A Study of the Complex of Human Protein IRF3 and Viral Protein (SARS-CoV-2) ORF7a

Shelke, Suneha (School: Sylvania Northview High School)

COVID-19 and its several strains caused millions of infections and deaths worldwide, making it vital to understand how the virus interacts with human cells. Determining binding site locations is a crucial first step in developing effective treatments. Studies can be performed in-vitro (experimentation occurring outside a living organism) or in-silico (experimentation through computer programs). This study used in-silico methods to speed up the process by using protein docking softwares to reduce the area of each protein that must be searched to determine (or rule out) binding sites. SWISS-MODEL was used to convert the amino acid sequences of both IRF3 and ORF7a to a .pdb file. These files were then entered into ZDOCK, which generated the top 10 predicted complexes of the two proteins. Next, the top predictions were entered into VMD, allowing the sequences and where they correlate on the 3D model to be viewed. The amino acids that corresponded to potential binding sites were selected and recorded. The top prediction complexes were then entered into PRODIGY, which determines the binding affinity of each complex. By obtaining likely binding site locations from top predicted complexes, future in-vitro studies can confirm the accurate binding site. The interaction location is essential for future studies where a protein or drug can be added to this site to weaken the interaction of the human-viral complex. If this interaction can be weakened, life-threatening symptoms of COVID-19 could be reduced or the manifestation of this virus could be entirely inhibited in the first place.

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