Prediksi interaksi antibodi-antigen(vaksin) virus H1N1 melalui metode molecular docking secara in silico

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Abstrak

Flu babi H1N1 merupakan salah satu penyakit menular akibat virus influenza tipe A yang telah menjadi pandemik dan mortalitasnya sangat tinggi pada manusia. Salah satu pencegahan penularan penyakit tersebut dengan cara vaksinasi. Mengetahui bagian antigenik (epitope) suatu virus merupakan hal penting untuk merancang suatu vaksin. Beberapa epitope telah diprediksi dari perwakilan protein hemagglutinin (HA), neuramidase (NA), dan matrik 2 (M2). Pendekatan in silico dilakukan melalui kombinasi prediksi pada tahap-tahap respon imun oleh adanya antigen yaitu; proteasomal cleavage (NetChop), Transporter Antigen Processing (TAP) binding (TAPPred), dan Major Histocompatibility complex (MHCPred). Upaya meningkatkan respon imun juga dilakukan dengan memprediksi epitope sel B menggunakan server DiscoTope (conformational epitope) dan BepiPred (sequential epitope). Enam vaksin, yaitu NHM, MHN, HNM, MNH, HMN, dan NMH diperoleh dari 21 kombinasi terbaik epitope sel T dan sel B sebagai representasi variasi allele Human Leukocyte Antigen (HLA) dan protein virus sehingga diharapkan mampu memberikan respon imun. Struktur 3D vaksin diprediksi dan dimodeling menggunakan server CPHModels dan program Swiss-Pdb Viewer (Deep View). Hasil struktur 3D vaksin dievaluasi menggunakan Ramachandran Plot, BLASTp (database PDB virus), dan FeatureMap3D. Vaksin terdiri dari 258 asam amino dan memiliki kesamaan struktur 3D dengan protein dalam database lebih besar dari 50 %. Terakhir dilakukan molecular docking antara vaksin dengan antibodi dalam database diperoleh 14 clustering dengan waktu yang dibutuhkan sekitar 18 detik dan data energi minimum interaksi antibodi dengan vaksin NHM sebesar -13,6859 kkal/mol.

.....Swine flu H1N1 is one of the diseases due to influenza type A virus that has become pandemic and very high mortality to humans. One of the prevention of this disease with a vaccination. Knowing the antigenic (epitope) of a virus is important for designing a vaccine. Some have predicted epitope of representatives from protein hemagglutinin (HA), neuramidase (NA), and matrix 2 (M2). In silico approach was undertaken through a combination of input stages by immune response, namely antigen; proteasomal cleavage (NetChop), Transporter Antigen Processing (TAP) binding (TAPPred), and Major Histocompatibility Complex (MHCPred). An effort to improve the immune response is also conducted to predict the B-cell epitope using DiscoTope (conformational epitope) and BepiPred (sequential epitope) server. Six vaccines (vaccine NHM, MHN, HNM, MNH, HMN, and NMH) are the best combinations of 21 B-cell epitope and T-cell variations in allele representation as Human Leukocyte antigen (HLA) and protein the virus are expected to provide the immune response. The 3D structure and predicted vaccine was modeled by CPHModels program and the Swiss-PDB Viewer (Deep View). The results of 3D structure of vaccines evaluated using the Ramachandran Plot, BLASTp (protein database human - virus GDP), and FeatureMap3D. Vaccines consist of 258 amino acids have a similar 3D structure with protein in the database bigger than 50 %. The last performed molecular docking between vaccines and antibody was found in the database received 14 of clustering with the time needed about 18 seconds and the minimum energy of

antibody interaction with NHM vaccine was -13,6859 kkal/mol.