

عنوان مقاله:

Molecular docking and ADME studies of natural compounds against prime targets of HIV

محل انتشار:

یازدهمین همایش ملی و دومین همایش بین المللی بیوانفورماتیک ایران (سال: 1401)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

The human immunodeficiency viruses (HIV) are two species of Lentivirus (a subgroup of retrovirus) that infect humans. They cause acquired immunodeficiency syndrome (AIDS), in which progressive immune system failure allows life-threatening opportunistic infections and cancers to thrive. AIDS is multifaceted, and this underlying complexity hampers its complete cure. The toxicity of existing drugs and the emergence of the multidrug resistant virus worsen the treatment. The development of effective, safe and low-cost anti-HIV drugs is among the top global priority. Exploration of natural resources may give a ray of hope to develop new anti-HIV leads. Among the various therapeutic targets for HIV treatment, reverse transcriptase, protease and integrase receptors is the prime focus. In the present study, we predicted potential plant-derived natural molecules for HIV treatment using a computational approach (molecular docking, in silico ADMET and drug-likeness) to inhibit the effects of HIV. Receptor-ligand binding studies were performed using Schrodinger. Seventeen natural product-based compounds were selected from several natural compounds by pharmacophore screening from the PubChem database and docked against the HIV targets. In this study, the Glide docking program was applied and extra precision (XP) was used. Docking scores revealed that mulberroside A (-9.744, -9.868, -8.958 Kcal/-mol), chlorogenic acid (-11.566, -11.360, -8.406 Kcal/mol) and gallic acid (-7.049, -7.533, -7.193 Kcal/mol) are promising candidates that bind with multi-targets of HIV, while Ca²⁺ic acid, Curcumin, and Silymarin were target-specific candidates. From molecular docking results, we have identified few potent molecules of natural origin against identified targets, which may give new drugs to combat HIV infection after wet lab validation

کلمات کلیدی:

HIV, Molecular Docking, ADMET, Natural Compound

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