Virtual screening of *Carica papaya L*. extracts: Identifying multi-target lead molecules against SARS-CoV-2.

Shahid Jah*

Department of Pharmaceutical Sciences, University of Toronto, Toronto, Canada

Received: *29 January, 2024, Manuscript No. AJPTI-24-130380;* ***Editor assigned:*** *31 January, 2024, Pre QC No. AJPTI-24-130380 (PQ);* ***Reviewed:*** *14 February, 2024, QC No. AJPTI-24-130380;* ***Revised:*** *21 February, 2024, Manuscript No. AJPTI-24-130380 (R);* ***Published:*** *28 February, 2024.*

Accepted on 25th February, 2024

Description

The ongoing COVID-19 pandemic, caused by the Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2), has prompted an urgent need for effective treatments. Traditional medicinal plants have long been a source of bioactive compounds with therapeutic potential. *Carica papaya L*., commonly known as papaya, is one such plant known for its diverse pharmacological properties. In this essay, we explore the identification of lead molecules against multiple targets of SARS-CoV-2 from *Carica papaya L*. through *In-Silico* methods.

Introduction: The emergence of SARS-CoV-2 has led to an unprecedented global health crisis, highlighting the importance of developing effective antiviral therapies. Traditional medicinal plants offer a vast reservoir of bioactive compounds that can potentially inhibit viral replication or alleviate symptoms associated with viral infections. *Carica papaya L*., a widely cultivated tropical fruit, has been traditionally used in various medicinal preparations due to its broad spectrum of pharmacological activities, including antimicrobial, anti-inflammatory, and immunomodulatory effects.

In-Silico methods, also known as computational or computer-aided drug design, play a crucial role in modern drug discovery by facilitating the rapid and cost-effective screening of large chemical libraries for potential drug candidates. These methods utilize computational algorithms and molecular modeling techniques to predict the interaction between small molecules and biological targets, thereby identifying lead compounds with therapeutic potential. In the context of SARS-CoV-2, *In-Silico* methods have been instrumental in the search for novel antiviral agents. SARS-CoV-2 infects host cells through the binding of its spike (S) protein to the Angiotensin-Converting Enzyme 2 (ACE2) receptor on the surface of human cells. Additionally, several other viral proteins, such as the Main Protease (Mpro) and RNA-dependent RNA polymerase (RdRp), are essential for viral replication and transcription. Targeting multiple viral proteins simultaneously can enhance the efficacy of antiviral therapies and reduce the likelihood of drug resistance. Therefore, identifying lead molecules that can interact with multiple targets of SARS-CoV-2 is crucial for developing effective treatments.

Carica papaya L. is rich in bioactive compounds, including flavonoids, alkaloids, terpenoids, and phenolic compounds, which possess diverse pharmacological activities. Several studies have reported the antiviral properties of papaya extracts against a range of viruses, including dengue virus, herpes simplex virus, and human immunodeficiency virus (HIV). These antiviral effects are attributed to the presence of bioactive compounds that inhibit viral replication or modulate host immune responses. *In-Silico* screening involves the virtual screening of compounds from natural sources against specific drug targets using molecular docking simulations and other computational techniques. By analyzing the binding interactions between compounds and target proteins, potential lead molecules can be identified based on their predicted binding affinities and pharmacological properties. In the case of SARS-CoV-2, molecular docking studies have been conducted to screen natural compounds for their ability to inhibit viral proteins, such as the S protein, Mpro, and RdRp.

Conclusion

The identification of lead molecules against multiple targets of SARS-CoV-2 from *Carica papaya L*. through *In-Silico* methods represents a promising approach to drug discovery. By harnessing the diverse pharmacological properties of papaya bioactive compounds, such as flavonoids and alkaloids, novel antiviral agents can be developed to combat COVID-19. However, further experimental validation, including *in vitro* and *in vivo* studies, is required to confirm the efficacy and safety of these lead molecules. Nevertheless, the integration of *In-Silico* screening with traditional medicinal plant research holds great potential for accelerating the discovery of effective treatments for emerging viral infections like COVID-19. In summary, the use of *In-Silico* methods to identify lead molecules against SARS-CoV-2 targets from *Carica papaya L*. underscores the importance of interdisciplinary approaches in drug discovery. By leveraging computational techniques and traditional medicinal plant knowledge, researchers can expedite the search for novel antiviral therapies, ultimately contributing to the global efforts to combat the COVID-19 pandemic.

***Correspondence to:**

Feng Jun

Department of Pharmacy,

University of California,

San Francisco, USA

E-mail: jungeng@uofc.edu

Citation: *Jah S. Virtual screening of Carica papaya L. extracts: Identifying multi-target lead molecules against SARS-CoV-2. AJPTI 2024;12 (46):1*