Analisis pathigenisitas virus Avian Influenza tipe a neuraminidase subtipe 2 (N2) dengan simulasi dinamika molekuler = Molecular dynamic simulation of subtype 2 neuraminidase (n2) of Avian Influenza a virus pathogenicity analysis

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Abstrak

Neuraminidase (NA) memiliki peran penting dalam melepaskan virion yang menggantung pada sialic acid (SA) sel inang sehingga dapat menginfeksi sel inang lainnya dan meningkatkan pathogenisitas virus. Untuk dapat mengetahui lebih dalam tentang pengaruh kontribusi residu fungsional terhadap ikatan antara NA dengan SA dilakukan simulasi permodelan molekuler dengan membandingkan NA Low Paihogenic Avian Influenza (LPAI) A/Mallard/Pennsylvania/10218/84 dan High Paihogenic Avian Influenza (HPAI) A/Tokyo/3/67. Dari penelitian diperoleh energi bebas ikatan NA-SA HPAI dan LPAI sebesar -231.59 kcal/mol dan -350.62 kcal/mol. Analisis okupansi dan energi ikatan menunjukkan bahwa Asp151, Arg152, Glu276, Arg292 dan Arg371 merupakan residu fungsional yang berperan penting pada aktivitas enzimatik NA virus dan berperan besar dalam menentukan pathogenisitas virus. Kemudian dari analisis murasi dikerahui D147G, V1491, I194V, K19911, V2751, I290V, V3031, T346N, Q347P, L370S, S400N, D401N, R4o3W dan K431P memiliki pengamh yang signiikan terhadap kestabilan ikatan di wilayah aktif.

.....Neurciminidcise (NA) has a significant role in releasing virions that are attached to the sialic acid (SA) of the host cells so that the new virions could infect other cells and increasing the virus pathogenicity. To gain insight on the effects of the contribution of the functional residues towards the binding of NA with SA, we conducted a molecular dynamics simulation and compared Low Pathogenic Avian Influenza (LPAI) NA A/Mallard/Pennsylvania/lO2l8/84[l] with High Pathogenic Avian Influenza (HPAI) NA A/Tokyo/3/67[2]. From this study we obtained the binding free energy of the NA-SA HPAI and LPAI with the value of -231.59 kcal/mol and -350.62 kcal/mol respectively. Hydrogen bond occupancy analysis and binding energy showed that Aspl5l, Argl52, Glu276, Arg292 and Arg37l are functional residues that have a significant role on the enzymatic activities of the NA and also have a big responsibility to detennine virus pathogenicity. And then from the mutation analysis it was observed that Dl47G, Vl49I, Il94V, K19911, v2751, 129ov, v3o31, T346N, Q347P, L370S, S400N, D40lN, R4o3w and K43 lP mutations has the most influence on bond stability at the active site.