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Pharmacophore-based Molecular Docking of Usnic Acid Derivatives to Discover Anti-viral drugs Against Influenza A Virus

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Abstract

For decades, influenza virus infection has been a serious health concern due to seasonal epidemics and pandemics, and it is continuing on the rise today, yet there is no gold-standard medication available for treating influenza viral infection. As a result, better influenza medicine is necessary to prevent illness. The purpose of this work was to investigate how effective usnic acid derivatives were as antiviral medications against the influenza virus in a computational approach. To discover the prospective medication as an anti-influenza agent, we employed pharmacophore-based molecular docking, ADMET, and drug-likeness studies, CYP isoform analysis and MD simulation approaches. Using pharmacophore filtering processes, twenty-three (23) usnic acid derivatives were acquired from an in-house database of 340 usnic acid derivatives. A docking simulation on the Influenza A H1N1 polymerase resulted in four molecules with a high affinity for the protein. The pharmacokinetics and drug-likeness predictions yielded two hit compounds, which were then subjected to cytochrome P450 enzyme screening to provide the lead molecule, denoted as compound-4. In addition, MD simulation of lead compound (Compound-4) was performed to verify the stability of the docked complex and the binding posture acquired in docking experiments. The findings revealed that compound-4 is a promising option for antiviral treatment of influenza illness in the future. © 2023 Marmara University Press.

Author Keywords

Influenza; MD Simulation; Molecular docking; Pharmacophore; Usnic acid

Index Keywords

cytochrome P450, usnic acid; antiviral activity, antiviral therapy, Article, crystal structure, human, Influenza A virus, Influenza A virus (H1N1), molecular docking, molecular dynamics, nonhuman, pharmacophore, prediction, protein structure, structure activity relation

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