PULSUS
WWW.PULSUSCONFERENCE.COM
35 YEARS IN ASSESING THE IMPACT OF HEALTHCARE RESEARCH

ISSN: 2161-0398, Volume 07

Webinar on

Nanomedicine: Nanotechnology and Pharmaceutics

March 07, 2022

Working goal of Brazilein sappan wood as a candidate for SARS-coV-2 antiviral drug against spike (S) glycoprotein, papain-like protease, and main protease: In silico study

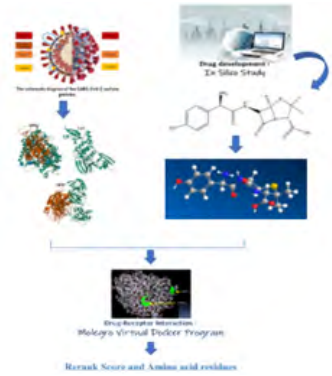
Dwi Krihariyani
Surabaya Health Polytechnic, Indonesia

Statement of the Problem: SARS-CoV-2 antiviral medicines that can decrease virus attachment, replication, and transcription in the human body are expected to be developed from Brazilein sappan wood. Brazilein has potential as an immunomodulator, has favorable pharmacokinetic properties, and generates relatively low toxicity, according to earlier studies employed in silico tests. Corona viruses connect to ACE2 on human host cells with Spike (S) glycoprotein and then employ Main Protease (MPro) and Papain-like protease (PLpro) to start their life cycle and impair the host response. Using the comparative medicine hydroxychloroquine, the goal of this work was to predict in silico the target of sappan wood brazilein as a candidate for SARS-CoV-2 antiviral treatments against S, PLpro, and MPro proteins.

Methodology & Theoretical Orientation: An in silico test was performed by docking using the Molegro Virtual Docker computer application. The goal of the in silico study is to use a computer to predict the physical chemical properties of chemicals (absorption, distribution, metabolism, and excretion = ADME), as well as their toxicity and biological activity against the target receptor. The bond energy of the docking results between the ligands on the target receptor was compared for data analysis. The lower the ligand's binding energy with the target receptor, the more stable the connection established, and thus the compound's biological activity can be predicted.

Findings: On the Spike (S) glycoprotein target, brazilein offers lower energy than the ligand but greater than hydroxychloroquine, while brazilein provides higher energy than the ligand and hydroxychloroquine on the Papain-like protease and Main protease targets.

Conclusion & Significance: The in silico test revealed that sappan wood brazilein was a viable SARS-CoV-2 therapeutic candidate with stable binding and greater biological activity against S protein than PLpro and Mpro proteins.



Biography

Dwi Krihariyani is a medical laboratory technology lecturer at Surabaya Health Polytechnic who is also interested in health microbiology. My research group and I are currently working on developing Covid-19 antibodies based on pathotype analysis and cloning of the SARS-CoV-2 specific gene, which will be used to generate rapid diagnostic tests.

dwikrihariyani@gmail.com