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Dermaseptin-Based Antiviral Peptides to Prevent COVID-19 through *In Silico* Molecular Docking Studies against SARS-CoV-2 Spike Protein

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ABSTRACT

A pandemic coronavirus disease of 2019 (COVID-19) caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has now been declared a global pandemic by the World Health Organization. The search for new drugs, especially by utilizing antiviral peptides is a very potential area. Through this study, protein-peptide docking and protein-protein docking simulations were conducted using *in silico* methods to identify, evaluate, and explore the molecular affinity and interaction of dermaseptin peptide molecules produced by frogs of the genus *Phyllomedusa* against the SARS-CoV-2 spike protein macromolecule, and its effect on attachment to the surface of the ACE-2 (Angiotensin Converting Enzyme-2) receptor. Protein-peptide docking simulation results show that dermaseptin-S9 peptide molecule has the best affinity to the active site of SARS-CoV-2 spike protein macromolecule binding site, with a binding free energy value of −792.93 kJ/mol. Then the results of protein-protein docking simulations proved that dermaseptin-S9 peptide molecule was able to prevent the attachment of SARS-CoV-2 spike protein to the surface of the ACE-2 receptor, with a total energy value of 517.85 kJ/mol. Therefore, it is hoped that dermaseptin-S9 peptide molecule can be further studied in the development of novel antiviral peptide candidates for the control of COVID-19 infectious disease.

Keywords: *COVID-19; SARS-CoV-2 spike protein; dermaseptin; antiviral peptide; in silico study*

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INTRODUCTION

The World Health Organization has now declared a global emergency and a pandemic for novel coronavirus disease of 2019 (COVID-19, formerly called 2019-nCoV) which has been actively spreading throughout the world. The COVID-19 infectious disease caused by the SARS-CoV-2 virus can cause symptoms such as fever, cough, pneumonia, nausea, and fatigue. To date, SARS-CoV-2 has spread to almost 24 countries worldwide and more than 8,061,550 people have been reported to be infected by 17 June 2020. Among these, there have been 440,290 deaths reported to be related to COVID-19 (Gabutti et al., 2020).

The main epidemiological cause of the SARS-CoV-2 virus is thought to originate from the seafood market in Wuhan City, Hubei Province, China (Chen et al., 2020). However, the true center of the initial transfer to humans is still unknown. At present, there are more than 100 complete genome sequences known in NCBI GenBank obtained from approximately 10 countries. Later it was also found that the variation between these sequences was less than 1% (Lu et al., 2020; Sah et al., 2020).

The SARS-CoV-2 virus is closely related to SARS-CoV and this allows the use of a known protein structure to quickly study models to find candidate compounds in the prevention and treatment of this SARS-CoV-2 virus (Hui et al., 2020). While traditional methods of drug discovery can take years, the approach that can be utilized here to find a predictable drug for SARS-CoV-2 is to use *in silico* protein-peptide docking studies of the most variable target proteins in SARS-CoV-2, which is spike protein from SARS-CoV-2 (Tahir ul Qamar et al., 2020; Wu et al., 2020).

SARS-CoV-2 spike protein is responsible for controlling some of the main functions of the virus and has a catalytic domain that is highly conserved from the SARS-CoV virus (Zhang et al., 2020). Some other functions include the virus replication process which makes it an ideal target in drug development (Das et al., 2020; Ton et al., 2020). It has been computationally proven that SARS-CoV-2 has a mechanism that is identical to the SARS-CoV virus and has a high affinity for ACE-2 (Angiotensin Converting Enzyme-2) receptor (Xu et al., 2020). Besides, there are structural similarities between SARS-CoV-2 and SARS-CoV spike proteins, which conservation is only 73% with most of the variability in the area of host cell protein interaction (Hall & Ji, 2020).

Dermaseptin is an antiviral peptide produced by frogs of the genus *Phyllomedusa*. The antiviral activity of this peptide has been described for HSV-1, HSV-2, and HIV-1, in which the virus envelope appears to be the