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Molecular Docking Study of Ver-1 Binding Compounds for the Mitigation of Aflatoxin B_1 Toxicity

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Abstract

Food safety has become a global health issue due to mycotoxins that occur naturally in agricultural products. The most dangerous of these toxins is Aflatoxin B_1 (AFB_1). Aflatoxin B_1 is a potent mycotoxin produced by Aspergillus flavus that exhibits toxic effects in the liver. In this study, the binding potential of 18 natural compounds to the Ver-1 protein, which is involved in the biosynthesis of AFB_1, was investigated using the Molecular Docking method. In analyses conducted using Gaussian and AutoDock/Vina software, the molecule apiol showed the strongest binding. The findings suggest that certain natural compounds may act as potential inhibitors by binding to the VER-1 protein, thereby reducing toxicity. The study presents a preliminary in silico analysis that evaluates the antifungal potential of natural compounds and could contribute to the drug development process.

Keywords: *Aflatoxin B_1, Ver-1 protein, Molecular docking*

1. Introduction

Mycotoxins are toxic secondary metabolites synthesized by fungi belonging to the genera Aspergillus, Alternaria, Fusarium, and Penicillium [1,2]. These naturally occurring compounds contaminate agricultural products, threatening both crop yields and the quality of animal feed, while also posing serious health risks [2]. The main factors contributing to mycotoxin formation include high temperature and humidity levels, improper storage conditions, incorrect agricultural practices, and damage caused by pests [3]. To date, over 500 mycotoxins have been identified in natural environments and food products (C.P. Wild, 2010). Among the most commonly known groups of these toxins are: aflatoxins (AFB_1, AFB_2, AFG_1, AFG_2, AFM_1, and AFM_2), ochratoxins (OTA, OTB, OTC), trichothecenes (deoxynivalenol, T-2 toxin, HT-2 toxin, nivalenol), fumonisins (FB_1, FB_2, FB_3), zearalenone (ZEN), fusarins (fusarin A, C, D), ergot alkaloids (e.g., ergotamine), and other toxins (e.g., paxillin, paspalin) [4]. Aflatoxins (AFs) are a group of mycotoxins produced primarily by toxigenic Aspergillus species such as Aspergillus flavus, Aspergillus parasiticus, and rarely Aspergillus nomius [5]. Aflatoxins are primarily divided into three groups based on the fluorescent color they emit under ultraviolet light: aflatoxin B group (AFB_1 and AFB_2), aflatoxin G group (AFG_1 and AFG_2), and aflatoxin M group (AFM_1 and AFM_2) [2]. To date, 21 different types of aflatoxins have been identified, among which AFB_1, AFB_2, AFG_1, AFG_2, and AFM_1, which is commonly found in dairy products, are particularly prominent [6]. The compound with the highest toxicity in this group is Aflatoxin B_1 (AFB_1). The two dihydrofuran rings in the structure of this molecule are a unique structural feature that distinguishes it from other types of aflatoxins [7]. This specific structure of AFB_1 is directly related to its high toxic effects. The literature emphasizes that exposure to AFB_1 can lead to chronic nervous system disorders and that long-term exposure can cause neurotoxicity [8,9]. In vitro studies using cell cultures have also shown that AFB_1 can directly damage human brain microvascular endothelial cells, disrupting the structural integrity of the blood-brain barrier and facilitating the passage of the toxin into brain tissue [10]. Studies have shown that aflatoxin G_1 is more prevalent than the B_2 and G_2 types. However, the type with the highest carcinogenic and lethal effects is AFB_1, followed by AFG_1, AFB_2, and AFG_2, respectively [11,12]. Experimental studies have reported that AFG_1 administered orally to laboratory mice caused hepatic carcinomas, kidney cell tumors, increased triglyceride levels, and cell autolysis [11]. The Ver-1 protein is a key oxidoreductase enzyme involved in the

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production of aflatoxin B_1 (AFB_1) synthesized by Aspergillus flavus. This enzyme catalyzes the conversion of versicolorin A to dimethylsterigmatocystine (DMST), a key step in the aflatoxin biosynthesis pathway, representing a decisive step in the biosynthetic chain [13]. The structure of the Ver-1 (Versicolorin 1) protein is shown in **Figure 1**. The enzyme's central position in this biochemical process has made it a target for natural antifungal compounds. Molecular docking studies have revealed that various plant-derived compounds (e.g., eugenol, geraniol, terpineol) bind to the active site of Ver-1. These compounds bind to the protein via hydrogen bonds and van der Waals interactions, leading to conformational changes in the active site and thus contributing to the suppression of aflatoxin biosynthesis [14,15].

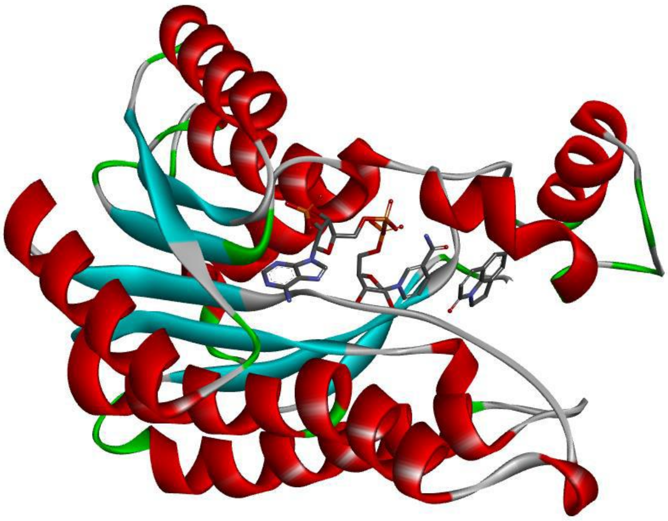


Figure 1. Structure of the Ver-1 protein.

In this study, the molecular structure of the Ver-1 protein was considered and the binding potential of various small molecules to this protein was evaluated using molecular docking. Docking is a modeling technique based on computer-aided simulations that predicts potential interactions between a target protein and a ligand molecule. In this study, we used Gaussian, GaussView, and AutoDock/Vina software to optimize the ligands and calculate their interactions with the protein. Selected ligands were determined among compounds of natural origin and potential inhibitory properties, and their binding affinities with Ver-1 protein were analyzed.

2. Material and Method

In this study, the interaction potential of a ligand molecule with a target protein was investigated computationally using molecular docking. In the first step, the three-dimensional structure of the ligand was modeled using GaussView 5.0 software, and then geometry optimization was performed using the PM6 semi-empirical method in Gaussian 09W [16]. This process resulted in the most stable, minimum-energy conformation of the molecule. The optimized structure was transferred to AutoDock/Vina, where potential interactions with the target protein were investigated [17]. In the docking analysis, potential ligand binding sites on the target protein were evaluated, the most suitable binding positions were determined, and binding energies were calculated. The resulting docking scores were interpreted to understand the nature of ligand-protein interactions. This approach allows for the theoretical assessment of biological interaction potential before proceeding with the experimental phases.

Selected Molecules

Apiol

Apiol, also known as liquid apiol or green oil of parsley, is extracted from parsley in the form of an oleoresin (oleoresin) rather than an essential oil obtained by distillation. Care should be taken to avoid confusion due to its similarity to the term "apiole" [18].

Caravan

Carvone occurs naturally in many essential oils, but the most abundant sources are caraway (Carum carvi), peppermint (Mentha spicata), and dill seed oils [19].

Citral

Citral, also known as 3,7-dimethyl-2,6-octadienal or limonal, consists of terpenoids that exist as a pair or mixture with the molecular formula $C_{10}H_{16}O$ [20].

Citronellal

Citronellal or rodinal ($C_{10}H_{18}O$) is a monoterpenoid aldehyde and the main component of the mixture of terpenoid chemical compounds that give citronella oil its distinctive lemon scent [21].

Elemicin

Elemicin is a compound found in the oleoresin and essential oil of the Canarium luzonicum tree (also known as elemi). It is named after this tree [22].

Eugenol

Eugenol is an allyl-chain-substituted guaiacol derivative and belongs to the allylbenzene class of chemical compounds. It is a colorless to pale yellow, aromatic, oily liquid; it is extracted from certain essential oils, particularly those from cloves, nutmeg, cinnamon, basil, and bay leaves [23].

Fenchone

Fenchone is an organic compound classified as a monoterpenoid and a ketone. It is a colorless, oily liquid with a structure and odor similar to camphor. Fenchone is a component of absinthe (a spirit similar to arrack) and fennel essential oil [24].

Geraniol

Geraniol is a monoterpenoid and alcohol. It is the primary component of citronella, rose, and palmarosa oils. It is a colorless oil, although commercial forms may appear yellow [25].

Limonen

Limonene is a colorless liquid classified as a cyclic monoterpene in the aliphatic hydrocarbon class. It is the main component of the oil in the peel of citrus fruits [26].

Linalool

Linalool is the name given to two enantiomers of a natural terpene alcohol found in many flowers and spice plants. Its pleasant (with a slight floral touch) odor has many commercial applications [27].

Menthol

Menthol is an organic compound, a monoterpenoid, found naturally in the oils of several plants, particularly those in the mint family. It occurs as a white or clear, wax-like crystalline substance that is solid at room temperature and melts at slightly higher temperatures [22].

Methyl Palmitate

Methyl palmitate is the methyl ester of palmitic acid. It is a saturated fatty acid ester commonly found in vegetable oils. It is a white, odorless, melt-in-the-mold substance that can appear as a liquid or wax [28].

Methyl Cinnamate

Methyl cinnamate is the methyl ester of cinnamic acid and is a white or transparent solid with a strong, aromatic odor. Its aroma is fruity and strawberry-like, and its odor is sweet, balsamic, and fruity, reminiscent of cinnamon and strawberries [29].

***p*-Cymene**

p-Cymene is a naturally occurring aromatic organic compound. It is classified as an alkylbenzene linked to monocyclic monoterpenes [30].

Terpineol

Terpineol is the name given to each of four isomeric monoterpenoids. Terpineols have been isolated from various sources, including cardamom, cajuput oil, pine oil, and petitgrain oil. Four isomers exist: α-terpineol, β-terpineol, γ-terpineol, and terpinen-4-ol. β-terpineol and γ-terpineol differ only in the location of the double bond. Terpineol is usually a mixture of these isomers, with α-terpineol as the major component [31].

Terpinolene

Terpinolene belongs to the group of naturally occurring menthadienes, that is, terpenes with a β-menthane skeleton and two double bonds. In various forms, α-Terpinolene is also called δ-Terpinene and is thus considered among the isomeric terpines [32].

Thymol

Thymol (also 2-isopropyl-5-methylphenol) is a natural monoterpenoid phenol derivative of p-cymene and isomer of carvacrol. It occurs naturally in oil of oregano and is extracted from Thymus vulgaris (common oregano) and various other herbs as a white crystalline substance with a pleasant aromatic odor and strong antiseptic properties [33].

Trans-anethole

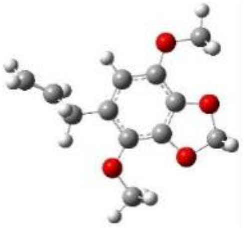
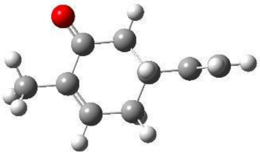
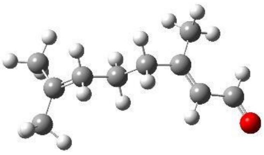
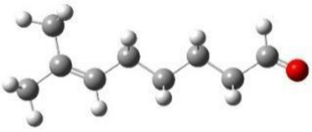
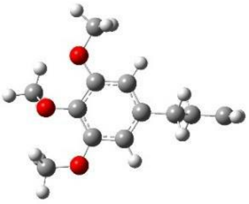
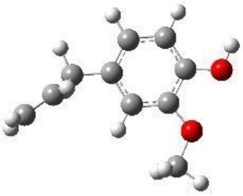
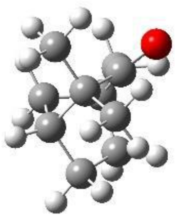
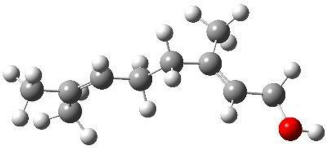
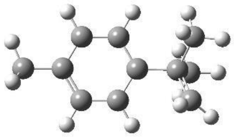
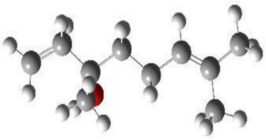
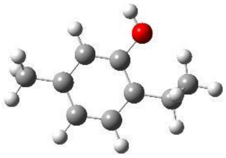
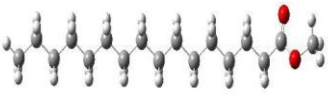
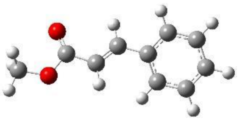
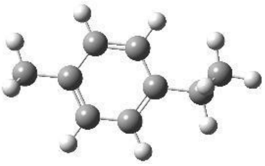
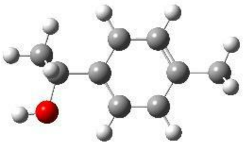
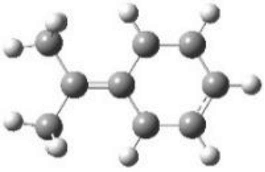
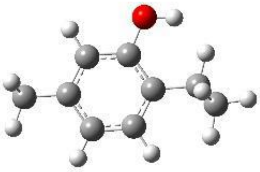
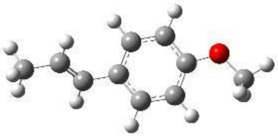
Anethole (also known as fennel camphor) is an organic compound widely used as a flavoring agent. It is a derivative of the aromatic compound allylbenzene and is widely found in the essential oils of plants [34].

3. Results and Discussion

In this study, the binding of 18 different small molecules to the Ver-1 protein (PDB ID: 1JA9), which is involved in the biosynthesis of aflatoxin B_1, was analyzed using molecular docking. The molecules used were selected from volatile compounds commonly found in nature, some of which are known for their antimicrobial or antifungal properties. The structure of the ligand molecule was modeled three-dimensionally using GaussView 5.0 and optimized using the semi-empirical PM6 method using Gaussian 09W software (**Table 1**).

The interactions of the molecules with the Ver-1 protein (**Figure 2**) were evaluated based on the binding affinities (kcal/mol) and the amino acid residues they interact with, calculated using AutoDock/Vina software.

Table 1. Optimized structure of molecules

Apiol	Carvone	Citral	Citronellal
			
Elemicin	Eugenol	Fenchone	Geraniol
			
Limonen	Linalool	Menthol	Methyl Palmitate
			
Methyl Cinnamate	*p*-Cymene	Terpineol	Terpinolene
			
Thymol	Trans-anethole		
			

Molecular docking studies have detailed the amino acid residues to which 18 different compounds interact with the Ver-1 protein. The findings reveal that some residues interact with multiple molecules, and that these regions play a key role in the binding site.

Apiol interacted with the Ver-1 protein through residues THR213, PHE216, PRO208, and SER164. This molecule, with the highest binding energy, exhibited strong affinity due to π-π stacking interactions, particularly with aromatic residues such as PHE216. This suggests that apiol binds tightly to the protein through both hydrogen bonds and hydrophobic interactions. Carvone interacted only with SER164 and TYR223, resulting in a weaker binding profile.

Citral bound to GLY209, VAL211, THR213, PHE216, and MET215, demonstrating its adaptability to the binding site thanks to its flexible structure and functional groups. Citronellal interacted with residues SER164, TYR178, TYR223, and PHE216. Its long-chain structure and hydroxyl group facilitated the molecule's attachment to various binding sites. Elemicin was observed to bind to many residues, including PRO208, SER164, GLY210, PHE216, TYR223, VAL211, and THR213.

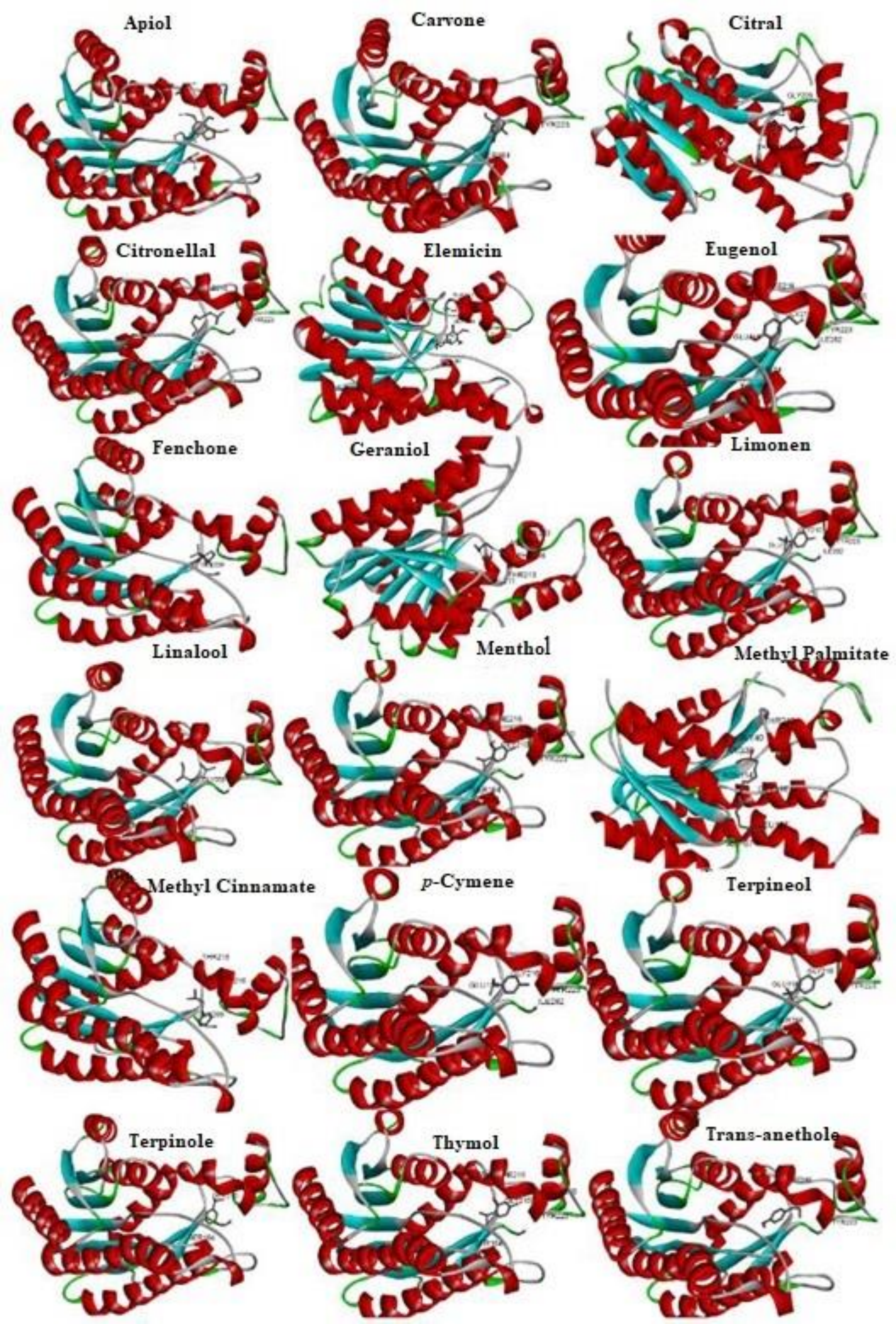


Figure 2. Interaction of molecules with the Ver-1 protein.

Eugenol, due to its phenolic OH group, interacted with TYR178, SER164, ILE282, TYR223, GLU118, LEU240, GLY210, PHE216, and MET215. π-π interactions with aromatic amino acids significantly increased binding strength. Fenchone formed a limited number of interactions with MET215 and GLY209. Geraniol bound with VAL211, THR213, PHE216, MET215, and TYR223; these interactions were supported by the molecule's hydrogen bonding capacity and aliphatic structure.

Limonene interacted with GLU118, GLY210, TYR223, and ILE282. Despite its nonpolar structure, its bonds with negatively charged residues such as GLU118 suggest that electrostatic interactions may also play a role. Linalool interacted only with GLY209, suggesting its limited binding capacity.

Menthol exhibited a broad binding profile with TYR178, SER164, TYR223, GLY210, SER220, LEU240, MET215, and PHE216. This is attributed to the molecule's flexible structure and ability to form hydrogen bonds. Methyl palmitate interacted with residues further away from the binding site, such as THR213, GLY40, ARG39, ASN114, GLY116, LEU137, and ASP87. This suggests that methyl palmitate is directed toward superficial regions rather than the binding pocket.

Methyl cinnamate bound with THR213, MET215, GLY209, PHE216, and VAL211, and its aromatic structure was observed to favor π-interactions with PHE216. p-Cimene showed hydrophobic binding with GLU118, GLY210, ILE282, and TYR223. Terpineol interacted with GLY210, GLU118, LEU240, TYR223, SER164, and TYR178, and this broad interaction profile reflects the structural flexibility of the molecule. Terpinolene bound only with GLY210 and SER164.

Thymol exhibited strong binding with SER164, TYR178, TYR223, LEU240, GLY210, MET215, and PHE216. Its aromatic structure stabilized these interactions. Trans-anethole formed π-π interactions with PHE216, TYR223, and TYR178, increasing binding stability.

Overall, residues SER164, PHE216, TYR223, MET215, GLY210, and THR213 appear to share bonds with multiple molecules. It is believed that these residues are located in the active site of the Ver-1 protein, and directing potential inhibitors to these regions may yield more effective results. Furthermore, aromatic compounds were observed to generally form more and stronger bonds, demonstrating that π-π interactions are an important factor to consider in inhibitor design.

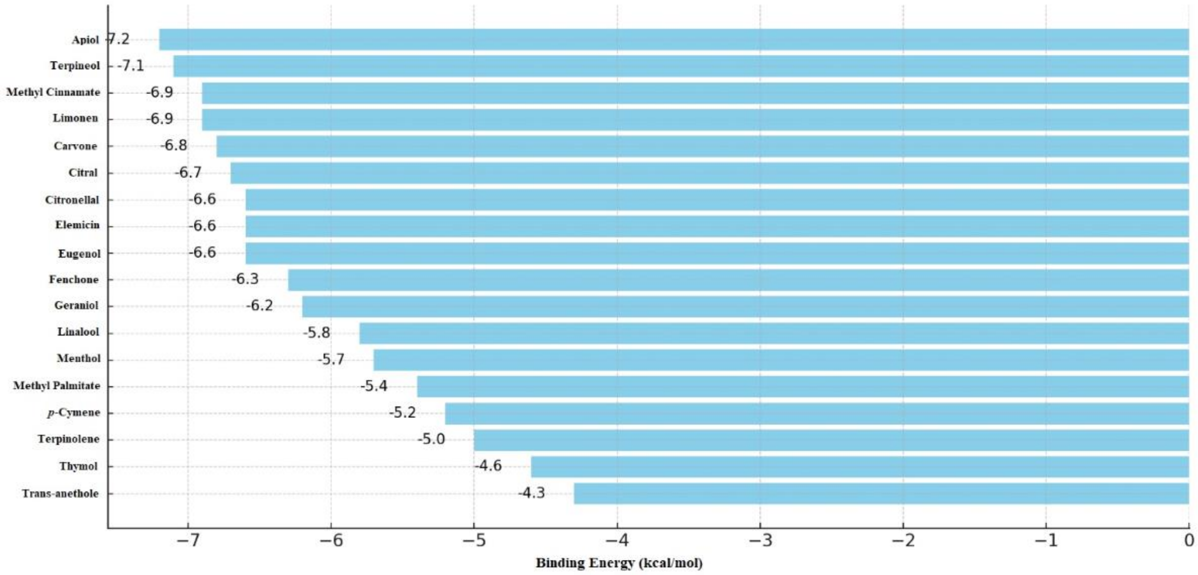


Figure 3. Binding energies of native molecules to Ver-1 protein.

According to the docking analyses, apiol was the molecule that showed the strongest interaction with Ver-1 protein among the tested compounds. This compound reached the highest affinity value with a binding energy of -7.2 kcal/mol. Terpineol (-7.1 kcal/mol), methyl cinnamate, and limonene (both -6.9 kcal/mol) followed apiol, respectively. Carvone came second with a value of -6.8 kcal/mol. The binding energies of the other compounds ranged from -6.6 to -4.3 kcal/mol. These findings suggest that apiol has the potential to be a potent inhibitor of Ver-1 protein. All binding energies of the molecules are presented in **Table 2**.

Table 2. Binding energies of molecules and amino acids interacting with Ver-1 protein

Receptor Protein	Molecule Name	Binding Energy (kcal/mol)	Hydrogen bonding with amino acids
VER-1	Apiol	-7.2	THR213, PHE216, PRO208, SER164
	Terpineol	-7.1	GLY210, GLU118, LEU240, TYR223, SER164, TYR178
	Methyl Cinnamate	-6.9	THR213, MET215, GLY209, PHE216, VAL211
	Limonene	-6.9	GLU118, GLY210, TYR223, ILE282
	Carvone	-6.8	SER164, TYR223
	Terpinolen	-6.6	GLY210, SER164
	Thymol	-6.6	SER164, TYR178, TYR223, LEU240, GLY210, MET215, PHE216
	Menthol	-6.6	TYR178, SER164, TYR223, GLY210, SER220, LEU240, MET215, PHE216
	Eugenol	-6.5	TYR178, SER164, ILE282, TYR223, GLU118, LEU240, GLY210, PHE216 MET215
	Fenchone	-6.5	MET215, GLY209
	p-Cymen	-6.5	GLU118, GLY210, ILE282, TYR223
	Elemicin	-6.3	PRO208, SER164, GLY210, PHE216, TYR223, VAL211 THR21
	Geraniol	-5.9	VAL211, THR213, PHE216, MET215, TYR223
	Trans-anethole	-5.9	PHE216, TYR223, TYR178
	Linalool	-5.7	GLY209
	Citral	-5.4	GLY209, VAL211, THR213, PHE216 MET215
	Citronellal	-4.7	SER164, TYR178, TYR223, PHE216
	Methyl Palmitate	-4.3	THR213, GLY40, ARG39, ASN114, GLY116, LEU137, ASP87

4. Conclusions

Molecular docking analyses of 18 different natural molecules bound by the Ver-1 protein revealed that certain amino acid residues interact repetitively with multiple ligands. This suggests that some amino acids in the Ver-1 protein are functionally prominent in the binding site.

Residues such as PHE216, SER164, and TYR223, in particular, interacted with more than 11 molecules. These residues appear to occupy a central position in the binding pocket and form strong bonds with ligands through both π-π stacking and hydrogen bonding. Their aromatic structure and favorable functional groups make these residues crucial for inhibitor binding.

Additionally, amino acids such as GLY210, MET215, and THR213 stand out as complementary components of the binding site, interacting with many molecules. These small and/or polar residues are thought to contribute to the proper positioning of molecules by increasing the flexibility of the binding site.

Overall, these common residues stand out as key targets for inhibitor binding of the Ver-1 protein and are important structural elements that should be taken into account in future drug or prophylactic design.

This study, conducted on the Ver-1 protein, which is involved in aflatoxin B_1 biosynthesis, aimed to evaluate the inhibitory potential of various natural small molecules using in silico methods. Binding energy analyses revealed that each molecule's affinity for the protein varies, and some compounds may have high inhibitory potential.

Compounds such as apiol, thymol, eugenol, and terpineol, in particular, have attracted attention due to their high binding scores and interactions with numerous amino acid residues. These results support the notion that natural compounds can exhibit antimycotoxigenic activity and that this effect is predictable at the molecular level.

Protein-ligand interactions are determined not only by binding energy but also by the structure, chemical properties, and three-dimensional conformation of the amino acids in the binding site. In this context, targeting frequently interacting residues, such as PHE216, TYR223, SER164, and THR213, could enable the design of more effective new inhibitors.

This study, which is an important step for the development of environmentally friendly and low-toxic inhibitors, has the potential to contribute to food safety practices with future experimental verifications.

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