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Fatemeh Karimzadeh, Seyed Abbas Mirzaei

Shahrekord University of Medical Sciences, Shahrekord, Iran

Repositioning of FDA-Approved Pharmaceuticals against Epstein–Barr Virus Nuclear Antigen 1 (EBNA1): A Molecular Docking and Molecular Dynamics Study

Epstein-Barr virus (EBV) is known as a malignancy-inducing oncovirus in cancers involving lymphoid and epithelial cells.Currently, there are no FDA-approved anti-EBV drugs on the market. On the other hand, the development of new molecules is a slow process with high costs. One promising strategy that has attracted widespread attention in recent years is the identification of new applications for clinically approved drugs. In this study, based on a review of previous studies, seven compounds identified as being able to block EBNA1-DNA binding were selected and used as templates in SwissSimilarity. Drugs were identified by SwissSimilarity based on their similarity score values to the templates, FDA-approved drugs were selected and then used for molecular docking analysis. A total of 204 drugs were identified based on structural similarity to the introduced patterns, of which 20 FDA-approved drugs were selected. The active binding sites of the EBNA1 protein, as well as the amino acids involved in their formation, were predicted using the online server PrankWeb. The molecular docking results were interpreted, and five ligands with the lowest binding energy (in kcal/mol) and the strongest binding affinity were selected. The stability behavior of selected docked complexes (drugs- EBNA1) was checked using MD simulations. Although some potential compounds related to other diseases have been identified, confirmation of their activity against EBV requires further investigation through in vitro, in vivo, and preclinical studies.

Keywords

Epstein–Barr virus (EBV), Malignancy, Drug repurposing, Molecular docking, MD simulations

Biography

Fatemeh Karimzadeh is presently a Ph.D. candidate in the Department of Medical Biotechnology at Shahrekord University of Medical Sciences. His research project is presently supervised by Prof. Seyed Abbas Mirzaei, focusing on the design of cell-penetrating peptides aimed at enhancing gene transfer using liposome nanoparticles to combat cancer drug resistance.

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