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Research Article

In silico Identification of Characteristics Spike Glycoprotein of SARS-CoV-2 in the Development Novel Therapeutic Candidates for COVID-19 Infectious Diseases

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Abstract

Background: The emergence of infectious diseases caused by SARS-CoV-2 has resulted in more than 90,000 infections and 3,000 deaths. The coronavirus spike glycoprotein encourages the entry of SARS-CoV-2 into cells and is the main target of antivirals. SARS-CoV-2 uses ACE2 to enter cells with an affinity similar to SARS-CoV, correlated with the efficient spread of SARS-CoV-2 among humans.

Objective: In the research were performed identification, evaluation, and exploration of the structure of SARS-CoV and SARS-CoV-2 spike glycoprotein macromolecules and their effects on Angiotensin-Converting Enzyme 2 (ACE-2) using *in silico* studies.

Methods: The spike glycoproteins of the two coronaviruses were prepared using the BIOVIA Discovery Studio 2020. Further identification of the three-dimensional structure and sequencing of the macromolecular spike glycoprotein structure using Chimera 1.14 and Notepad++. To ensure the affinity and molecular interactions between the SARS-CoV and SARS-CoV-2 spike glycoproteins against ACE-2 protein-protein docking simulations using PatchDock was accomplished. The results of the simulations were verified using the BIOVIA Discovery Studio 2020.

Results: Based on the results of the identification of the macromolecular structure of the spike glycoprotein, it was found that there are some similarities in characteristics between SARS-CoV and SARS-CoV-2. Protein-protein docking simulations resulted that SARS-COV-2 spike glycoprotein has the strongest bond with ACE-2, with an ACE score of −1509.13 kJ/mol.

Conclusion: Therefore, some information obtained from the results of this research can be used as a reference in the development of SARS-CoV-2 spike glycoprotein inhibitor candidates for the treatment of infectious diseases of COVID-19.

Keywords: COVID-19; SARS-CoV-2; spike glycoprotein; ACE-2, *in silico* study.
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INTRODUCTION

Three types of coronaviruses have caused deadly pneumonia in humans since the beginning of the 21st century, including severe acute respiratory syndrome coronavirus (SARS-CoV), Middle-Eastern respiratory syndrome coronavirus (MERS-CoV), and SARS-CoV-2.[1]

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SARS-CoV appeared in Guangdong province in China in 2002, infecting 8098 people and causing 774 deaths. In 2012, MERS-CoV appeared in the Arabian Peninsula, infecting a total of 2,494 individuals and claimed 858 lives.[2] Recently appeared a coronavirus named SARS-CoV-2 which was discovered in December 2019 in Wuhan, Hubei province of China. SARS-CoV-2 is linked to an ongoing atypical pneumonia outbreak (COVID-19) which has affected more than 90,000 people and killed more than 3,000 people affected in 60 countries.[3] The World Health Organization (WHO)