ABSTRAK

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Program Studi : Farmasi
Judul : Analisis Sel T & Sel B Pada *3-Chymotrypsin-Like Proteinase* SARS-CoV-2 Sebagai Kandidat Vaksin Covid-19: Pendekatan Imunoinformatika

Salah satu langkah paling efektif dalam menangani pandemic COVID-19 yaitu melalui vaksinasi. Berbagai jenis vaksin yang digunakan masih banyak menimbulkan efek samping. Vaksin subunit memiliki keunggulan yaitu hanya menggunakan komponen antigenik dengan penambahan *adjuvant* dan penghubung. *3-Chymotrypsin-Like Proteinase* pada SARS-CoV-2 bertanggung jawab dalam replikasi dan transkripsi virus yang diprediksi memiliki antigenisitas dan berpotensi dijadikan sebagai antigen dalam pengembangan vaksin COVID-19. Penelitian ini bertujuan untuk menentukan urutan epitop dan posisi yang berpotensi sebagai kandidat vaksin COVID-19 melalui pendekatan imunoinformatika. Epitop Sel T Sitotoksik, Sel T Penolong dan Sel B diprediksi menggunakan situs web Vaxijen 2.0, AllerTOP, ToxinPred, NCBI BLAST, ExPasy ProtParam. Seluruh epitop terpilih digabungkan menggunakan linker dan penambahan adjuvant untuk membentuk desain vaksin multi-epitop. Hasil desain protein vaksin dilakukan prediksi struktur sekunder menggunakan PSIPRED dan pemodelan struktur 3D menggunakan GalaxyRefine dan dilakukan analisis molekular *docking* pada TLR3 dengan protein vaksin melalui YASARA dan melihat interaksi menggunakan LigPLot. Desain vaksin multi-epitop terdiri dari 2 epitop sel T sitotoksik QTFSVLACY dan GSVGFNIDY, 2 epitop sel T penolong KSNHNFLVQAGNVQL dan SNHNFLVQAGNVQLR, serta 2 sel B EDMLNPNYEDL dan TANPKTPKYKFVRIQPG. Hasil analisis molekular *docking* menunjukkan bahwa adanya interaksi antara protein vaksin dengan TLR3 yang ditunjukkan dengan adanya ikatan hidrogen.

Kata Kunci: COVID-19, Epitop, Kandidat Vaksin, SARS-CoV-2.

ABSTRACT

Nama : Nurul Maulia
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Judul : Analysis of T Cells & B Cells in *3-Chymotrypsin-Like Proteinase* of SARS-Cov-2 as Covid-19 Vaccine Candidates: An Immunoinformatics Approach

One of the most effective steps in dealing with the COVID-19 pandemic is through vaccination. Various types of vaccines used still cause many side effects. Subunit vaccines have the advantage of only using antigenic components with the addition of adjuvants and linkers. 3-Chymotrypsin-Like Proteinase in SARS-CoV-2 is responsible for viral replication and transcription which is predicted to have antigenicity and has the potential to be used as an antigen in the development of the COVID-19 vaccine. This study aims to determine the epitope sequence and position as a potential candidate for the COVID-19 vaccine through an immunoinformatics approach. Cytotoxic T Cell Epitopes, Helper T Cells and B Cells were predicted using Vaxijen 2.0, AllerTOP, ToxinPred, NCBI BLAST, ExPasy ProtParam servers. All selected epitopes are combined using a linker and the addition of adjuvants to form a multi-epitope vaccine design. The results of the vaccine protein design were carried out by predicting the secondary structure using PSIPRED and 3D structure modeling using GalaxyRefine and molecular docking analysis was carried out on TLR3 with the vaccine protein via YASARA and viewing interactions using LigPLot. The multiepitope vaccine design consisted of 2 cytotoxic T cell epitopes QTFSVLACY and GSVGFNIDY, 2 helper T cell epitopes KSNHNFLVQAGNVQL and SNHNFLVQAGNVQLR, and 2 B cells EDMLNPNYEDL and TANPKTPKYKFVRIQPG. The results of the molecular docking analysis showed that there was an interaction between the vaccine protein and TLR3 as indicated by the presence of hydrogen bonds.

Keywords: COVID-19, Epitope, SARS-CoV-2, Vaccine Candidate.