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Magainin as an Antiviral Peptide of SARS-CoV-2 Main Protease for Potential Inhibitor: An In Silico Approach

TAUFIK MUHAMMAD FAKIH*, MENTARI LUTHFIKA DEWI, EKY SYAHRONI
Department of Pharmacy, Faculty of Mathematics and Natural Sciences, Universitas Islam Bandung, Indonesia
Jl. Tamansari No.1, Tamansari, Bandung, West Java, Indonesia. 40116
*Email: taufikmuhammadf@gmail.com

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ABSTRACT

The new coronavirus (SARS-CoV-2) which caused the global pandemic Coronavirus Disease-2019 (COVID-2019) has infected nearly 206 countries. There is still little information about molecular compounds that can inhibit the development of infections caused by this disease. It is important to achieve the discovery of effective natural inhibitor candidates, such as antiviral peptides because they have a variety of biological activities and have evolved to target biochemical machinery from different pathogens or host cell structures. In this research, in silico studies will be carried out, including protein-peptide docking and protein-protein docking, to identify, evaluate, and explore the affinity and molecular interactions of the Magainin-1 and Magainin-2 peptide molecules derived from frog skin (Xenopus laevis) to the main protease macromolecule (Mpro) SARS-CoV-2, and its effect on the ACE-2 receptor (Angiotensin Converting Enzyme-2 Receptor). Protein-peptide docking simulations show that both peptide molecules have a good affinity for the active site area of the SARS-CoV-2 Mpro macromolecule. These results were then confirmed using protein-protein docking simulations to observe the ability of the peptide molecule in preventing attachment to the ACE-2 receptor surface area. In silico studies show that Magainin-2 has the best affinity, with a bond free energy value of −3054.53 kJ/mol. Then the protein-protein docking simulation results showed Magainin-2 was able to prevent the attachment of ACE-2 receptors, with an ACE score of 1697.99 kJ/mol. Thus, through in silico research, it is hoped that the Magainin peptide molecule can be further investigated in the development of new antiviral peptides for the treatment of infectious diseases of COVID-19.

Keywords**:** antiviral peptide; COVID-19; In silico; Magainin; SARS-CoV-2

INTRODUCTION

The emergence of symptoms such as fever, cough, fatigue, sputum production, shortness of breath, sore throat, headache along with several reports of diarrhea and vomiting began to increase as a cause of pneumonia cases since December 2019 and later identified as a new coronavirus in Wuhan, Hubei Province, China (Guan et al., 2020; Wang et al., 2020). On 12 January 2020 the WHO first named the 2019-novel coronavirus (2019-nCoV) and officially referred to this disease as the coronavirus 2019 (COVID-19) and as a global emergency disease as a result of concern globally. The International Committee of Coronavirus Study Group (CSG) recommends using the name as SARS-CoV-2, published on 11 February 2020 (Guo et al., 2020).

Two overlapping polyproteins function to encode the SARS-CoV-2 genome consisting of ~30,000 nucleotides, namely pp1a and pp1ab. Both polyproteins are needed by coronavirus for replication and transcription (Lu et al., 2020). Through this polyprotein, a functional polypeptide is released through a proteolytic process involving the main protease (Mpro) of SARS-CoV-2 (Ge et al., 2013). Previous studies have shown that the functional structure between SARS-CoV-2 and SARS-CoV is identical based on the complete phylogenetic analysis of the genome (Chen et al., 2009; Letko et al., 2020). By analyzing the order and analysis of the evolution of this coronavirus, it is suspected that bats act as coronavirus's natural hosts. The coronavirus may have been transferred to humans as an intermediate host by binding to