# Analisis aktivitas epitope netralisasi hemaglutinin virus H5N1 strain non-Indonesia dan Indonesia dengan introduksi antibodi 8H5 menggunakan simulasi dinamika molekuler = Analysis of neutralising epitope activity of a non-Indonesian and an Indonesia H5N1 virus' hemagglutinin introduced with an 8H5 antibody using molecular dynamics simulation

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Abstrak

Sebagai upaya dalam memahami netralisasi virus H5N1 oleh antibodi manusia, simulasi dinamika molekuler dua kompleks antibodi-antigen dilakukan. Tiga struktur molekul yang membentuk dua kompleks tersbeut dibentuk termasuk antigen hemagglutinin Vietnam 2IBX, hemagglutinin Indonesia CDC, dan fragmen variabel dari antibodi 8H5 atau 8H5Fv.

Dalam penelitian ini komplesks 8H5Fv-2IBX dan 8H5Fv-CDC diproduksi melalui pemodelan struktur molekul, homology modeling, dan molecular docking. Dua kompleks tersebut lalu melewati simulasi dinamika molekuler selama 2 nanosekon untuk menginvestigasi kestabilan struktur kompleks dan aktivitas netralisasi yang dapat diamati dengan berfokus pada epitope netralisasi masing ? masing hemagglutinin yang didapatkan hasil molecular docking.

Didapatkan bahwa sifat dinamis atom ? atom pembentuk molekul tidak menihilkan aktivitas netralisasi. Dengan mengamati epitope netralisasi masing ? masing hemagglutinin juga didapatkan bahwa aktivitas netralisasi lebih efektif pada hemagglutinin 2IBX (Vietnam) dibandingkan dengan hemagglutinin Indonesia (CDC) berdasarkan kalkulasi solvent accessible surface (SAS), energi, root mean square displacement (RMSD), dan analisis okupansi ikatan hidrogen.
<hr><i>In an effort to study the H5N1 virus neutralisation by a human antibody, molecular dynamics simulations on two antibody-antigen complexes were conducted. Three molecular structures were formed in this study including the Vietnamese hemagglutinin 2IBX, the Indonesian hemagglutinin CDC, and a variable fragment of the 8H5 antibody or 8H5Fv.

In this study the complexes 8H5Fv-2IBX and 8H5Fv-CDC, that were produced by molecular modeling, homology modeling and molecular docking, was subjected to a 2 nanosecond molecular dynamics simulation each to investigate the stability of such complexes and the maintenance of the neutralising activity that was observed by focusing on the neutralising epitopes that were predicted by molecular docking.

It is was found that the dynamic nature of the molecules in study did not negate the steric hindrance occuring from the antibody variable fragment 8H5Fv with the hemagglutinins, therefore suggesting that the 8H5 antibody should be able to neutralise these two hemagglutinins. By solvent accessible surface (SAS) calculations, energy analysis, root mean square displacement (RMSD) analysis, and also hydrogen bond

occupance it was also found that the the 8H5Fv seem to be more effective against the 2IBX (Vietnamese) hemagglutinin than against the CDC (Indonesian) hemagglutinin.</i>