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Molecular Docking Analysis of Christanoate and Christene from *Christia vespertilionis* Plants as Potential Inhibitors of Covid-19

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Abstract

Covid-19 is a global pandemic caused by SARS-CoV-2 virus that caused mortality and world economic collapse. It is almost impossible to break the chain of infection with no intervention except vaccines to prevent worsening symptoms and to build herd immunity in people. Efforts to discover a therapeutic drug to combat the virus are still ongoing. Various medicinal phytoconstituents are also researched for their pharmacological action as antiviral agents against Covid-19. This study explored the antiviral potential of *Christia vespertilionis* bioactive compounds (christene and christanoate) for treating Covid-19 using molecular docking analysis. The Covid-19 protein crystal structures (PDB ID: 6LU7, PDB ID: 6CS2, PDB ID: M1D, PDB ID: 2GHV and PDB ID: 6M71) obtained from the protein data bank were docked to christene and christanoate. The analyses were carried out using the Autodock tool 1.5.6. The control docking was done using favipiravir as the reference drug. The binding interaction of the protein and ligand was observed using the Biovia Discovery visualizer. The binding affinity and interactions indicate that the observed compounds have antiviral action suggesting their potential as Covid-19 inhibitors and can be further considered for therapeutic applications.

Keywords: SARS-CoV-2, *Christia vespertilionis*, molecular docking, Covid-19

Introduction

The outbreak of coronavirus disease (COVID-19) caused a global health emergency at the end of 2019 (1). The RNA virus has caused significant economic and social repercussions providing a significant threat globally (2). According to Chen et al., (3), the virus was most likely transmitted to humans through infected droplets from bats. The majority of those infected with COVID-19 will experience mild to moderate respiratory symptoms and will recover without the need for additional treatment. However, COVID-19 can develop serious illnesses in older people, those suffering from medical conditions such as heart disease, diabetes, chronic pulmonary illness, and cancer. Currently, vaccination has been approved for mass immunization. However, there is decreasing vaccine coverage and an increasing risk of vaccine-preventable disease outbreaks and epidemics due to vaccine hesitancy. Vaccination is perceived as unnecessary by many individuals due to their belief, lack of confidence, and presumed unsafe (4). The key goals to fight against the rapidly evolving virus are developing new therapies or repurposing drugs (5,6).

The SARS-CoV-2 virus belongs to the Coronaviridae family, subfamily coronavirinae and Nidovirales order. It is a protein-sense RNA virus with a single linear RNA segment on a sin-