Analisis In Silico Senyawa Tripeptida sebagai Penghambat Reseptor Angiotensin Converting Enzyme 2 (ACE 2) terhadap SARS-CoV-2 = In Silico Analysis of Tripeptides as Angiotensin Converting Enzyme 2 (ACE 2) Receptor Inhibitor against SARS-CoV-2

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Abstrak

Penyakit Coronavirus 2019 (COVID-19) merupakan penyakit pernafasan yang baru ditemukan di Wuhan, China pada akhir tahun 2019. Penyakit ini menjadi pandemik secara global pada Maret 2020. Penyakit COVID-19 disebabkan oleh severe acute repiratory syndrome coronavirus 2 (SARS-CoV-2) yang masuk melalui reseptor angiotensin converting enzyme 2 (ACE 2). Penelitian ini dilakukan untuk mencari kandidat senyawa yang dapat menghambat masuknya SARS-CoV-2 ke dalam tubuh melalui reseptor ACE 2. Penelitian ini menggunakan kandidat senyawa yang berasal dari tripeptida. Metode yang digunakan adalah penapisan virtual menggunakan target molekul dengan ID 6M17 yang didapatkan melalui laman RSCB PDB. Kesimpulan penelitian ini adalah perolehan 8 kandidat senyawa tripeptida dengan energi ikatan yang paling rendah yaitu tripeptida FWW (-9,8 kkal/mol); tripeptida WFF (-9,6 kkal/mol); tripeptida WYY (-9,6 kkal/mol); tripeptida HWW (-9,5 kkal/mol); tripeptida WFW(-9,5 kkal/mol); tripeptida WWT (-9,5 kkal/mol); tripeptida WWY (-9,5 kkal/mol); tripeptida YYW (-9,5 kkal/mol). Hasil dari visualisasi interaksi makromolekul dan ligan, ditemukan 15 residu asam amino yang penting adalah Gln102, Asp206, Glu208, Gly205, Val209, Tyr196, Lys562, Pro565, Ala396, Trp566, Leu95, Val212, Ala99, Asn210, dan Gln98.

.....Coronavirus disease 2019 (COVID-19) is a respiratory disease which found in Wuhan China at the end of 2019. This disease has become a global pandemic at March 2020. COVID-19 caused by a virus called severe acute repiratory syndrome coronavirus 2 (SARS-CoV-2) which enters the body through angiotensin converting enzyme 2 (ACE 2) receptor. This study was conducted to find potential candidates of compounds that can inhibit SARS-CoV-2 entry through ACE 2. This study used tripeptides as the ACE 2 inhibitor candidates. The method used was virtual screening using macromolecular target named ID 6M17 obtained from the RSCB PDB. The result of this study, 8 compound candidates were found to have the lowest binding energy, namely tripeptide FWW (-9,8 kcal/mol); tripeptide WFF (-9,6 kcal/mol); tripeptide WYY(-9,6 kcal/mol); tripeptide HWW (-9,5 kcal/mol); tripeptide WFW (-9,5 kcal/mol); tripeptide WWT (-9,5 kcal/mol); tripeptide WWY (-9,5 kcal/mol); tripeptide YYW (-9,5 kcal/mol). Based on the result of visualization macromolecule and ligand interaction, there are 15 crucial amino acid residues which are Gln102, Asp206, Glu208, Gly205, Val209, Tyr196, Lys562, Pro565, Ala396, Trp566, Leu95, Val212, Ala99, Asn210, dan Gln98.