STUDI PENAMBATAN MOLEKUL SENYAWA TURUNAN FLAVONOL SEBAGAI KANDIDAT INHIBITOR PROTEASE UTAMA (M^{pro}) COVID-19

Salsabila Firdausi
17/409488/PA/17795

INTISARI

Penelitian tentang studi penambatan molekul senyawa turunan flavonol sebagai kandidat inhibitor M^{pro} Covid-19 telah dilakukan. Penelitian ini bertujuan untuk memprediksi beberapa senyawa turunan flavonol sebagai kandidat inhibitor Covid-19 dengan penambatan molekul dan mempelajari interaksi yang terjadi antara senyawa turunan flavonol terhadap protease utama (M^{pro}) SARS-CoV-2 sebagai kandidat inhibitor Covid-19. Penelitian ini menggunakan protein 6W63 dengan ligan alami X77. Protein 6W63 di *re-docking* menggunakan AutoDockTools-1.5.6. Selanjutnya ligan baru dari senyawa turunan flavonol (fisetin, gosipetin, kaemferol, mirisetin, pachypodol dan kuersetin) ditambatkan pada protein 6W63 dengan AutoDockTools-1.5.6. Hasil interaksi antar protein dan ligan divisualisasikan dengan Biovia Discovery Studio 2020.

Hasil yang diperoleh dari penelitian ini yaitu nilai energi ikat (ΔG) fisetin, gosipetin, kaemferol, mirisetin, pachypodol dan kuersetin secara berturut-turut -4,77; -3,65; -2,29; -2,70; -5,33 dan -2,72 kkal/mol serta nilai RMSD masing-masing turunan flavonol yaitu 1,91; 1,33; 1,98; 1,69; 1,84 dan 1,83 Å. Senyawa turunan flavonol (fisetin, gosipetin, kaemferol, mirisetin, pachypodol dan kuersetin) memiliki interaksi π-alkil dengan Cys145 dan/atau His41 serta interaksi ikatan hidrogen yang dapat menghambat kerja (M^{pro}) SARS-CoV-2. Senyawa turunan flavonol yang dapat berpotensi sebagai inhibitor (M^{pro}) SARS-CoV-2 yaitu pachypodol dengan nilai energi ikat dan RMSD yaitu -5,33 kkal/mol dan 1,84 Å serta memiliki interaksi π-alkil dan ikatan hidrogen dengan Cys145 dan/atau His41.

Kata kunci: covid-19, flavonol, inhibitor, penambatan molekul

MOLECULAR DOCKING STUDY OF THE FLAVONOL DERIVATIVES AS INHIBITOR CANDIDATE OF THE MAIN PROTEASE (M^{pro}) COVID-19

Salsabila Firdausi
17/409488/PA/17795

ABSTRACT

Molecular docking study of flavonol derivatives as candidate inhibitor of main protease Covid-19 has been done. The purpose of this research was to predict several flavonol derivatives as candidates for Covid-19 inhibitors with molecular docking and to study interactions between flavonol derivatives and the main protease (M^{pro}) SARS-CoV-2 as a candidate for Covid-19 inhibitors. This research used 6W63 protein with native ligand X77. The 6W63 protein was re-docked using AutoDockTools-1.5.6. Furthermore, new ligands from flavonol-derived compounds (fisetin, gosipetin, kaemferol, mirisetin, pachypodol and kuersetin) were docked 6W63 protein with AutoDockTools-1.5.6. The results of interactions between proteins and ligands were visualized with Biovia Discovery Studio 2020.

The results from this research showed that the binding energy (ΔG) value fisetin, gosipetin, kaemferol, mirisetin, pachypodol and kuersetin respectively -4.77; -3.65; -2.29; -2.70; -5.33 and -2.72 kcal/mol and the RMSD value of each flavonol derivatives namely 1.91; 1.33; 1.98; 1.69; 1.84 and 1.83 Å. Flavonol derivatives (fisetin, gosipetin, kaemferol, mirisetin, pachypodol and kuersetin) had π-alkyl interactions with Cys145 and/or His41 as well as hydrogen bond interactions that can inhibit the action of (M^{pro}) SARS-CoV-2. Flavonol derivatives that have the potential as an inhibitor (M^{pro}) SARS-CoV-2 are pachypodol with binding energy and RMSD values of -5.33 kcal/mol and 1.84 Å, which also have π-alkyl and hydrogen bond interactions with Cys145 and/or His41.

Keywords: covid-19, flavonol, inhibitor, molecular docking