of studied essential oils components with Prx5 indicated that all major components had negative binding scores, suggesting stable interactions with Prx5 **(detailed docking results are available at Supplementary Table 2).** Among these, phytol had the strongest binding affinity (S = -5.4440 kcal/mol), followed by Cedrelanol (-4.9524 kcal/mol) and cis-β-farnesene (-4.7075 kcal/mol), supporting the practically observed antioxidant activity (**Table 2**, **Figure 3 and Figure 4**).

ADME analysis: ADME analysis revealed that compounds such as phytol and Cedrelanol showed good gastrointestinal absorption and potential for blood-brain barrier (BBB) penetration **(Table 3, Table 4 and Figure 5).**

Toxicity analysis: Toxicity profiling indicated that most compounds were classified as safe, with phytol and Cedrelanol showing low toxicity (Class IV). However, phytol and Cedrelanol raised some concerns regarding carcinogenicity (51% and 76%, respectively), while fenchone and humulene displayed some potential for immunotoxicity (50% and 69%, respectively) **(Table 5).**

Discussion

This study examines the antioxidant potential and bioactive composition of essential oils from four different cultivars of *Ocimum basilicum* L. basil, essential oils were obtained from collected plant leaves using steam distillation, a method known for its ability to preserve the volatile components of plant materials [29].

Considerable antioxidant activity was observed in all the extracted essential oils, with notable variations between cultivars. Of particular interest, cinnamon basil exhibited the greatest antioxidant activity, which aligns with prior reports suggesting that cultivars with elevated levels of eugenol, methyl eugenol, and phytol show enhanced antioxidant properties [29-31], and is confirmed by GC-MS analysis of these essential oils. This is further supported by the IC_{50} values, where samples ranked in the following order of potency: Vitamin E > Cinnamon basil > Green basil > Lemon basil > Purple basil, indicating that cinnamon basil required the lowest concentration to achieve 50% inhibition of radicals compared to other cultivar oils, and thus possessed the highest antioxidant potential. These results are consistent with previous studies reporting that cinnamon basil essential oil exhibits superior antioxidant activity, with IC_{50} values as low as 8.9 µg/mL in Thiobarbituric Acid Reactive Substances (TBARs) assays, compared to synthetic antioxidants like Trolox [20].

Table (2): RMSD, binding energies, and Interaction of selected phytochemicals with amino acid residues in the binding pocket of human Peroxiredoxin 5.

Compound	S (Kcal/mol)	RMSD	Interacting residues
Estragole	-4.1403	1.6331	Phe-120, Thr-44, Pro-45, Gly-46, Ile119, Arg-127, Thr-147
Methyl eugenol	-4.4364	0.8127	Phe-120, Ile-119, Arg-127, Thr-44, Pro-45, Gly-46, Thr-147, Cys-47, Leu-149
Humulene	-4.3719	1.9689	Phe-120, Arg-127, Pro-40, Gly-46, Thr-147, Pro-45, Thr-44, Leu-149, Ile-119, Leu-116, Leu-149
(-)-β-caryophyllene	-4.5234	1.7791	Ile-119, Leu-149, Arg-127, Gly-46, Thr-147, Pro-45, Phe-120, Pro-40, Thr-44
7-epi-cis-sesquisabinene hydrate	-4.8463	1.7243	Ile-119, Pro-40, Gly-46, Phe-120, Thr-147, Arg-127, Gly-148, Cys-47, Pro-45, Leu-149, Thr-44
Cedrelanol	-4.9524	2.2177	Pro-45, Thr-44,Phe-120, Ile-119, Leu-116, Pro-40, Thr147, Cys-47, Arg-127, Gly-46
Cis- β -Farnesene	-4.7075	1.4055	Thr-147, Cys-47, Gly-148, Pro-40, Thr-44, Phe-120, Arg-127, Pro-45, Ile-119
Phytol	-5.4440	2.3426	Pro-45, Pro-40, Thr-44, Gly-46, Cys-47, Arg-127, Thr-147, Leu-116, Phe-120, Ile-119

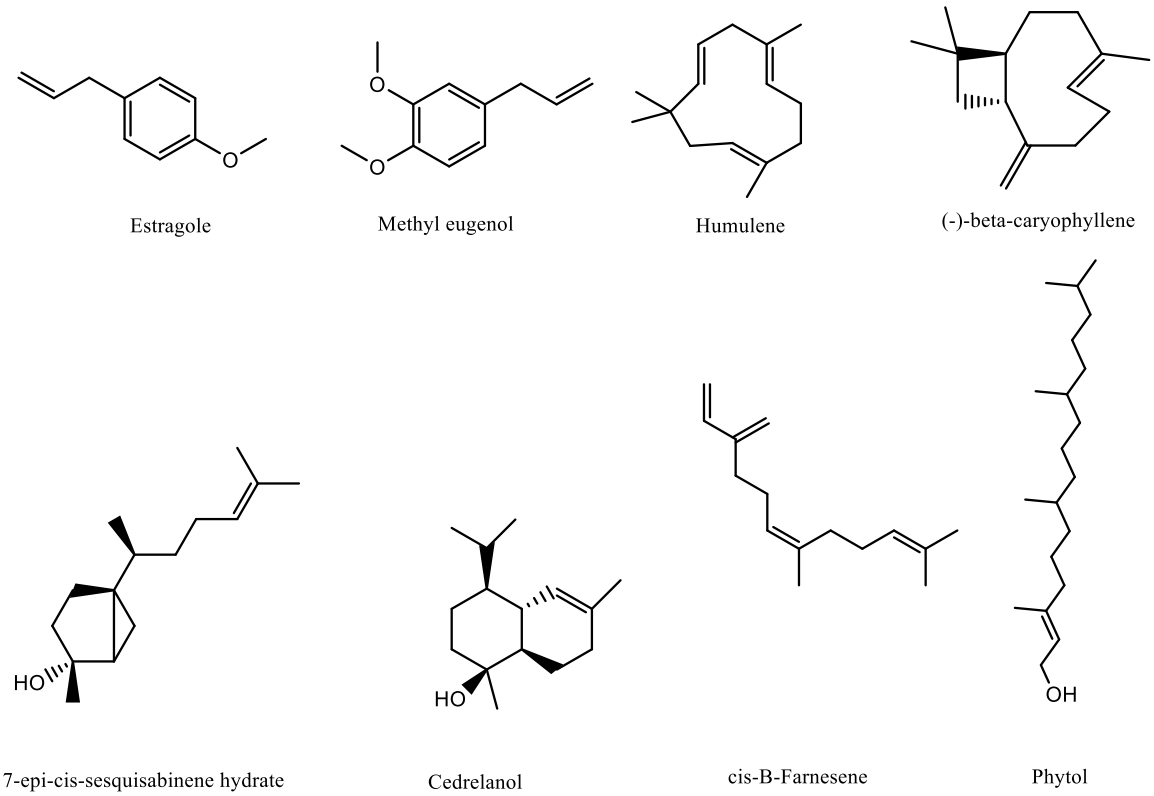

Figure (3): Chemical structures of the major volatile phytochemicals, as well as those having the four top docking scores present within the four species of *Ocimum basilicum* L. essential oil.

In contrast, other cultivars, such as *Ocimum basilicum* cv. Citriodorum have shown weaker antioxidant activity, which clearly highlights the effect of different chemical components within each cultivar on their bioactivity [20]. These observations also suggest that the observed antioxidant activity likely arises not solely from an individual component, but rather from a synergistic interaction between multiple bioactive constituents within the essential oils, which work together to neutralize free radicals and reduce oxidative stress. This finding agrees with previous studies highlighting the importance of synergistic interactions between phytochemicals in determining overall biological activity [32-34]. For instance, in Rosmarinus officinalis, the combined effects of phenolic acids have been shown to greatly improve antioxidant activity [34]. A similar synergistic interaction likely occurs in basil essential oils, where compounds like methyl eugenol a major compound identified in our analysis, have been linked to strong antioxidant properties [35]. Additionally, compounds such as methyl chavicol, anethole, Cedrelanol, and phytol, often present in basil oil, work together more effectively to neutralize free radicals than individual compounds alone [16]. These bioactive components may exert their antioxidant effect through different mechanisms, such as free radical scavenging, or metal ion chelation, or even boosting the endogenous antioxidant enzymes [17].To create more powerful natural antioxidant treatments, it's crucial to understand how different antioxidant components work together; therefore, molecular docking investigations were performed to identify the molecular mechanisms underlying the antioxidant potential of basil essential oils. These simulations investigated the interactions between key bioactive components, such as phytol and methyl eugenol, and peroxiredoxin 5 (Prx5), an antioxidant enzyme involved in cellular defences against oxidative stress [6]. The docking results indicated that phytol, Cedrelanol, and 7-epi-cis-sesquisabinene hydrate formed stable interactions with critical residues within the Prx5 active site: Thr-44, Gly-46, and Arg-127 **(Figure 4),** which are critical for the enzyme's antioxidant function.

These results suggest that basil essential oils' components may enhance the antioxidant activity of Prx5 through stabilizing its structure and enhancing its ability to neutralize reactive oxygen species (ROS). This aligns with the observed antioxidant activity, suggesting a possible link between the predicted protein-ligand interactions and the biological activity of these compounds.

Furthermore, the *in-silico* analysis revealed favourable pharmacokinetic properties for several compounds, including good gastrointestinal absorption, which is crucial for oral bioavailability. However, potential drug-drug interactions were predicted for some compounds due to their potential to inhibit key cytochrome P450 enzymes. While most compounds have shown low toxicity, some have shown possible carcinogenicity, immunotoxicity, or mutagenicity, thus necessitating further safety assessments.

However, the study does have several limitations. Even though a qualified taxonomist identified the plant cultivars, external verification is not possible because no voucher numbers were issued at the time of identification. Furthermore, the lack of n-alkane standards during GC-MS analysis meant that retention index values could not be calculated. These limitations will be improved in future studies to strengthen reproducibility and reference accuracy. In addition, since the *in-silico* predictions rely on computational models, they may not fully reflect the complex nature of the biological system. Additionally, using other antioxidant activity assays, along with the DPPH assay, could enhance our understanding of the antioxidant activities.

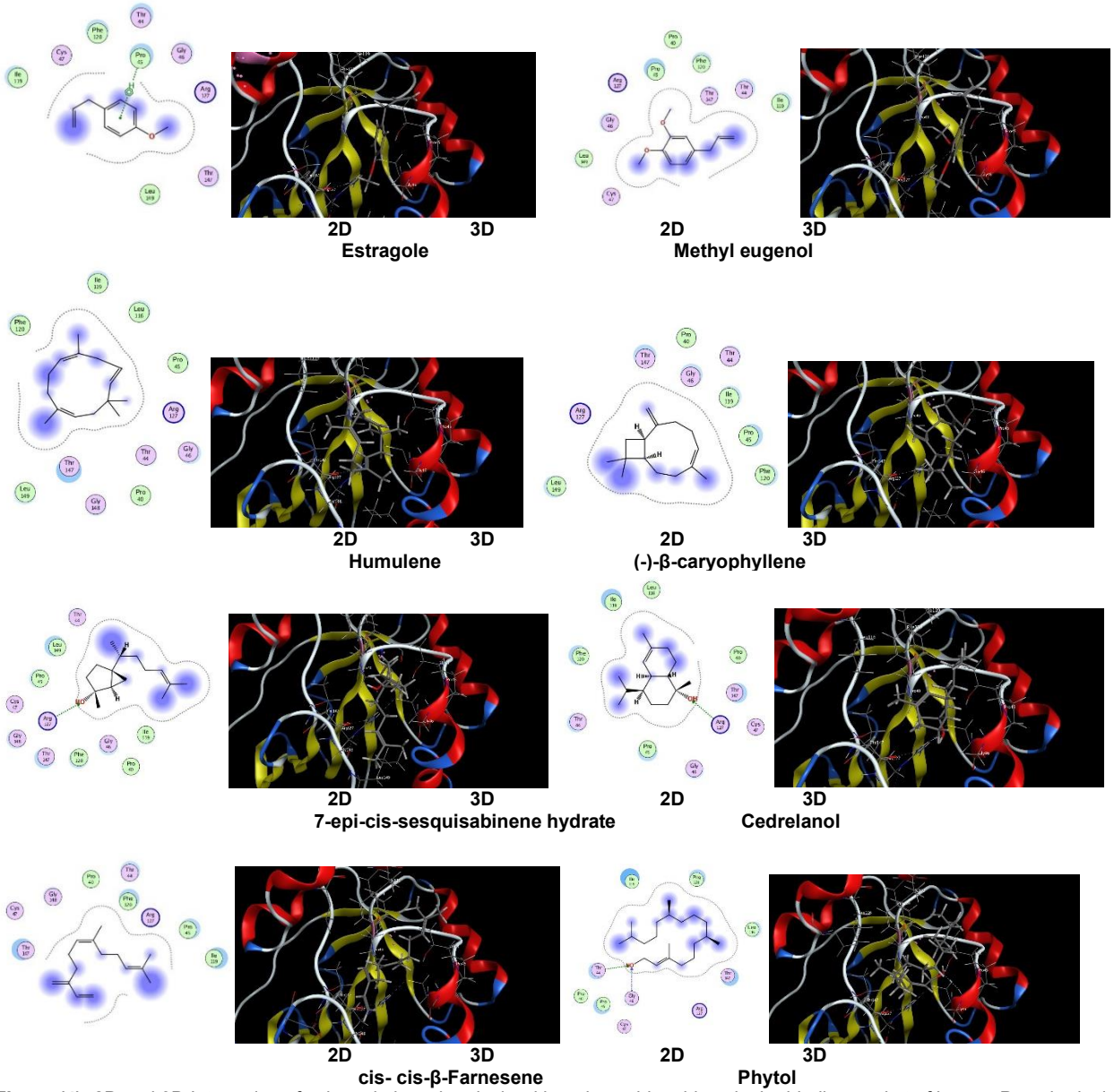

Figure (4): 2D and 3D Interaction of selected phytochemicals with amino acid residues in the binding pocket of human Peroxiredoxin 5

Table (3): Physicochemical properties of selected compounds, according to Swiss ADME software.

Physicochemical properties	Compounds							
	Estragole	Methyl eugenol	Humulene	(-)-β-caryophyllene	7-epi-cis-sesquisabinene hydrate	Cedrelanol	cis- β - Farnesene	Phytol
MWT (g/mol)	148.20	178.23	204.35	220.39	222.37	222.37	294.35	296.53
H bond acceptor	1	2	0	0	1	1	0	1
H bond donor	0	0	0	0	1	1	0	1
Fraction C sp3	0.36	0.27	0.60	0.75	0.87	0.87	0.47	0.90
Rotatable bonds	3	4	0	0	4	1	7	13
TPSA (A^2)	9.23	18.46	0.00	0.00	20.23	20.23	0.00	20.23
Molar refractivity	47.04	53.53	70.42	75.70	70.46	20.72	72.32	98.94
Log P o/w (consensus)	2.78	2.85	4.26	3.89	3.81	3.43	4.97	6.21
Log S (ali)	-3.24	-2.55	-4.27	-4.77	-3.22	-2.73	-3.74	-8.47

Table (4): Pharmacokinetics and drug-likeness of four selected compounds, according to Swiss ADME software.

ADME properties	Compounds							
	1	2	3	4	5	6	7	8
GI absorption	High	High	low	low	high	high	low	low
BBB permeant	Yes	Yes	no	no	yes	yes	no	no
P-gp substrate	No	No	No	yes	no	no	no	yes
CYP1A2 inhibitor	Yes	yes	No	no	no	no	yes	no
CYP2C19 inhibitor	No	No	No	No	yes	yes	no	no
CYP2C9 inhibitor	No	No	yes	No	yes	no	yes	yes
CYP2D6 inhibitor	No	no	No	No	no	no	no	no
CYP3A4 inhibitor.	No	No	No	No	no	no	no	no
Skin permeation (cm/s)	-4.81	-5.60	-4.32	-4.07	-4.76	-5.29	-3.27	-2.29
Drug likeliness LIPINSKI	Yes, 0 violation	Yes, 0 violation	Yes, 1 violation	Yes, 1 violation	Yes, 0 violations	Yes, 0 violations	Yes; 1 violation	Yes, 1 violation
Bioavailability score	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55

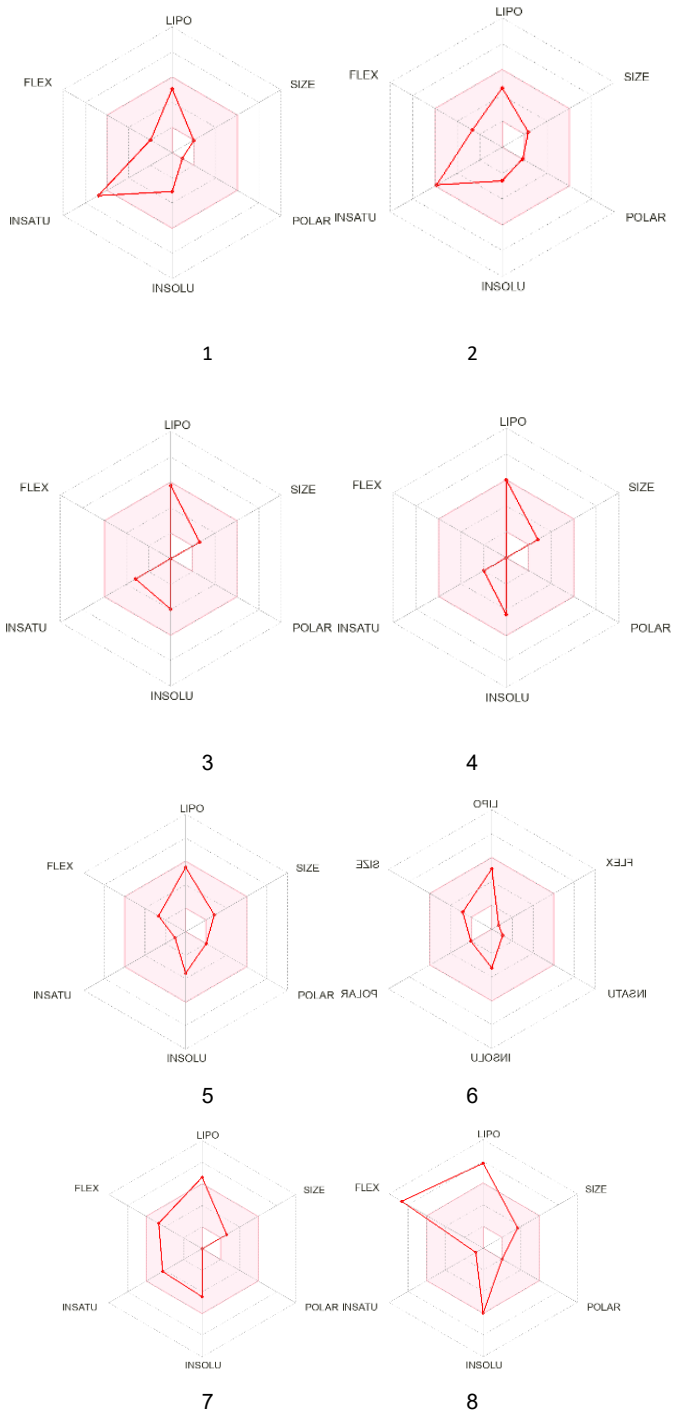

Figure (5): Bioavailability radar of the selected phytoconstituents. 1: Estragole, 2: methyl eugenol, 3: Humulene, 4: Caryophyllene, 5: 7-epi-cis-sesquisabinene hydrate, 6: Cedrelanol, 7: cis-beta-Farnesene, 8: Phytol.

Table (5): Toxicity parameters of studied compounds.

Toxicity parameters	Compounds							
	1	2	3	4	5	6	7	8
LD50 (mg/kg)	1230	810	3650	5300	3450	2830	5000	5000
Prediction accuracy (%)	100	100	70.97	70.97	70.97	72.9	70.97	100
Hepatotoxicity	- a	-	-	-	-	-	-	-
Carcinogenicity	+ b)	+	-	-	-	-	-	-
Immunotoxicity	-	-	-	+	-	+	-	-
Mutagenicity	-	-	-	-	-	-	-	-
Cytotoxicity	-	-	-	-	-	-	-	-
Toxicity class	IV	IV	V	V	V	V	V	V

a non-toxic, b toxic

Conclusion

This study highlights the significant antioxidant potential of essential oils extracted from different basil cultivars, with cinnamon basil showing the strongest activity among these basil oils in terms of IC_{50} value. Synergistic interactions among different bioactive components are likely driving the observed activity rather than relying solely on the most active compound within the essential oils, suggests that these oils hold promise as natural sources of antioxidants, which could contribute to managing oxidative stress-related conditions. Additional *in vitro* and *in vivo* studies are required to confirm these findings, assess their safety and efficacy, and fully clarify the underlying mechanisms of their antioxidant activity before they can be recommended for therapeutic use. These findings highlight the therapeutic potential of basil essential oils, particularly Cinnamon basil, as an accessible natural source of antioxidants, offering a promising approach to alleviating oxidative stress.

Disclosure statement

- **Ethics approval:** This study required no ethical approval.
- **Consent for publication:** Not applicable
- **Availability of data and materials:** The raw data required to reproduce these findings are available in the body and illustrations of this manuscript.
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