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Protein-Ligand Docking for Atherosclerosis to Uncover Phytochemicals as Therapeutic Exercise

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Atherosclerosis is one of the primary reasons of the global leading cause of death, cardiovascular disease (CVD), and stroke, the world's second cause of mortality. It is an advancing disease with lipid and fibre accumulation in large arteries. PCSK9 (PDB ID:6U26) has become an attributable target that regulates the pathogenesis of atherosclerosis. Inhibition of PCSK9 significantly diminished the development of atherosclerosis. This study is aimed to discover naturally occurring PCSK9 antagonists as potential drug candidates to treat atherosclerosis. In this study, docking of 102 ligands was performed using Autodock vina 1.2.6 to detect PCSK9 inhibitors from NCBI PubChem database. Through a single config.txt file and *.BAT file, vina docking for multiple ligands was executed. BIOVIA DS was used for the visualization of the receptor-ligand interactions. SwissADME web tool was utilized to categorize and filter potential candidates based on Lipinski's Rule of Five against atherosclerosis and GI absorption for oral administration was evaluated. The docking result of phytochemicals showed Silibinin, Canadin, and Manoalide (-10.7, -10.0, -9.7 kcal/mol) respectively and other 99 compounds (binding affinity ranges from -5.7 to -9.7 kcal/mol). TRP461, VAL 460, PRO 438, and PRO 331 amino acid residues were identified as the most common active sites within the binding pocket of the PCSK9 receptor. The study founds Silibinin, Canadine, Manoalide and most of the compounds respect all drug-likeliness rules and can be used as effective molecules for PCSK9 receptor antagonists based on the docking method. *In vitro* study can be conducted in the future based on this research.

Keywords: **.BAT file, PCSK9, silibinin, vina*