Simulasi Penambatan dan Dinamika Molekuler Senyawa dari Tumbuhan Anredera cordifolia (Binahong) Terhadap Target Mpro (Enzim Main Protease) Virus SARS-CoV-2 = Molecular Docking and Molecular Dynamics Simulation of Natural Compounds from Anredera Cordifolia (Binahong) to Mpro (Main Protease Enzyme) of SARS-CoV-2

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Abstrak

Penyakit COVID-19 yang merebak di seluruh dunia pada akhir tahun 2019 diakibatkan oleh virus SARS-CoV-2. Penelitian ini membahas simulasi penambatan serta dinamika molekuler dari beberapa senyawa herbal dari tumbuhan Anredera cordifolia (binahong) yaitu procyanidin, metil linoleat, asam oleat dan vitexin dengan protein target (Mpro SARS-CoV-2). Simulasi dinamika molekuler dilakukan selama 20 ns. Selain itu, analisis toksikologi dan farmakologi (ADMET) dilakukan untuk setiap ligan. Hasil simulasi ini dibandingkan dengan ligan kontrol quercetin yang sudah terbukti memiliki interaksi yang baik dengan protein target (Mpro SARS-CoV-2). Hasil prediksi ADMET menunjukkan bahwa semua ligan baik untuk dijadikan obat, kecuali metil linoleat dan asam oleat. Simulasi penambatan molekuler menunjukkan procyanidin serta vitexin memiliki skor penambatan dan binding energy paling baik. Hasil dinamika molekuler juga membuktikan procyanidin, vitexin dan quercetin memiliki nilai RMSD dan RMSF paling baik dan menunjukkan interaksi paling stabil dan kompleks dengan protein target. Sehingga, secara keseluruhan, procyanidin dan vitexin berpotensi untuk menjadi inhibitor Mpro SARS-CoV-2.
.....COVID-19 that spread across the globe at the end of 2019 is caused by the SARS-CoV-2. This virus attacks human respiratory cell. Until now, there is no efficacious drug to treat this disease. This sudy discusses molecular docking and molecular dynamics simulations of four herbal compounds from Anredera cordifolia (binahong), which are procyanidin, methyl linoleate, oleic acid, as well as vitexin with Mpro SARS-CoV-2 as the protein target. The molecular dynamics simulations were carried out for 20 ns. In addition, toxicological and pharmacological analyses (ADMET) were performed for each ligand. The results were compared to quercetin as the control ligand, which has been shown to have good interaction with the protein target. ADMET prediction results show that all ligands are good for use as drugs, except methyl linoleic and oleic acid. Molecular docking simulation results show that procyanidin and vitexin have the docking scores and binding energy scores. The results of molecular dynamics also prove that procyanidin, vitexin and quercetin have the best RMSD and RMSF values and show the most stable as well as complex interactions with target proteins. Thus, procyanidin and vitexin have the potential to be Mpro SARS-CoV-2 inhibitors.