INTISARI

RENALDY, 2022, ANALISIS PENAMBATAN MOLEKULER SENYAWA KANDUNGAN TANAMAN BUAH ANGGUR *(Vitis vinifera)* TERHADAP RESEPTOR COVID-19 DAN PREDIKSI PROFIL FARMAKOKINETIKA, SKRIPSI, PROGRAM STUDI S1 FARMASI, FAKULTAS FARMASI, UNIVERSITAS SETIA BUDI, SURAKARTA. Dibimbing oleh Dr. Nuraini Harmastuti, S.Si., M.Si. dan apt. Fransiska Leviana, S.Farm., M.Sc.

Covid-19 *(Coronavirus disease)* adalah suatu penyakit yang disebabkan oleh virus SARS-COV-2 yang saat ini belum ditemukan obatnya, tetapi telah dilaporkan bahwa senyawa aktif buah anggur dapat menghambat protein SARS-COV-2. Penelitian ini bertujuan untuk memprediksi afinitas dan pola interaksi senyawa kimia buah anggur dengan protein target dan prediksi profil farmakokinetika sebagai kandidat antivirus Covid-19.

Dilakukan analisis penambatan molekuler dengan metode Autodock Vina. Pemilihan senyawa uji berdasarkan studi literatur dan *web server* Phytochem dan Pubchem dengan melihat parameter *Lipinski'*s *rule of five*. Pemilihan protein target Covid-19 berdasarkan studi literatur dan *web server* Protein Data Bank (PDB). Visualisasi hasil penambatan molekuler menggunakan Autodock PyRx, PyMOL, dan Biovia DS. Prediksi profil sifat farmakokinetik menggunakan *web server* ADMETLab 2.0.

Hasil prediksi penambatan molekuler menunjukkan bahwa beberapa senyawa kimia buah anggur yaitu senyawa *ellagic acid*, myricetin, dan resveratrol memiliki hasil interaksi yang baik pada protein target PLpro (PDB:7CJM). Senyawa cinnamaldehyde, *ferullic acid*, dan vanillin memiliki hasil interaksi yang baik pada protein target 3CLpro (PDB:6M2N). Senyawa *ellagic acid* dan *gallic acid* memiliki hasil interaksi yang baik pada protein target RdRp (PDB:7ED5). Senyawa *ellagic acid*, resveratrol, *ferullic acid*, dan *gallic acid* memiliki prediksi profil farmakokinetika dan toksisitas yang baik.

Kata Kunci : Covid-19, buah anggur *(Vitis Vinifera)*, penambatan molekuler, Autodock Vina, ADMETLab 2.0

ABSTRACT

RENALDY, 2022, ANALYSIS OF DOCKING MOLECULAR OF GRAPE PLANT CONTENT COMPOUNDS (*Vitis vinifera*) AGAINST COVID-19 RECEPTORS AND PREDICTION OF PHARMACOKINETIC PROFILE, THESIS, PHARMACY UNDERGRADUATE STUDY PROGRAM, FACULTY OF PHARMACY, SETIA BUDI UNIVERSITY, SURAKARTA. Guided by Dr. Nuraini Harmastuti, S.Si., M.Si. and apt. Fransiska Leviana, S.Farm., M.Sc.

Covid-19 *(Coronavirus disease)* is a disease caused by the SARS-COV-2 virus for which no cure has been found, but it has been reported that the active compounds of grapes can inhibit the SARS-COV-2 protein. This study aims to predict the affinity and interaction patterns of grape fruit chemical compounds with target proteins and predict their pharmacokinetic profiles as covid-19 antiviral candidates.

Molecular tethering analysis was carried out by the Autodock Vina method. Selection of test compounds based on literature studies and *web servers* of Phytochem and Pubchem by looking at the parameters of *Lipinski's rule of five*. The selection of covid-19 target proteins is based on literature studies and the Protein Data Bank (PDB) *web server*. Visualization of molecular tethering results using Autodock PyRx, PyMOL, and Biovia DS. Prediction of pharmacokinetic properties profiles using the ADMETLab 2 web server.

The results of the prediction of molecular tethering show that several chemical compounds of grapes, namely ellagic acid, myricetin, and resveratrol compounds, have good interaction results on the target protein PLpro (PDB: 7CJM). The compounds cinnamaldehyde, ferullic acid, and vanillin had good interaction results on the target protein 3CLpro (PDB:6M2N). Ellagic acid and gallic acid compounds have good interaction results on the target protein RdRp (PDB:7ED5). Compounds of ellagic acid, resveratrol, ferullic acid, and gallic acid have good predictions of pharmacokinetic profile and toxicity.

Keywords: Covid-19, grape (*Vitis Vinifera*), docking molecular, Autodock Vina, ADMETLab 2.0