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Molecular Interaction Study of *Punica granatum*-Derived Phytochemicals Targeting H1N1 Influenza A Virus Neuraminidase Using Docking Simulations

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Structured Abstract

Background: Influenza viruses often develop resistance to antiviral drugs, requiring constant discovery of new drug sources. By utilising natural resources as a component in the development of the drug to inhibit the virus function, it can provide researchers with more options. Antiviral drugs are created based on the principle of molecular docking which analyse orientation of a molecule that will bind to the specific target site designated. This study explores using *Punica granatum* extract as a natural bioactive component to inhibit viral neuraminidase through molecular docking analysis. The aim is to identify bioactive compounds from *Punica granatum* that can act as ligands and analyse their interactions with neuraminidase using computer software.

Methods: Application software needed for the docking were installed. The ligand files were downloaded from PubChem and the neuraminidase downloaded from Protein Data Bank. The files were converted into pdbqt format using Biovia Discovery. The coordinate and the size of the grid box of the ligand were determined and the information were put in a config file using notepad software. Molecular redocking were carried out of oseltamivir using AutoDock Vina and docking scores were obtained. Next, molecular docking of 20 ligands were carried out followed by the visualisation using PyMol and analysis of the interactions were carried out using AutoDock Tools.

Results: This study shows the distance of rmsd of the oseltamivir and neuraminidase for the redocking process is 0 Å which indicates high similarity between original ligand and downloaded ligand. Next, all 20 ligands were docked into the neuraminidase successfully and the three bioactive compounds with the highest binding affinity are ellagic acid, catechin and delphinidin. The visualisation result shows that ligands were bonded into the neuraminidase. The types of interactions involve in the docking are hydrogen binding, hydrophobic and electrostatic interactions.

Conclusion: In conclusion, the findings of this simulation indicated that the bioactive compounds in *Punica granatum* extract are able to bind to the neuraminidase and inhibit the protein function. The interactions involved has been determined. This shows that components from natural resources can be used an alternative to create antiviral drugs in modern research.

Keywords: Molecular docking, *Punica granatum*, Influenza virus, Neuraminidase, Bioactive compound

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