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Bioinformatic study of the antiviral properties of thyme and eucalyptus against the coat protein of Mimosa yellow vein virus

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A B S T R A C T

Objective: The *Geminiviridae* family comprises significant plant pathogens causing severe economic losses worldwide. Among them, *Begomovirus* species, like *Mimosa yellow leaf curl virus* (MiYLCV), threaten crops and ornamental plants. Natural compounds, such as thyme and eucalyptus essential oils, may offer antiviral solutions. This study investigates the inhibitory potential of thyme and eucalyptus essential oils against MiYLCV coat protein using molecular docking, providing insights into eco-friendly antiviral strategies.

Materials: In this study, first, the three-dimensional structure of phytochemical compounds present in the two medicinal plants, Thymus vulgaris and Eucalyptus grandis, was obtained from the PubChem database. Next, the three-dimensional structure of the virus coat protein was optimized using the Swiss-MODEL online tool. The ability of the selected chemical compounds to inhibit the coat protein associated with pathogen virulence was explored using the molecular docking method using the specialized software autodock4.2.6.

Results: Phylogenetic analysis of *Mimosa yellow vein virus* coat protein revealed close relationships between some *Begomovirus* sequences (e.g., NP_808548.1 and NP_803540.1), while others (YP_00358491.1, ADW83758.1) showed divergence. The 3D protein model exhibited stable Ramachandran plot angles. Among thyme compounds, β-Myrcene had the highest permeability (logP=2.89), while γ-Terpinene showed the highest solubility (logS=-3.45). In eucalyptus, Isoamyl isovalerate (logP=3.05) and alpha-Terpinene (logS=-3.30) exhibited extreme values. Molecular docking identified strong binding interactions: Endo-borneol (-4.75 kcal/mol), α-Terpineol (-4.96 kcal/mol), and Terpinen-4-ol (-4.78 kcal/mol) from thyme, and beta-Terpineol (-5.14 kcal/mol), trans-Carveol (-5.15 kcal/mol), and Carvotanacetone (-5.21 kcal/mol) from eucalyptus exhibited the highest affinity for the viral coat protein. These findings suggest potential antiviral activity against *Mimosa yellow vein* ***virus*****.**

Conclusion: The results revealed that the combination of a-Terpineol and Carvotanacetone act as the strongest binding molecules in thyme and eucalyptus plants, respectively. These compounds can be proposed as potent antagonists targeting the coat protein of Mimosa yellow vein virus, effectively impeding its function.

Keywords: a-Terpineol, Carvotanacetone, β-Myrcene, Virulence, geminiviruses

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Introduction

The Geminiviridae constitute a prominent and expansive group within phytopathogenic viruses. Virions in this family encapsulate either a monopartite or bipartite circular single-stranded DNA genome, typically ranging from 2.5 to 2.7 kilobases in length, characterized by their distinctive twin icosahedral coat morphology [1]. The monopartite genome of these viruses harbors the complete complement of viral open reading frames. In bipartite configurations, the genome is typically divided into two components, designated DNA-A and DNA-B, each encoding distinct gene subsets. Segment A predominantly contains genes responsible for viral replication, transcriptional

regulation, and coat assembly, whereas segment B encodes factors essential for intra- and intercellular viral trafficking, host specificity, and symptom expression [2].

In the latest classification of the International Committee on Virus Nomenclature (ICTV), geminiviruses have been divided into 9 genera based on host range, vector insects, and genome characteristics [3]. Members of this family infect annual as well as perennial plants and even fruit trees in different parts of the world [4]. The economic damage caused by viruses in this family is extremely high. It has been reported in important crops such as tomato, bean, squash, sugar beet, tobacco, and corn. The extent of this damage has been estimated to be 20 to 100%, depending on the number of infected plants and the age of infection. The damage caused by this virus has been reported mostly in tropical, subtropical, and to some extent in temperate climates [5].

Leaf spot, yellow mosaic, twisting, and malformation are the most common symptoms of plants infected with geminiviruses. In young and old plants, symptoms such as clumping and reduced fruit formation have been reported, respectively [6]. The genus Begomovirus, which is one of the most important genera in this family, has 132 species. Recently, nine new begomoviruses have been reported, one of them being Mimosa yellow leaf curl virus (MiYLCV), which is capable of infecting mimosa [7, 8]. Mimosa pudica is an annual or perennial herbaceous plant which is considered an ornamental and medicinal plant [1]. The protein coat plays a key role in many processes of geminivirus pathogenesis, including specificity of association with insects and virus transmission [9].

The three-dimensional structure of the protein coat of viruses has been more conserved than their sequences in the course of evolution, and this is the basis of homology modeling [10]. Identification and introduction of various compounds with antiviral effects can be important in inhibiting the activity of this virus. In particular in recent decades, the use of natural compounds, especially plant compounds, has received more attention owing to their natural origin. Thyme (Thymus vulgaris L.) is a plant from the mint family that has fragrant and evergreen leaves. The lower surface of the leaf is covered with abundant essential oil glands. Its major part consists of phenols, monoterpene hydrocarbons, and alcohols. Thyme essential oil has antibacterial, antiviral, and antifungal properties. This essential oil is one of the ten famous essential oils that claim a special place in world trade [11]. The genus Eucalyptus belongs to the Myrtaceae family. This plant has alternate, lanceolate, and relatively beta-extended leaves. The essential oil secreting glands in its leaves are small and distributed in equal numbers on both leaf surfaces [12]. Essential oils have a direct or indirect defensive role in plants. Their antimicrobial properties have been reported in various studies [13].

Currently, one of the innovative strategies for managing phytopathogens involves rational drug design facilitated by computational modeling and bioinformatics approaches [14]. Specifically, molecular docking simulations enable the in-silico evaluation of ligand-protein interactions prior to empirical validation, allowing identification of candidate molecules with high binding affinity to target proteins. Following this computational screening, promising compounds can be subjected to in vitro and in vivo analyses. Molecular docking quantitatively assesses the binding dynamics between a ligand and its receptor [15]. Leveraging this methodology, researchers can pinpoint antiviral agents with efficacy against viral coat proteins [16]. In this computational investigation, the antiviral potential of phytochemicals derived from thyme and eucalyptus was examined in relation to the coat protein of Mimosa yellow vein virus.

Materials and Methods

Phylogenetic Characterization of the Targeted Protein Sequence via Computational Tools

The coat protein (CP) sequence of Mimosa yellow vein virus was initially subjected to comparative analysis against homologous CP sequences from various begomoviruses retrieved from the NCBI (National Center for Biotechnology Information) repository [4]. Multiple sequence alignment of the CP sequences, including reference type strains, was conducted utilizing the Clustal W algorithm [17]. Subsequent phylogenetic reconstruction was carried out employing the Neighbor-Joining (NJ) approach implemented in MEGA version 6 software, with statistical support assessed through 1,000 bootstrap replicates [18].

Detection and optimization of the three-dimensional structure of the CP of Mimosa yellow vein virus

The coat protein (CP) of *Mimosa yellow vein virus* exhibited maximal structural homology to *Ageratum yellow vein virus* CP through BLASTp analysis against the Protein Data Bank (PDB) repository. Consequently, a

tertiary structural model was constructed using Swiss-MODEL, utilizing the *Ageratum yellow vein virus* CP (PDB ID: 6F2S) as a structural template. The model underwent energy minimization via 3Drefine to optimize atomic coordinates. Ramachandran plot analysis was conducted to evaluate backbone dihedral angle distributions (φ/ψ) and validate the model's stereochemical quality. Structural visualizations were performed using UCSF Chimera 1.8 computational suite [19].

Preparation and examination of physicochemical properties of plant compounds

The molecular architectures of principal phytoconstituents from Thymus and Eucalyptus species were retrieved from the PubChem repository, a comprehensive database for chemical and pharmacologically active entities. To facilitate downstream computational analyses, Python Viewer 1.5 was employed for the conversion of three-dimensional molecular files from Structure Data File (SDF) format to Protein Data Bank (pdb) format. This software suite was further utilized to dissociate ligand entities from macromolecular complexes, incorporate polar hydrogen atoms, assess ligand orientation within catalytic domains, and visualize electrostatic surface potentials of the analyzed molecules [20].

Prior to interrogating ligand-macromolecule binding dynamics, the selected botanical derivatives underwent rigorous in silico profiling for their physicochemical attributes and toxicity liabilities. Parameters such as aqueous solubility, partition coefficient (Log Po/w), predicted solubility via ESOL (Log S), and inhibitory potential against key cytochrome P450 isoforms—including CYP2C19, CYP3A4, CYP2D6, CYP2C9, and CYP1A2—were systematically evaluated for genotoxic and cytotoxic risk using the SwissADME web-based platform. Only those candidates meeting stringent criteria across these pharmacokinetic and safety endpoints were advanced for further study. SwissADME provides robust computational tools for forecasting molecular physicochemical properties and cytotoxicity profiles, accepting chemical descriptors in mol or SMILES notation [20].

The octanol-water partition coefficient (LogP) serves as a critical metric for estimating compound lipophilicity and hydrophilicity, thereby informing solubility predictions. Subsequently, all candidate ligands and target proteins were subjected to structural and energetic optimization using the Avogadro molecular editor. This step ensured that molecular docking simulations were conducted with conformers representing energetically favorable and structurally stable states, thereby minimizing the likelihood of artifactual positive or negative interaction results (20).

Molecular docking

The application of expedited in silico methodologies, including molecular docking techniques, is indispensable for the rational prediction and design of bioactive agents capable of suppressing pathogenic proliferation. Accordingly, this investigation employed molecular docking simulations to evaluate the inhibitory potential of select phytochemicals with documented antiviral efficacy against the coat protein of Mimosa yellow vein virus. The docking procedures were conducted utilizing the specialized computational platform AutoDock version 4.2.6 (2014 release). For ligand binding site exploration, a cubic grid box with dimensions of 60 × 60 × 60 Å was defined. The conformational landscape of the candidate inhibitors was exhaustively sampled using the Lamarckian Genetic Algorithm embedded within AutoDock 4.2.6. Post-docking analyses and visualization of binding interactions were performed through AutoDockTools [21] and LigPlot [15] software suites, facilitating comprehensive interpretation of ligand-protein affinities and interaction profiles.

Results

The phylogenetic tree of the protein sequences studied in the study is displayed in Figure 1. Accession numbers with high similarity (e.g., CAD90081.1) may belong to the same subfamily or species. Sequences like AEA10361.1 could represent divergent branch (different organism or functional variants).

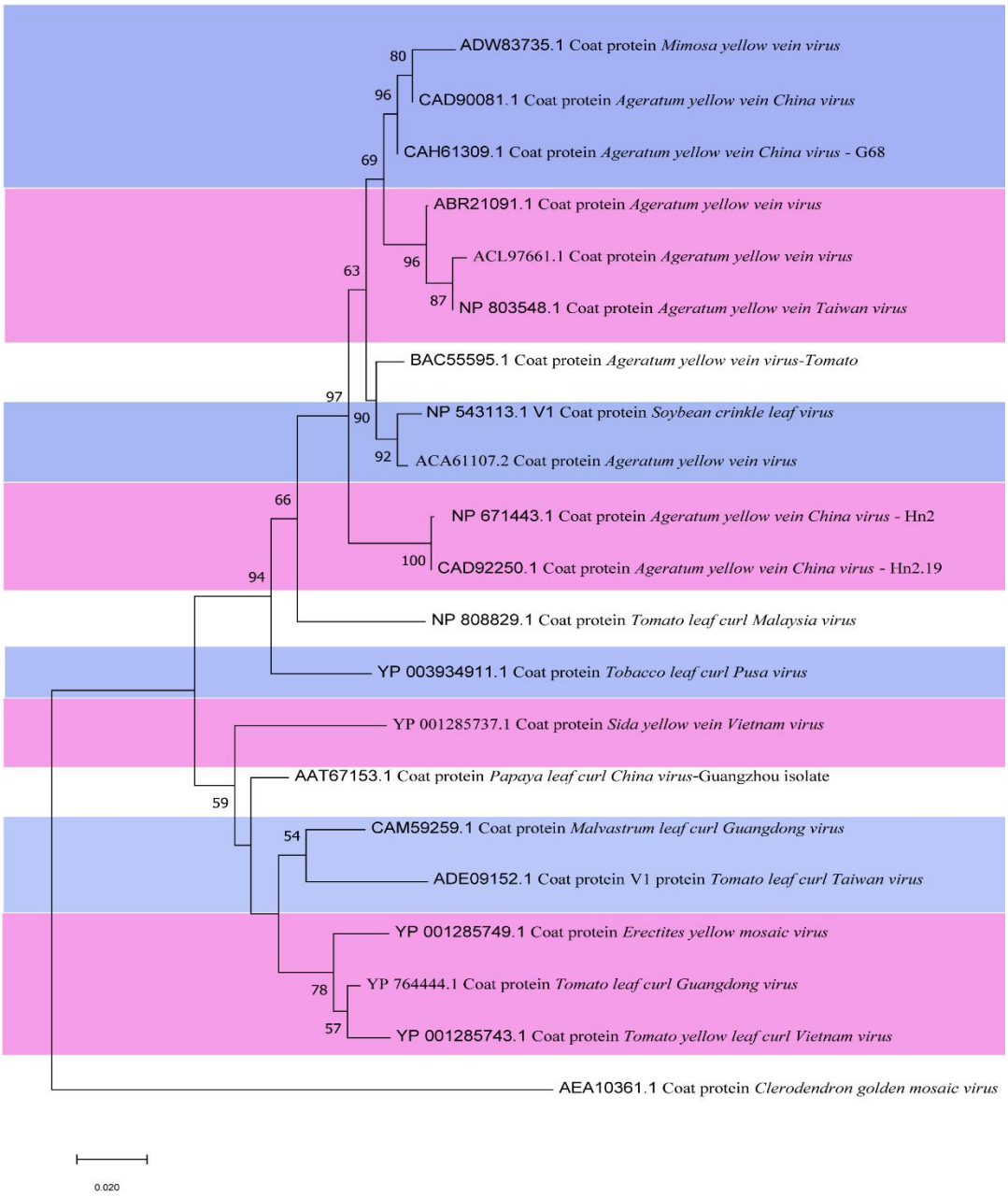


Figure 1: A phylogenetic reconstruction was conducted utilizing the envelope protein sequence of Mimosa yellow vein virus (accession number ADW83735) alongside various Begomovirus sequences retrieved from the GenBank repository. The evolutionary relationships were inferred employing the Neighbor-Joining algorithm implemented within the MEGA version 6 software platform.

The three-dimensional structure of the target protein, generated via the Swiss-MODEL computational platform and subsequently refined through the 3D-Refine algorithm, is illustrated in Figure 2.

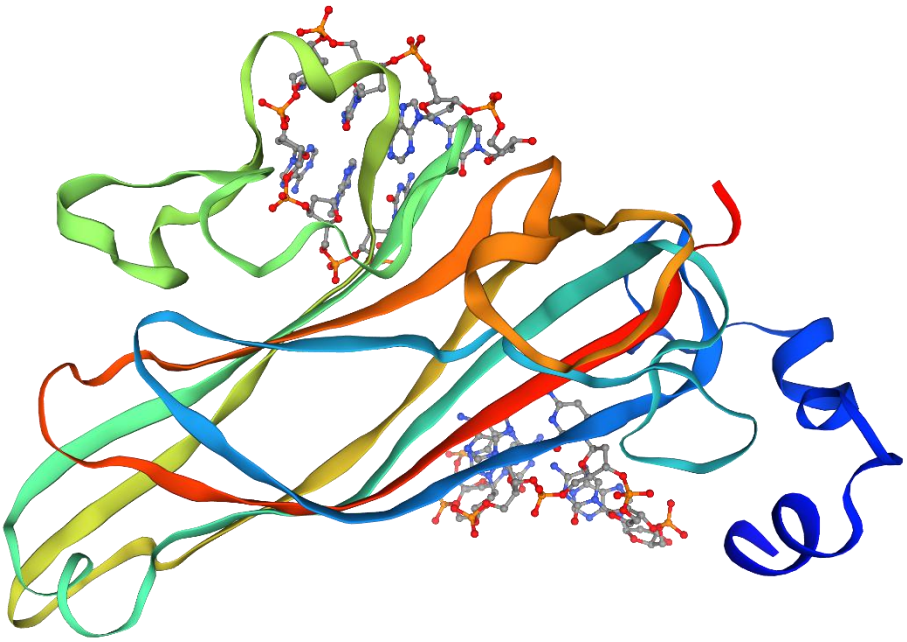


Figure 2. Three-dimensional structure of the Mimosa yellow vein virus envelope protein

The energy level and stability in terms of the two angles of Phi and Cy of the mentioned proteins from the Ramachandran plot.

Prediction of physicochemical properties and toxicity potential of the studied compounds

The quantity logP (logarithm of the octanol/water partition coefficient) as a factor in the study of the physicochemical properties of plant compounds, indicates the solubility in water and glycerol. The lower the hydrophilicity criterion (cLogP), the weaker its absorption. Based on logP, b-Myrcene and Cyclohexane compounds presented the highest and lowest permeability in thyme, respectively, and Isoamyl isovalerate and 4-Isopropyl-2-cyclohexenone indicated the highest and lowest permeability in eucalyptus. In addition, it was found that the solubility of the evaluated compounds based on logS showed that g-Terpinene compound had the highest while 3-Octano had the lowest solubility in thyme. Considering this index, in eucalyptus, the highest and lowest solubility were observed for alpha-Terpinene and alpha-Campholenal compounds, respectively. Cyclohexane, β-Myrcene, 3-Octanol, γ-Terpinene, Linalool, Endo-borneol, Terpinen-4-ol, and α-Terpineol have no significant pharmaceutical properties related to inhibition of the cytochrome P450 enzymes CYP1A2, CYP2C19, CYP2C9, CYP2D6, and CYP3A4. Available data indicate that these compounds do not inhibit these key drug-metabolizing enzymes, suggesting they lack relevant inhibitory effects on these CYP isoforms involved in drug metabolism. Although β-Myrcene shows potent inhibition of CYP2B1 in some models, it does not significantly inhibit CYP1A2, CYP2C19, CYP2C9, CYP2D6, or CYP3A4, and the other listed compounds similarly show no inhibitory activity on these CYP enzymes.

The compounds listed (Cyclohexane, β-Myrcene, 3-Octanol, γ-Terpinene, Linalool, Endo-borneol, Terpinen-4-ol, and α-Terpineol) exhibit a range of lipophilicity values, with penetration log values spanning from 2.10 for Cyclohexane to 2.89 for β-Myrcene, reflecting varying affinities for lipid environments. β-Myrcene, with the highest lipophilicity, suggests a stronger potential to traverse lipid membranes compared to the other compounds. Most substances show moderate lipophilicity around 2.5 to 2.7, indicating balanced characteristics that favor both membrane permeability and aqueous solubility, which are essential for effective pharmaceutical activity. In terms of water solubility, all compounds are classified as soluble, with solubility log values ranging from -2.07 for 3-Octanol to -3.45 for γ-Terpinene. The lower solubility of γ-Terpinene suggests it has reduced aqueous solubility, which could influence its absorption and bioavailability. Conversely, 3-Octanol's relatively higher solubility may facilitate better dissolution in biological fluids, potentially enhancing its pharmacokinetic profile. Linalool and Endo-borneol also demonstrate favorable solubility, supporting their use in formulations requiring balanced hydrophilic and lipophilic

properties. Skin penetration rates vary notably among these compounds, with Endo-borneol showing the highest rate at 5.31 cm/s, followed closely by Linalool at 5.13 cm/s and 3-Octanol at 5.12 cm/s. These elevated penetration values indicate their strong potential for transdermal delivery applications. In contrast, γ-Terpinene exhibits the lowest skin penetration rate at 3.94 cm/s, which may limit its effectiveness in topical formulations. Compounds like Terpinen-4-ol and α-Terpineol, with moderate penetration rates near 4.9 to 5.0 cm/s, offer a balanced profile for skin absorption, making them promising candidates for pharmaceutical and cosmetic use.

All the listed compounds, including alpha-Thujene, Verbenene, Sabinene, beta-Phellandrene, alpha-Phellandrene, alpha-Terpinene, Eucalyptol, beta-Terpinene, Linalool, Isoamyl isovalerate, Thujone, alpha-Campholenal, beta-Terpineol, Pinocarvone, Borneol, Terpinen-4-ol, 4-Isopropyl-2-cyclohexenone, alpha-Terpineol, cis-Piperitol, trans-Carveol, cis-Carveol, Carvotanacetone, Piperitone, and Phellandral have no significant pharmaceutical properties related to inhibition of the cytochrome P450 enzymes CYP2C19, CYP2C9, CYP2D6, and CYP3A4. Specifically, studies and databases indicate these compounds do not inhibit these key drug-metabolizing enzymes, suggesting they lack relevant inhibitory effects on CYP2C19, CYP2C9, CYP2D6, and CYP3A4 activities.

The compounds listed (alpha-Thujene, Verbenene, Sabinene, beta-Phellandrene, alpha-Phellandrene, alpha-Terpinene, Eucalyptol, beta-Terpinene, Linalool, Isoamyl isovalerate, Thujone, alpha-Campholenal, beta-Terpineol, Pinocarvone, Borneol, Terpinen-4-ol, 4-Isopropyl-2-cyclohexenone, alpha-Terpineol, cis-Piperitol, trans-Carveol, cis-Carveol, Carvotanacetone, Piperitone, and Phellandral) exhibit a range of lipophilicity values, with penetration log values spanning from 2.05 to 3.05, indicating moderate to relatively high affinity for lipid environments. Isoamyl isovalerate stands out with the highest lipophilicity (penetration log 3.05), suggesting it may penetrate lipid membranes more efficiently than others. Most compounds fall within a narrow lipophilicity range around 2.2 to 2.7, consistent with their classification as soluble substances. This balance between lipophilicity and solubility is crucial for their potential bioavailability and interaction with biological membranes. Regarding water solubility, the majority of these compounds are classified as soluble, with solubility log values generally between -1.82 and -3.30. Alpha-campholenal and 4-isopropyl-2-cyclohexenone are noted as highly soluble, with solubility log values of -1.82 and -1.90, respectively, indicating a greater ability to dissolve in aqueous environments compared to others. This enhanced solubility may facilitate faster absorption and distribution in biological systems. Conversely, compounds like alpha-terpinene with a solubility log of -3.30 are less water-soluble, which could affect their transport and bioavailability. In terms of skin penetration, the compounds demonstrate penetration rates ranging from approximately 4.11 cm/s to 5.91 cm/s. Alpha-campholenal exhibits the highest skin penetration rate at 5.91 cm/s, followed closely by 4-isopropyl-2-cyclohexenone and cis-piperitol, suggesting these molecules can effectively permeate the skin barrier. In contrast, alpha-terpinene shows the lowest penetration rate of 4.11 cm/s, which might limit its transdermal delivery potential. Overall, these physicochemical properties highlight the diverse capabilities of these compounds in terms of solubility, lipophilicity, and skin permeability, which are critical factors for their pharmaceutical and therapeutic applications.

Molecular docking

Molecular docking calculations were carried out using AutoDock software. Indeed, in this software, using force field functions, the number of chemical interactions between the ligand and the macromolecule is calculated based on the free energy of binding. The free energy of binding, which is provided in terms of kilocalories per mole in Tables 1 and 2, can indicate a measure of the affinity and binding of a compound to a macromolecular receptor. Data related to changes in binding energy; ligand interactions including hydrogen bonds and hydrophobic interactions were recorded. All compounds present in the thyme and eucalyptus medicinal plants were docked with the virus coat protein. In the case of these plants, the highest binding energy of 3 compounds in each case with the coat protein is reported in Tables 1 and 2. In relation to thyme, the compounds Endo-borneol, a-Terpineol and Terpinen-4-ol and considering eucalyptus, the compounds beta-Terpineol, trans-Carveol, and Carvotanacetone had the strongest interaction.

Table 1: Binding energy and interactions between the active site of the protein and the effective compounds of the thyme plant with the highest binding energy

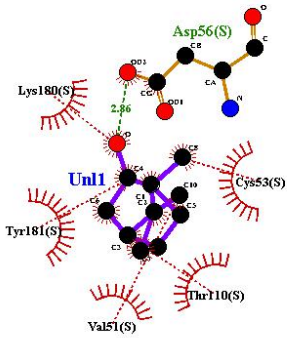
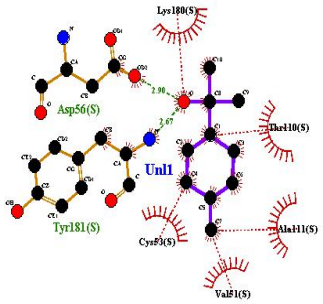
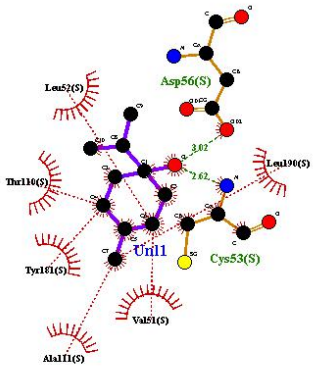
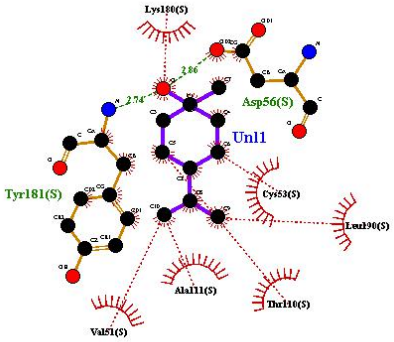
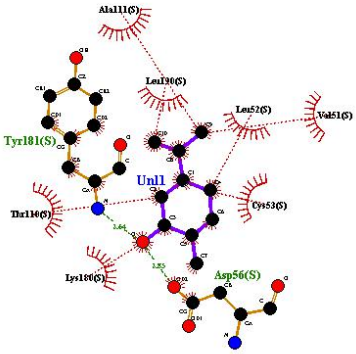
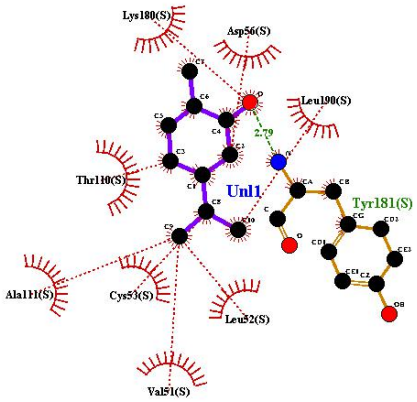
Compound Name	Accession Number	Binding Energy (kcal/mol)	Inhibition Constant (Ki)	Amino Acids Involved in Interaction	
Endo-borneol	120518	-4.75	328.88uM	Asp56 Lys180 Cys53 Thr110 Val51 Tyr181	
a-Terpineol	17100	-4.96	232.79uM	ASP56, Lys180 Val51 CYS53, TYR181, ALA111, THR110,	
Terpinen-4-ol	11230	-4.78	315.67uM	Asp56 Leu52 Thr110 Tyr181 Ala111 Val51 Cys53 Leu190	

Table 2. Binding energy and interactions between the active site of the protein and the effective compounds of eucalyptus with the highest binding energy

Compound Name	Accession Number	Binding Energy (kcal/mol)	Inhibition Constant (Ki)	Amino Acids Involved in Interaction	
beta-Terpineol	8748	-5.14	171.67 uM	Lys180 Tyr181 Val51 Ala111 Cys53 Thr110 Leu190 Asp56	
trans-Carveol	94221	-5.15	166.83 uM	Ala111 Leu190 Leu52 Val51 Lys53 Asp56 Lys180 Thr110 Tyr181	

Carvotanacetone	6432475	-5.21	151.54 uM	Lys180 Asp56 Leu190 Tyr181 Leu52 Val51 Cys53 Ala111 Thr110	

Discussion

In today's world, where resistance to viruses is progressively increasing, finding plant compounds with antiviral properties is very valuable [17]. Thanks to their multiple effects, various bioactive compounds present in medicinal plants can limit the synthesis of viral proteins in addition to affecting the stages of virus replication. Thus, active chemical compounds can be considered as new drug structures to combat a wide range of target molecules. On the other hand, due to their low cost, high efficacy and few side effects, they claim a special place [22]. Studies have been conducted on the effect of medicinal plants on various viruses. In a study, the antiviral properties of 25 medicinal plants have been reported. Most of the medicinal plants belonged to the Asteraceae, Lamiaceae, Phyllanthaceae, Polygonaceae, and Acanthaceae families. Their dominant active ingredients were reported to include flavones, alkaloids, and polyphenols [17]. Farahani [23] in examining the antiviral effect of thyme and oleander plants on HSV virus in vitro found that thyme plant has a very good antiviral effect on HSV-1 virus at non-toxic concentrations. In another study, the effect of thyme aquatic plant extract was investigated on herpes simplex virus types 1 and 2 and an acyclovir-resistant strain of HSV-1 (ACV(res)). The results revealed that thyme plant extract can be used topically in the treatment of recurrent HSV-1 infections [24]. It has been reported [25] that eucalyptus extract has significant antiviral properties at different stages of herpes simplex virus pathogenesis in the cell culture.

The examination of antiviral properties of medicinal plants by molecular docking method has received considerable attention in recent studies [26]. In a study, the effect of 47 compounds of plant secondary metabolites (12 metabolites and 35 derivative compounds) was tested to inhibit HIV and HTLV-1 protease using theoretical methods (molecular docking and dynamic simulation). Finally, 13 compounds with the best docking results with HTLV-1 protease were subjected to molecular dynamics simulation. Of them, 5 compounds remained bound to HTLV-1 protease by forming stable hydrogen bonds during the simulation. They concluded that these compounds have the ability to inhibit HTLV-1 protease and can be suitable options in the drug design process [27].

It has been studied [28] the interaction of Nia protein of wheat stripe mosaic virus and some plant compounds. The results of the protein interaction study in vitro demonstrated that among the extracts studied, licorice extract had a greater effect on changing the protein absorption rate and therefore a possible change in its structure. Thereafter, the extracts of lemon balm and marigold plants, respectively, led to a change in the absorption rate of NIa protein. Also, the catechin compound had a greater effect on changing the protein absorption rate compared to the caffeic acid compound. Comparing these results with the docking results indicated that each of the compounds that had a lower binding energy and hence a more stable complex in interaction with the NIa protein had a greater influence on the protein absorption rate and thus a structural change in vitro. They concluded that these compounds can be used in biological control of agricultural epidemic diseases.

It has been conducted [29] a bioinformatics study of the antiviral properties of 25 different medicinal plants on the Zika virus. The results of their research revealed that the most antiviral properties belonged to 5 compounds Repandusinic acid, Hesperidin, Tannic acid, Rosmarinic acid. The amino acids involved in the 5 compounds THR 95, LEU 96, ASP 98, ASP 247, HIS 249, ALA 250, LYS 251, ARG 252, GLU 274, GLU 276, LEU 284, and SER 285 are likely to be important in suppressing virus membrane fusion. Although the structures of the plant compounds differed from each other, the most important amino acids involved in the interaction were reported to include ARG 283, GLU 44, GLY 28, and VAL 46. In the present study, based on the docking results, the inhibitory potential of the studied compounds differed. The most important amino acids involved in relation to thyme included ASP56, Lys180, Val51, CYS53, TYR181, ALA111, THR110. On the other hand, considering eucalyptus, the amino acids involved Lys180, Asp56, Leu190, Tyr181, Leu52, Val51, Cys53, Ala111, and Thr110 showed the highest interaction.

An additional critical aspect in molecular docking analysis is the evaluation of binding free energy, where a more negative value indicates a reaction that is both more spontaneous and effectively irreversible. In this context, inhibitor molecules are particularly significant due to their enhanced propensity to engage in binding interactions. The strength and stability of these interactions are largely influenced by the quantity of hydrogen bonds and electrostatic forces formed, which facilitate a more robust and precise docking of inhibitors within the protein's active site. This enhanced binding affinity enables inhibitors to more effectively suppress the biological function of the target protein. In the current investigation, the most potent binding affinity observed for thyme was attributed to the α-Terpineol molecule, exhibiting a binding free energy of -4.96 kcal/mol. Similarly, for eucalyptus, the compound Carvotanacetone demonstrated the strongest interaction, with a binding free energy measured at -5.21 kcal/mol.

Conclusion

The results of molecular docking between plant compounds and the virus coat protein indicated that in relation to the thyme plant, Endo-borneol, a-Terpineol, and Terpinen-4-ol had the strongest interaction. On the other hand, it was found that the Cyclohexane compound in the mentioned plant created the weakest interaction with the evaluated protein. While in eucalyptus, Carvotanacetone, trans-Carveol, and beta-Terpineol had the strongest interaction, whereas the weakest interaction was related to the alpha-Thujene compound. The compounds a-Terpineol and Carvotanacetone in thyme and eucalyptus plants acted as the strongest binding molecules under in silico conditions. Such that they can be introduced and suggested as strong inhibitors for inhibiting the coat protein of the Mimosa yellow vein virus.

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