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Virtual screening for potential inhibitors of human hexokinase ii for the development of anti-dengue therapeutics (Review) (Open Access)

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Abstract

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Dengue fever, which is a disease caused by the dengue virus (DENV), is a major unsolved issue in many tropical and sub-tropical regions of the world. The absence of treatment that effectively prevent further viral propagation inside the human 's body resulted in a high number of deaths globally each year. Thus, novel anti-dengue therapies are required for effective treatment. Human hexokinase II (HKII), which is the first enzyme in the glycolytic pathway, is an important drug target due to its significant impact on viral replication and survival in host cells. In this study, 23.1 million compounds were computationally-screened against HKII using the Ultrafast Shape Recognition with a CREDO Atom Types (USRCAT) algorithm. In total, 300 compounds with the highest similarity scores relative to three reference molecules, known as Alpha-D-glucose (GLC), Beta-D-glucose-6-phosphate (BG6), and 2-deoxyglucose (2DG), were aligned. Of these 300 compounds, 165 were chosen for further structure-based screening , based on their similarity scores, ADME analysis, the Lipinski's Rule of Five, and virtual toxicity test results. The selected analogues were subsequently docked against each domain of the HKII structure (PDB ID: 2NZT) using AutoDock Vina programme. The three top-ranked compounds for each query were then selected from the docking results based on their binding energy, the number of hydrogen bonds formed, and the specific catalytic residues. The best docking results for each analogue were observed for the C-terminus of Chain B. The top-ranked analogues of GLC, compound 10, compound 26, and compound 58, showed predicted binding energies of –7.2, –7.0, and –6.10 kcal/mol and 7, 5, and 2 hydrogen bonds, respectively. The analogues of BG6, compound 30, compound 36, and compound 38, showed predicted binding energies of –7.8, –7.4, and –7.0 kcal/mol and 11, 9, and 5 hydrogen bonds, while the top three analogues of 2DG, known as compound 1, compound 4, and compound 31, showed predicted binding energies of –6.8, –6.3, and –6.3 kcal/mol and 4, 3, and 1 hydrogen bonds, sequentially. The highest-ranked compounds in the docking analysis were then selected for molecular dynamics simulation, where compound 10, compound 30, and compound 1, which are the analogues of GLC, BG6, and 2DG, have shown strong protein-ligand stability with an RMSD value of ±5.0 A° with a 5 H bond, ±4.0 A° with an 8 H bond, and ±0.5 A° with a 2 H bond, respectively, compared to the reference molecules throughout the 20 ns simulation time. Therefore, by using the computational studies, we proposed novel compounds, which may act as potential drugs against DENV by inhibiting HKII's activity.

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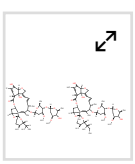
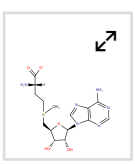
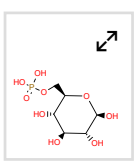
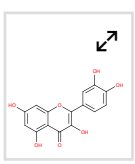
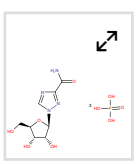
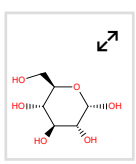

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