Perspective

iMedPub Journals
www.imedpub.com

American Journal of Computer Science and Information Technology
ISSN 2349-3917

2022
Vol.10 No.9:004

Computational Molecular Docking As a Virtual Design Strategy for Treating Ebola

Yujun Cui*

Department of Computer Science, School of Software, Tsinghua University, Beijing, China

***Corresponding author:** Yujun Cui, Department of Computer Science, School of Software, Tsinghua University, Beijing, China Email: yunjuncui34@yahoo.com

Received date: August 05, 2022, Manuscript No. IPACSIT-22-15005; **Editor assigned date**: August 08, 2022, PreQC No. IPACSIT-22-15005 (PQ); **Reviewed date**: August 17, 2022, QC No IPACSIT-22-15005; **Revised date:** August 25, 2022, Manuscript No. IPACSIT-22-15005 (R); **Published date:** September 06, 2022, DOI: 10.36648/ 2349-3917.10.9.4

Citation: Cui Y (2022) Computational Molecular Docking As a Virtual Design Strategy for Treating Ebola. Am J Compt Sci Inform Technol Vol. 10 Iss No.9:004.

Description

The Ebola virus, also known as EBOV, is a deadly human pathogen that is responsible for a severe form of hemorrhagic fever. Ebola Virus Disease (EVD) is caused by the EBOV infection. Ever since the EVD outbreak in 2014, it has remained the most common viral infection. Unfortunately, there are currently no antiviral medications available for EVD treatment. A surface trans membrane Glycoprotein (GP) that is acquired from infected cells during assembly is present in Ebola virions and is necessary for the viruses' binding to target cells and subsequent fusion with host-cell membranes. Spikes on the viral envelope are only produced by a single structural protein, the viral-surface trimeric GP. The GP1 (GP1EBOV) and GP2 (GP2EBOV) subunits of the trimeric GP are linked by a disulfide bond.GP1EBOV is responsible for binding receptors, whereas GP2EBOV is responsible for mediating the fusion of EBOV with the host cell membrane. A six-helix bundle formed by C-terminal coiled-coil regions (C-heptad repeat regions) on the surface of the virus-like particles is the central feature of the GP2EBOV ectodomain's pre-fusion structure. Previous research independently produced crystal structures of the GP that include the GP2EBOV ectodomain in the presumed post-fusion conformation. These two structures' GP2EBOV ectodomain regions are in good agreement and revealed a number of distinct helical bundle characteristics. An intermolecular disulfide bond stabilizes the short helix-turn-helix motif that connects the GP2EBOV C-terminus coiled-coil regions. Moreover, the C-end wound loop locale is exceptionally monitored across the four kinds of EBOV.

Multiple Recognition Surfaces or Targeting Binding

RNA oligonucleotides that are able to bind to specific targets with high affinity are referred to as RNA aptamers. The majority of aptamers bind micro- or macromolecules, intact cells, viruses, and single-stranded DNA or RNA molecules with 20–90 bases. These single-stranded oligonucleotide sequences are capable of folding into a variety of secondary structures, such as stem loops, pseudo knots, kinks, bulges, double-stranded DNA (dsDNA), and so on. As a result, they provide multiple recognition surfaces for targeting binding. Chemical modifications can be used to increase the *in vivo* half-life of RNA aptamers, which are small oligonucleotides (usually 20–50 base pairs) that specifically bind with high affinity to proteins or small target molecules that are not immunogenic. New neutralization sites can be identified with the assistance of smaller ligands like aptamers, which can get to surfaces that antibodies cannot reach. Therefore, RNA aptamer binding to the C-terminal of GP2EBOV's coiled-coil region may prevent virus fusion with cell plasma membrane; thereby prevent the virus from entering permissive cells. According to previous research, aptamers successfully inhibit HIV replication by binding to the same region of the HIV-1 TM protein. These inhibitors are a component of the clinically prescribed HIV-1 antivirals.

Vaccination Straegies and Identify Potential EBOV GP Sites

For instance, V-1 Fire up protein contains 10 arginine buildups in its 34 to 50 piece. Similar to the full-length protein, the Rev Responsive Element (RRE) RNA IIB hairpin is bound by a 17-residue peptide that contains four arginine residues essential to defining specificity. Additionally, the C-heptad repeating region of GP2EBOV, which is thought to be unstructured and accessible in the pre-fusion GP structure, is highly conserved across the four strains of EBOV. Because this region of the protein is located extracellularly on both virions and infected cells, aptamers have ready access to the targeted regions of the protein, making the GP2EBOV an excellent target for them. EBOV-fighting compounds could be found using computational molecular docking as a virtual design strategy. Using molecular dynamics simulations, we created and improved RNA aptamers that were able to bind to a peptide derived from the C-terminus of GP2EBOV.After that, molecular docking using auto-dock was used to measure the interaction between the designed orthogonal RNA aptamers and GP2EBOV, where the simulated structure of GP2EBOV was based on a GP structure that had been reported. The RNA aptamers we planned have high partiality to the C-terminal helix area of GP2EBOV, accordingly had the option to additionally enhance the focusing of GPs. This study aims to provide vaccination strategies and identify potential EBOV GP sites that could be targeted by small molecule drugs. Innovative experimental methods could also be applied to other serious emerging viruses like Lassa and Nipah in future research.