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Plant lectin from *Dioclea altissima* as a potential SARS-CoV-2 inhibitor: insights from molecular docking studies

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ABSTRACT

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) remains a relevant target for the identification of novel antiviral compounds. In this study, we investigated the molecular interactions between a plant-derived lectin from *Dioclea altissima* (DAL) and two key viral targets: the main protease (Mpro) and the spike glycoprotein. Molecular docking simulations were performed using HEX 8.0.0 to explore protein–protein interactions between the lectin and SARS-CoV-2 targets. The results revealed a markedly higher docking score of DAL toward Mpro (−83.73) compared to the spike protein (−40.71). Structural analysis of the top-ranked docking poses indicated that DAL interacts with amino acid residues in regions proximal to the catalytic site of Mpro, suggesting a potential influence on substrate accessibility or local conformational dynamics. In contrast, interactions with the spike protein were observed within the S2 subunit, outside the canonical receptor-binding domain, involving regions associated with conformational rearrangements required for membrane fusion. Visualization and interaction analyses were conducted using PyMOL, enabling the identification of key contact residues and interaction patterns contributing to complex stabilization. The comparative binding profile suggests preferential interaction of DAL with Mpro, supporting its potential as a scaffold for the development of antiviral agents against SARS-CoV-2. These findings provide preliminary in silico evidence of selective interaction between *D. altissima* lectin and a key viral enzyme, warranting further biochemical and pharmacological investigations.

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INTRODUCTION

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), the etiological agent of COVID-19, remains a relevant target for the identification of novel antiviral compounds. Despite advances in therapeutic strategies, the search for effective molecules capable of interacting with key viral proteins is still ongoing. Among the most relevant molecular targets, the main protease (Mpro) plays a central role in viral polyprotein processing, while the spike glycoprotein is responsible for viral attachment and entry into host cells (JIN *et al.*, 2020; JAFARY *et al.*, 2021).

Natural products have emerged as an important source of bioactive compounds with potential antiviral activity. In this context, plant lectins have gained attention due to their ability to recognize and bind specific carbohydrate structures, which may interfere with viral mechanisms. The lectin obtained from *Dioclea altissima* has been previously described as a biomolecule with promising biochemical properties, supporting its potential application in biomedical research (ARAÚJO *et al.*, 2020).

Computational approaches, particularly molecular docking, have been widely used as efficient tools for the preliminary investigation of ligand–target interactions, allowing the evaluation of structural compatibility and binding profiles (HOSSEINI *et al.*, 2021). These methods have been successfully applied in the identification of potential antiviral targets and compounds against SARS-CoV-2 (ZIGOLO *et al.*, 2021).

In this study, we performed a comparative in silico analysis of the interaction between *D. altissima* lectin and two key SARS-CoV-2 proteins, namely the main protease (Mpro) and the spike glycoprotein, aiming to evaluate binding affinity and to identify possible interaction mechanisms. Protein–protein docking has been widely used to explore macromolecular interactions and identify potential binding interfaces in viral systems (MACINDOE *et al.*, 2010).

MATERIALS AND METHODS

The three-dimensional structures of the SARS-CoV-2 spike glycoprotein, main protease (Mpro), and *Dioclea altissima* lectin (DAL) were retrieved from the Protein Data Bank (PDB) under the accession codes 7DWZ, 7BAJ, and 7LJG, respectively. The lectin structure (PDB ID: 7LJG) is currently annotated as *Macropsychanthus violaceus* due to database classification; however, it represents a closely related lectin within the Diocleinae tribe, sharing high structural similarity with *Dioclea altissima*.

Molecular docking simulations were performed using HEX 8.0.0, a protein–protein docking software based on spherical polar Fourier correlations, which accounts for both shape and electrostatic complementarity (Macindoe et al., 2010). The docking search was conducted over the entire protein surface to identify potential interaction regions between DAL and the viral targets.

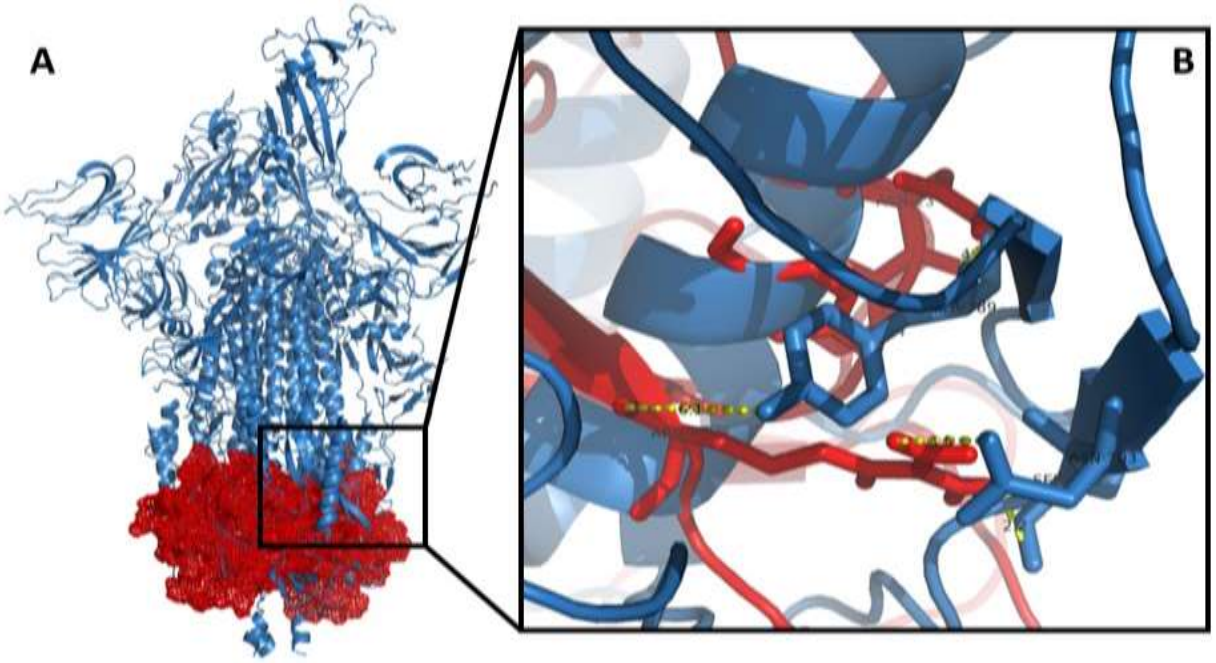
The resulting complexes were analyzed based on their docking poses and interaction patterns. Structural visualization and inspection of protein–protein interfaces were carried out using PyMOL (DeLano, 2014), enabling the identification of key amino acid residues involved in complex stabilization.

Docking scores were used as comparative parameters to evaluate the interaction profiles between DAL and each target protein. These values were interpreted comparatively within the same computational framework, rather than as absolute thermodynamic parameters. All structures were prepared by removing non-essential molecules and ensuring appropriate structural integrity prior to docking simulations.

RESULTS AND DISCUSSION

Molecular docking simulations revealed distinct interaction profiles between Dioclea altissima lectin (DAL) and the two SARS-CoV-2 targets evaluated. For the spike glycoprotein, DAL exhibited interactions within regions of the S2 subunit, rather than the canonical receptor-binding domain (RBD), which is primarily associated with viral attachment (WRAPP et al., 2020). The most favorable docking poses were located predominantly in α-helical regions with minimal steric hindrance (Figure 1).

Figure 1: Molecular docking of *Dioclea altissima* lectin (DAL) with the SARS-CoV-2 spike glycoprotein. (A) Overall view of the DAL–spike complex highlighting the binding region within the S2 subunit, outside the canonical receptor-binding domain (RBD). (B) Detailed view of the interaction site showing contacts with residues Asn703, Ser704, and Tyr769. Interaction distances range from 2.2 to 6.1 Å, consistent with stable protein–protein interactions.



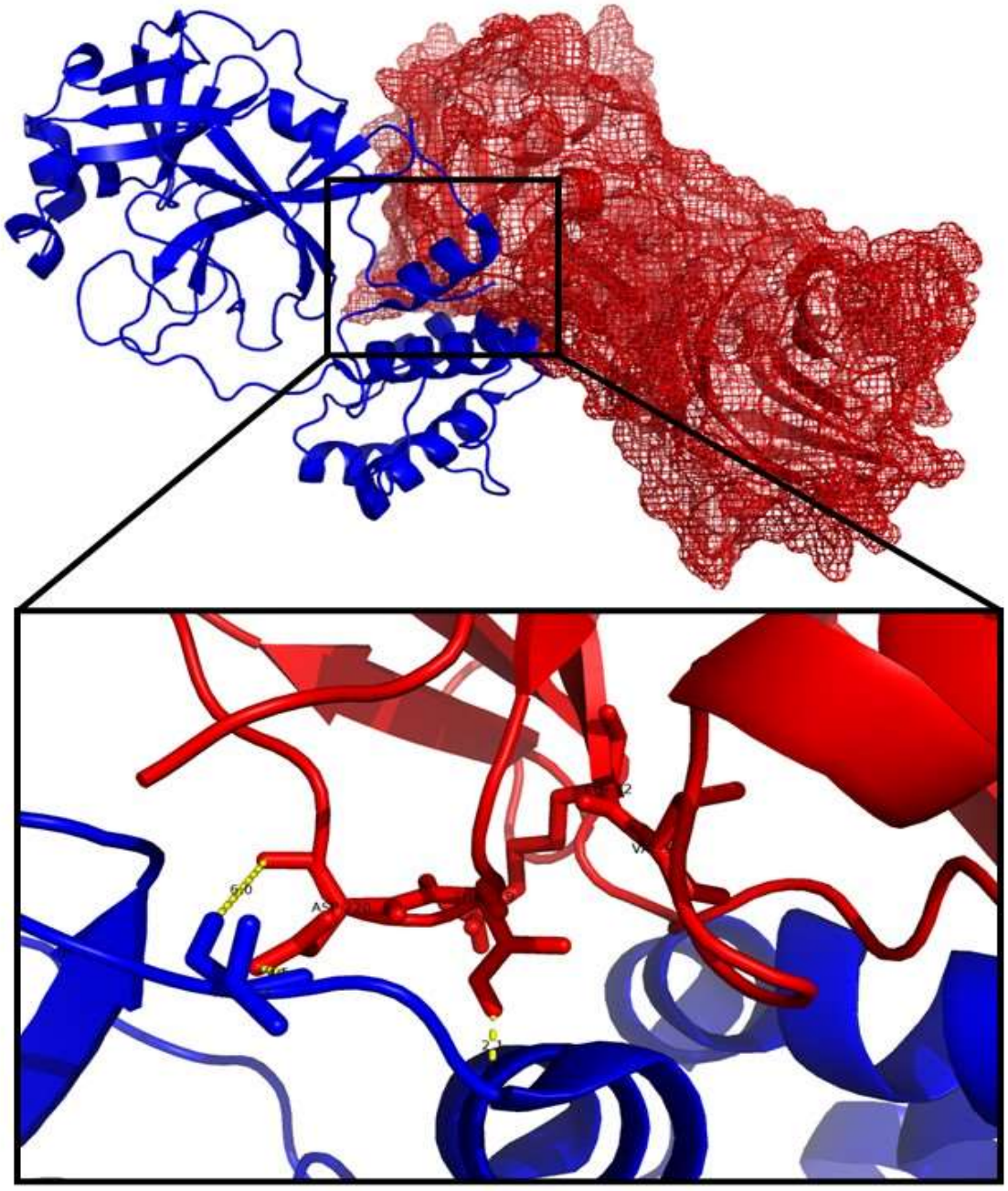
Source: Prepared by the authors.

Interaction analysis indicated that complex formation involved key amino acid residues, including Asn703, Ser704, and Tyr769, with interaction distances ranging from 2.2 to 6.1 Å (Figure 1B). These interactions suggest a consistent, although moderate, interaction profile, as reflected by the observed docking score (−40.71). The distribution of contacts and interaction distances indicates that DAL may associate with structurally relevant regions of the spike protein, potentially influencing local conformational dynamics.

In contrast, docking simulations with the main protease (Mpro) demonstrated a more consistent and favorable interaction pattern. Among the top-ranked docking clusters, a high level of convergence toward a specific binding region was observed, with 7 out of the 10 best-scoring poses occupying a similar site. This reproducibility suggests a preferential interaction region within the enzyme structure.

Detailed analysis of the best-ranked complex revealed that DAL interacts with multiple residues, including Ser1, Lys137, Thr169, Gly170, Val171, and Asn214 (Figure 2). These residues are located in structurally flexible regions composed of β-sheets and loop domains, which are often associated with conformational adaptability. The interaction network includes hydrogen bonds and hydrophobic contacts, with distances consistent with stable protein–protein interactions.

Figure 2: Molecular docking of *Dioclea altissima* lectin (DAL) with the SARS-CoV-2 main protease (Mpro). (A) Overall structure of the DAL–Mpro complex showing the preferential binding region. (B) Close-up view of the interaction site highlighting contacts with residues Ser1, Lys137, Thr169, Gly170, Val171, and Asn214, located in regions proximal to the catalytic site.



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The docking score observed for the DAL–Mpro complex (−83.73) indicates a substantially stronger interaction compared to the spike protein. Although docking scores should be interpreted comparatively within the same computational framework, this difference suggests a more favorable interaction profile toward Mpro. Additionally, the localization of interactions in regions proximal to functionally relevant areas of the enzyme supports the hypothesis that DAL may influence its structural dynamics or substrate accessibility.

Overall, the comparative analysis highlights a preferential interaction of DAL with Mpro over the spike glycoprotein, supported by both docking scores and interaction patterns. These findings are consistent with previous studies emphasizing the relevance of Mpro as a primary target for antiviral drug development against SARS-CoV-2 (JIN et al., 2020; ZIGOLO et al., 2021; HOSSEINI et al., 2021). Furthermore, recent investigations have reinforced the potential of computational approaches in identifying natural compounds with antiviral activity against SARS-CoV-2 targets (DAI et al., 2020; ZHANG et al., 2020; QAMAR et al., 2020).

Taken together, the results indicate that *D. altissima* lectin exhibits distinct interaction behavior toward SARS-CoV-2 proteins, with a more favorable and reproducible interaction profile for Mpro, supporting its potential as a candidate for further antiviral investigation.

CONCLUSION

This study provides a comparative in silico evaluation of the interactions between *Dioclea altissima* lectin (DAL) and two key SARS-CoV-2 proteins. The results indicate a preferential interaction profile of DAL toward the main protease (Mpro) over the spike glycoprotein, supported by higher docking scores and a more consistent interaction pattern.

Structural analysis suggests that DAL interacts with residues located in regions proximal to functionally relevant areas of Mpro, supporting its potential as a molecular scaffold for antiviral investigation. In contrast, interactions with the spike protein were observed in regions outside the canonical receptor-binding domain, indicating a distinct interaction profile.

Although these findings are based on computational approaches and should be interpreted comparatively within the same methodological framework, they highlight the relevance of plant-derived lectins as candidates for targeting viral proteins. Further experimental studies, including in vitro and in vivo assays, are required to validate the biological activity and therapeutic potential of DAL.

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