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Binding mode prediction of 8-hydroxyquinoline derivatives as inhibitors against Dengue Virus NS3 Protease using molecular dynamics simulations

NS3 protease (NS3pro) is an interesting target for discovering the new potent inhibitors of Dengue virus (DENV). The NS3pro is a serine protease consisting of catalytic triad (HIS51, ASP75, and SER135) and expresses role in the step for post-translational cleavage of substrate. Some derivatives of 8-hydroxyquinoline are found as potent NS3pro inhibitors. Molecular dynamics (MD) simulations were applied in order to investigate the structural information of these derivatives in NS3pro. From the results, MD simulations reveal key amino acids for the binding. H-bond interaction to catalytic amino acids (HIS51 and SER135) and H-bonds through other amino acids in NS3pro binding site are also found. Information from the study can indicate the structural effect of 8-hydroxyquinoline derivative during the binding and can use for further analysis in order to improve the activity of DENV inhibitor.

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