MECHANISM OF ACTION OF BIOACTIVE COMPOUNDS IN SOME ZINGIBERACEAE HERBAL PLANTS USING MOLECULAR DOCKING TECHNOLOGY IN SOME MAIN PROTEASE (MPRO) SARS-COV-2

by Nurfina Aznam, Retno Arianingrum, Sri Atun

ABSTRACT

Coronaviruses are a large family of viruses that cause illnesses ranging from the common cold to more severe illnesses such as Middle East respiratory syndrome (MERS-CoV) and severe acute respiratory syndrome (SARS-CoV). Corona virus is an infectious disease, with rapid and widespread spread, and no effective medicine has been found to kill the virus. Currently used antiviral drugs, such as remdesivir, ritonavir, and chloroquine, still show limited efficacy and have serious side effects. The problem of this research is to determine the bioactive compounds from herbal plants of the Zingiberaceae family, such as turmeric (Curcuma longa), ginger (Curcuma xanthorriza), and ginger (Zinger officinale) which can potentially be developed as anti-covid-19, as well as knowing the mechanism of activity of the bioactive compounds. in fighting viruses by molecular docking. The aim of this research is to determine potential bioactive compounds from several herbal extracts that have been used empirically by the public as anti-Covid-19, as well as to determine the mechanism of activity using computer virtual screening technology through molecular docking and molecular dynamics using several Covid-19 virus protein receptors. 19 contained in the data based RCSB PDB Database ((www.rcsb.org). Method: This research began with a literature study to search for bioactive compounds that have been found in turmeric, ginger and ginger plants via Pubchem and downloading their molecular structures (https: http://pubchem.ncbi.nlm.nih.gov/). Molecular docking was carried out using the PyRx computer program (based on AutoDock, Vina, and OpenBabel). The receptor chosen was a receptor that targets inhibition of the SARS-CoV-main protease (MPRO). 2 (PDB 6w63; PDB 6y2f; PDB 7vlq) which is an important part of the life cycle of the Covid-19 virus. The receptor structure can be obtained via the RCSB PDB Database website (www.rcsb.org). The expected results of this research can be to determine the mechanism of activity of bioactive compounds from herbal plants as potential anti-COVID-19 which are selected and evaluated for their absorption, distribution, metabolism and excretion (ADME) and Lipinski's rules. The target of this research is to publish at least 1 journal article published in a reputable international journal, such as Scopus Q3 Molecule. This research is basic research with the current level of technological readiness at TKT 1 and is expected to be at the end of the research at TKT 2.

Kata Kunci: *molekular docking; in siliko; protein virus; Covid-19; jahe; kunyit; temulawak*