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Molecular docking analysis of *Cupressus sempervirens* ligands against *Fusarium oxysporum* pathogenic proteins

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Abstract

This study utilized molecular docking via AutoDock Vina to investigate the inhibitory potential of eight ligands from *C. sempervirens*—comprising five flavonoids and three phenolic acids—against four critical *F. oxysporum* pathogenic proteins: 5AJH, 7T6A, 7T69, and 5OD4. The results revealed spontaneous and stable binding interactions for all complexes, with binding affinities (ΔG) ranging from -5.2 to -9.3 kcal.mol^{-1}. Flavonoids consistently exhibited stronger affinities than phenolic acids, with Hesperidin identified as the most promising bioactive compound. Hesperidin achieved exceptional binding scores, particularly against targets 7T6A (-9.3 kcal.mol^{-1}) and 5AJH (-9.0 kcal.mol^{-1}). These *in silico* findings provide a robust molecular basis for previously observed *in vitro* antifungal efficacy. The study concludes that *C. sempervirens*, and specifically Hesperidin, represents a viable and eco-friendly source for developing natural bio-fungicides to manage *F. oxysporum* infections.

Keywords: *Cupressus sempervirens*, *Fusarium oxysporum*, Molecular docking, Hesperidin, Antifungal activity, Bio-fungicides.

Analyse de docking moléculaire des ligands de *Cupressus sempervirens* contre les protéines pathogènes de *Fusarium oxysporum*

Résumé

Cette étude a utilisé le docking moléculaire via AutoDock Vina afin d'évaluer le potentiel inhibiteur de huit ligands issus de *Cupressus sempervirens* — comprenant cinq flavonoïdes et trois acides phénoliques — contre quatre protéines pathogènes essentielles de *Fusarium oxysporum* : 5AJH, 7T6A, 7T69 et 5OD4. Les résultats ont révélé des interactions de liaison spontanées et stables pour tous les complexes, avec des affinités de liaison (ΔG) variant de -5,2 à -9,3 kcal.mol^{-1}. Les flavonoïdes ont systématiquement présenté des affinités plus élevées que les acides phénoliques, l'hespéridine étant identifiée comme le composé bioactif le plus prometteur. L'hespéridine a montré des scores de liaison exceptionnels, notamment contre les cibles 7T6A (-9,3 kcal.mol^{-1}) et 5AJH (-9,0 kcal.mol^{-1}). Ces résultats *in silico* fournissent une base moléculaire solide aux activités antifongiques *in vitro* précédemment observées. L'étude conclut que *C. sempervirens*, et particulièrement l'hespéridine, représente une source viable et écologique pour le développement de biofongicides naturels destinés à lutter contre les infections causées par *F. oxysporum*.

Mots-clés : *Cupressus sempervirens*, *Fusarium oxysporum*, Docking moléculaire, Hespéridine, Activité antifongique, Biofongicides.

INTRODUCTION

Fusarium oxysporum, a ubiquitous soil-borne fungal pathogen, poses a significant threat to global agricultural productivity by causing vascular wilts and root rots in a wide range of economically important crops. The escalating concerns regarding conventional

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fungicide resistance and environmental impact necessitate the exploration of novel, sustainable antifungal strategies, such as those derived from natural plant sources (Yousafi et al., 2022). In this context, plant-derived small molecules are recognized for their crucial role in pathogen defense (Angelini, 2024).

The present study focuses on *Cupressus sempervirens*, commonly known as the Mediterranean cypress, which has been traditionally recognized for its medicinal properties, including antimicrobial activities. Specifically, this investigation employs molecular docking to elucidate the inhibitory potential of various ligands identified in *C. sempervirens* extracts against key pathogenic proteins of *F. oxysporum*, thereby providing a computational basis for its observed antifungal efficacy (**Omar et *al*., 2021**).

This in silico approach, utilizing Autodock Vina, allows for the prediction of binding affinities and interaction patterns between *C. sempervirens* compounds and critical *F. oxysporum* proteins, thereby identifying potential phytotherapeutic agents for agricultural applications. Such computational methodologies are instrumental in screening and prioritizing compounds based on their capacity to interact with specific fungal proteins implicated in virulence and pathogenicity, thereby streamlining the development of targeted antifungal interventions (**Shravani et *al*., 2024**).

The in vitro analysis conducted by Chihat et al. (2025) supports the efficacy of *Cupressus sempervirens* extract in inhibiting *F. oxysporum* growth, providing an empirical foundation for the present computational study. The subsequent molecular docking experiments utilized several *F. oxysporum* protein targets, including 5AJH, 7T6A, 7T69, and 5OD4, to assess their binding interactions with various *Cupressus sempervirens* derived ligands.

These proteins, often involved in critical metabolic pathways or virulence mechanisms, represent promising targets for antifungal intervention (**Aamir et *al*., 2018; Diass et *al*., 2024**).

MATERIAL AND METHODS

1. List of ligands

The screened compounds were selected to represent the metabolic diversity of *Cupressus sempervirens*. The classification and sources of the 08 ligands are detailed below (Table 1).

Table 1 : Classification of *C. sempervirens* ligands

Chemical category	Ligand	Molecule type
Flavonoids	Hesperidin	Flavonoid Heteroside
	Myricetin	Flavonol
	Quercetin	Flavonol
	Kaempferol	Flavonol
	Catechin	Flavanol (monomer)
Phenolic acids	Caffeic acid	Hydroxycinnamic acid
	Ferulic acid	Hydroxycinnamic acid
	Gallic acid	Hydroxybenzoic acid

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The ligand library used included primary and secondary metabolites documented for the species *Cupressus sempervirens* (**Yang et *al*., 2024**) it was composed of five flavonoids and three phenolic acids, allowing for the evaluation of a wide range of polarities and molecular sizes against target proteins.

2. Ligand preparation

The 3D structures of the phenolic, terpenic and steroidal compounds of *Cupressus sempervirens* were downloaded from PubChem (https://pubchem.ncbi.nlm.nih.gov) on Mai 09, 2026. The ligands were converted to PDBQT format with AutoDockTools-1.5.7©.

3. Preparation of target proteins

To effectively target the inhibition of *Fusarium oxysporum* growth and pathogenicity, the choice of proteins focused on four key pathogenic targets identified from the Protein Data Bank (PDB):

- **5AJH**: *Fusarium oxysporum* cutinase,
- **7T6A:** Crystal structure of Avr1 (SIX4) from *Fusarium oxysporum*,
- **7T69:** Crystal structure of Avr3 (SIX1) from *Fusarium oxysporum*,
- **5OD4:** Avr2 effector.

These proteins were selected for their essential roles in the survival, virulence, and metabolic pathways of the fungus, making them ideal candidates for molecular docking. Specifically, target 7T6A was included for its potential as a primary site of interaction, while 5AJH represents a crucial enzymatic regulator within the pathogen.

By utilizing this diverse panel of targets, the study covers various biological functions essential for fungal development, increasing the likelihood of identifying a potent bioactive molecule from cypress capable of a pleiotropic inhibitory action.

This *in silico* approach seeks to provide a molecular basis for the significant antifungal efficacy of *C. sempervirens* extracts previously observed in in vitro assays (**Chihat et *al*., 2025**).

The 3D structures of the proteins were downloaded from the *RCSB Protein Data Bank* (https://www.rcsb.org).

Pre-treatment was performed using AutoDock Tools and involved the removal of water molecules and co -crystallized ligands, the addition of polar hydrogens, and the addition of *Kollman charges*. Docking was performed with AutoDock Vina (**Trott , O. et *al* ., 2010**).

4. Definition of the Grid Box

The grid was defined so as to encompass the active site or presumed link domain (Table 2).

Table 2: Grid Box parameters for molecular docking

Target protein (PDB ID)	Coordinates of the center (x; y; z)	Dimensions ($Å^3$)	Spacing (Å)
5AJH	(-20.393; 11.164; -30.072)	40 × 40 × 40	0.375
5OD4	(-5.348; -5.582; 15.989)	40 × 40 × 40	0.375
7T6A	(4.077; 2.233; 55.276)	40 × 40 × 40	0.375
7T69	(26.027; 12.902; 46.166)	40 × 40 × 40	0.375

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These parameters define a 40×40×40 cubic Grid Box for each target, with a standard spacing of 0.375 Å. Using a box of this size is typical of a blind approach docking (extended docking), allowing exploration of a large part of the protein surface, rather than being limited to a very small known active site. The exhaustiveness was set at 8, and the *energy range* at 4 kcal.mol^{-1}, allowing efficient exploration of the conformational space of the ligand. The selection criterion is defined as the lowest bond free energy (ΔG, in kcal.mol^{-1}**)** provided by Vina (**Trott , O. et *al* ., 2010**).

5. Analysis of Interactions

The analysis of key interactions (hydrogen bonds, hydrophobic interactions, etc.) was performed using Discovery Studio 2024 Client.

RESULTS

1. General connection affinities

The *in silico* molecular docking analysis using AutoDock Vina revealed a wide range of binding affinities (Δ*G*) between the selected *Cupressus sempervirens* ligands and the four pathogenic targets of *Fusarium oxysporum*. The binding energies for all tested complexes ranged from -5.2 to -9.3 kcal.mol^{-1}, indicating spontaneous and stable interactions across the board (Table 3).

Table 3: Binding free energies (ΔG) for the main ligands

Protein target (PDB ID)	**Ligand**	**ΔG (kcal.mol^{-1})**
5AJH	Hesperidin	-9.0
	Myricetin	-8.1
	Quercetin	-8.0
	Kaempferol	-8.0
	Catechin	-7.8
	Caffeic acid	-6.0
	Ferulic acid	- 5.9
	Gallic acid	-5.6
7T6A	Hesperidin	-9.3
	Myricetin	-7.3
	Quercetin	-7.4
	Kaempferol	-7.2
	Catechin	-7.6
	Caffeic acid	-6.4
	Ferulic acid	-6.0
	Gallic acid	-5.6
7T69	Hesperidin	-7.8
	Myricetin	-6.8
	Quercetin	-6.9
	Kaempferol	-6.5
	Catechin	-6.6

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	Caffeic acid	-5.3
	Ferulic acid	-5.5
	Gallic acid	-5.2
5OD4	Hesperidin	-8.3
	Myricetin	-7.1
	Quercetin	-6.9
	Kaempferol	-6.7
	Catechin	-6.7
	Caffeic acid	-5.6
	Ferulic acid	-5.5
	Gallic acid	-5.2

A clear distinction was observed between the two chemical classes of ligands:

- **Flavonoids** (Hesperidin, Myricetin, Quercetin, Kaempferol, and Catechin) demonstrated the strongest affinities, with scores consistently below -6.5 kcal.mol^{-1}.

- **Phenolic acids** (Caffeic, Ferulic, and Gallic acid) showed more moderate binding strengths, generally ranging between -5.2 and -6.4 kcal.mol^{-1}.

Among the four targets, 7T6A and 5AJH appeared to be the most receptive to cypress bioactive compounds, yielding the highest negative ΔG values.

2. Identification of the most promising molecule

Based on the docking scores, *Hesperidin* was identified as the most promising bioactive molecule within the *C. sempervirens* extract. It consistently outperformed all other ligands by achieving the highest binding affinities for every single protein target:

- **Target 7T6A :** -9.3 kcal.mol^{-1}
- **Target 5AJH :** -9.0 kcal.mol^{-1}
- **Target 5OD4 :** -8.3 kcal.mol^{-1}
- **Target 7T69 :** -7.8 kcal.mol^{-1}

The exceptional score of -9.3 kcal.mol^{-1} against target 7T6A marks Hesperidin as a potent potential inhibitor of *Fusarium oxysporum* pathogenic pathways. Other flavonoids like Myricetin and Quercetin also showed strong potential (reaching -8.1 and -8.0 kcal.mol^{-1} respectively against 5AJH), but remained secondary to Hesperidin.

3. Molecular interaction analysis of Hesperidin

To elucidate the binding mechanism of the most promising molecule, Hesperidin, a detailed analysis of 2D and 3D interactions was performed for the four protein targets (Figure 1). Visual inspection confirms that Hesperidin effectively anchors within the binding cavities of the targets, stabilized by a dense network of non-covalent interactions.

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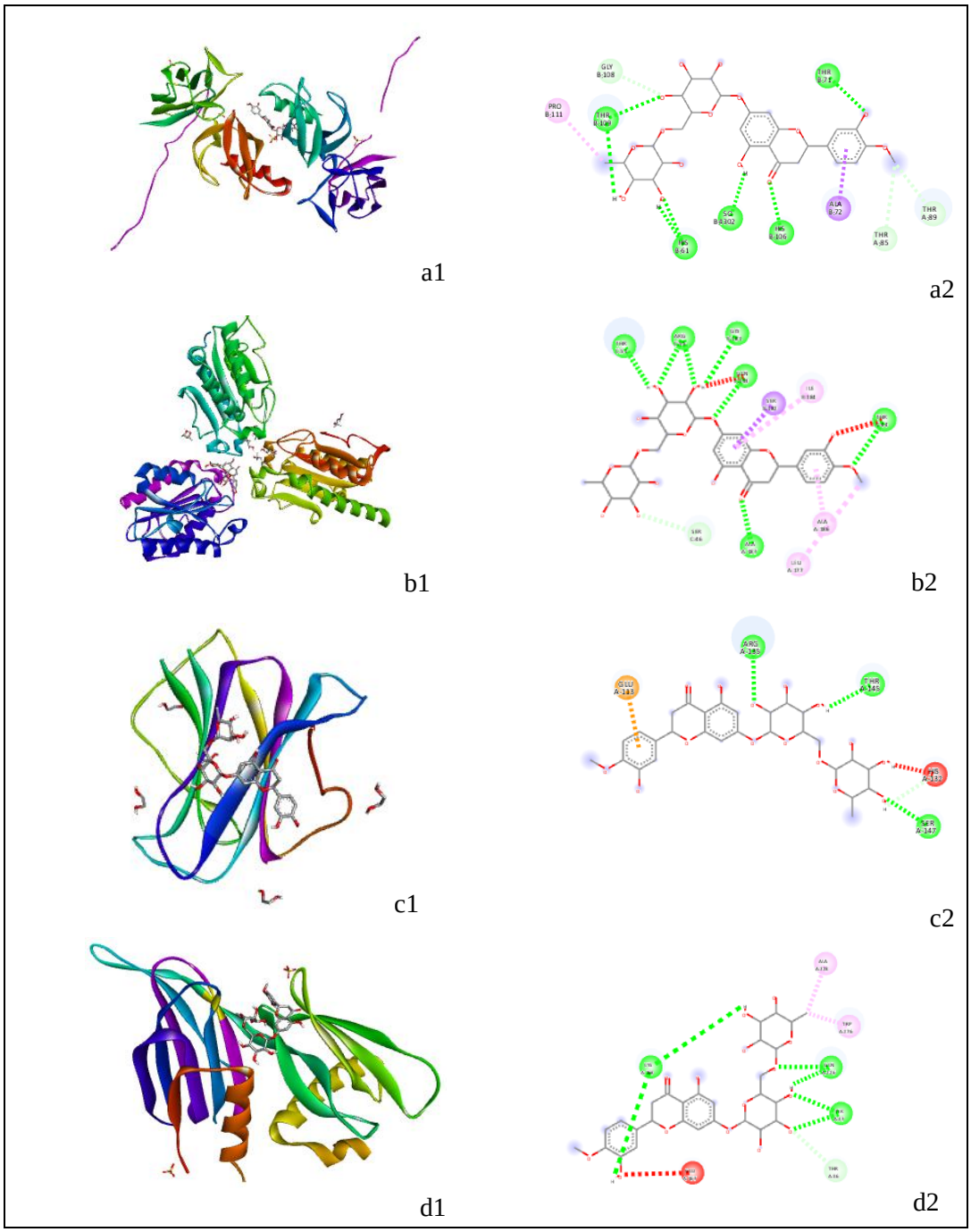


Figure 1: 3D visualization (left) and 2D interaction schemas* (right) of Hesperidin with *F. oxysporum* pathogenic proteins: (a) 7T6A, (b) 5AJH, (c) 5OD4, and (d) 7T69**.**

*Green dashed lines represent conventional hydrogen bonds, while pink/purple areas indicate hydrophobic interactions.

a) **Target 7T6A (-9.3 kcal.mol^{-1}):** The diagrams **a1** and **a2** illustrate the maximum affinity observed in this study. The complex is stabilized by multiple conventional hydrogen bonds with key residues, including *THR-109, HIS-61, HIS-106***,** and *THR-71*. A *Pi-Alkyl*

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interaction with *ALA-72* further enhances the hydrophobic stability of the flavonoid core.

b) **Target 5AJH (-9.0 kcal.mol⁻¹):** As shown in figures **b1** and **b2**, Hesperidin establishes strong hydrogen bonds with *THR-127*, *ARG-153***,** and *GLN-156*. These interactions within the enzymatic site suggest a direct potential for inhibiting the catalytic activity required for fungal penetration.

c) **Target 5OD4 (-8.3 kcal.mol⁻¹):** Analysis of figures **c1** and **c2** reveals a notable electrostatic interaction (Pi-Anion) with *GLU-113*, alongside hydrogen bonds with *ARG-155* and *THR-145*. Despite a minor unfavorable donor-donor interaction with *HIS-132*, the overall complex remains highly stable.

d) **Target 7T69 (-7.8 kcal.mol⁻¹):** Diagrams **d1** and **d2** show that Hesperidin interacts with residues *SER-148*, *GLN-126***,** and *SER-111* via hydrogen bonding. This stabilization is complemented by Pi-Alkyl interactions with *TRP-176* and *ALA-128*.

DISCUSSION

The molecular docking results reveal a clear hierarchy in the inhibitory potential of the eight ligands derived from *Cupressus sempervirens* against *Fusarium oxysporum* infection. The calculated binding affinities, ranging from −5.2 to −9.3 kcal·mol⁻¹, demonstrate that all compounds bind spontaneously to the target proteins, although their structural differences significantly influence their efficacy. A major finding is the consistent superiority of flavonoids (Hesperidin, Myricetin, Quercetin, Kaempferol and Catechin) over phenolic acids (Gallic, Caffeic, and Ferulic acids).

This observation is consistent with previous studies reporting that the benzo-γ-pyrone scaffold and polyphenolic structure of flavonoids favor stronger hydrophobic and π-based interactions within enzymatic binding pockets compared with simpler phenolic acids **(Panche et al., 2016; Xiao and Woods, 2023).**

Hesperidin emerged as the most potent ligand, particularly against targets 7T6A (−9.3 kcal·mol⁻¹) and 5AJH (−9.0 kcal·mol⁻¹). These values indicate highly stable ligand–protein complexes, as binding energies below −7.0 kcal·mol⁻¹ are generally considered indicative of significant biological activity in molecular docking studies (**Zare et al., 2024**). The exceptional stability of these complexes is supported by the dense network of hydrogen bonds and π-type interactions observed in the 2D interaction diagrams. In particular, π-alkyl and anion–π interactions involving residues such as ALA-72 and GLU-113 contribute substantially to ligand stabilization within the active site, as previously highlighted in studies examining non-covalent interactions in protein–ligand complexes **(Rosokha, 2023; Xiao and Woods, 2023).**

These *in silico* findings provide a molecular explanation for the antifungal activity experimentally observed for *Cupressus sempervirens* extracts against Fusarium oxysporum infection **(Chihat et al 2025)**. The strong interaction of Hesperidin with the 5AJH cutinase target suggests inhibition of fungal cuticle degradation mechanisms, thereby potentially limiting host penetration during the early stages of infection. Moreover, the variability in binding affinities across the four targets (5AJH, 7T6A, 7T69, and 5OD4) indicates that cypress-derived bioactive compounds may exert a multitarget or pleiotropic antifungal effect. Such multitarget activity is advantageous because it can disrupt several essential fungal metabolic pathways simultaneously, thereby reducing the likelihood of resistance development.

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Although phenolic acids exhibited lower affinities (average ≈ −5.8 kcal·mol⁻¹), they may still contribute indirectly to antifungal activity through synergistic mechanisms, including weakening of the fungal cell wall and enhancement of membrane permeability, which could facilitate the penetration of larger flavonoid molecules such as Hesperidin. Similar synergistic effects between phenolic acids and flavonoids have been widely described in phytochemical-based antifungal strategies. Overall, the strong agreement between the docking scores and previously reported antifungal activities supports the potential of *Cupressus sempervirens* as a promising source of eco-friendly antifungal compounds for sustainable plant disease management.

CONCLUSION

This *in silico* study establishes a definitive molecular link between the bioactive compounds of *Cupressus sempervirens* and the potent inhibition of *Fusarium oxysporum*. By identifying Hesperidin as a lead candidate with an exceptional binding affinity of -9.3 kcal.mol⁻¹ against the 7T6A target, our research provides the computational evidence necessary to explain the significant antifungal activity observed in experimental trials. These high-affinity interactions, particularly with targets 7T6A and 5AJH (-9.0 kcal.mol⁻¹), offer a robust molecular basis for the inhibition of mycelial growth reported in recent literature.

Furthermore, the stability of these flavonoid-protein complexes confirms that cypress leaf extracts are not merely a mixture of secondary metabolites, but a source of specialized molecules capable of disrupting multiple pathogenic pathways. In the face of rising pesticide resistance and the urgent need for food safety, this study validates *C. sempervirens* as an eco-friendly alternative to synthetic chemicals. Future research should focus on isolating Hesperidin for targeted field applications, paving the way for a new generation of sustainable agricultural treatments.

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