UNIVERSITY GRADUATE SCHOOL BULLETIN

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Florida International University

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Doctoral Dissertation Defense

Abstract

In-Silico Identification of Vaccine Candidates Against Viral Infections

by

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There are many viral diseases without effective treatments or vaccines. A critical step in the immune system fight against viruses involves an immunological protein molecule binding to a viral protein molecule. I investigate the atomic and molecular details of binding site recognition and binding interactions and dynamics for three important viruses.

An epitope is the part of an invading antigen molecule that is the site for antibody binding. In-silico identification is a powerful tool to facilitate the identification of potential epitope candidates and can decrease the time and expense spent on validation experiments. I employed several epitope computational prediction methods that are based upon the antigen protein’s amino acid sequence and conformation for the glycoprotein of the Lassa virus as well as for different proteins of the Marburg virus. The predicted epitopes are further filtered based on a consensus approach that resulted in the identification of new epitopes that have not yet been tested experimentally. I performed molecular dynamics computational simulations on the most promising epitopes to determine atomic-level details of the epitope’s interactions and dynamics.

In addition, I performed MD simulations to investigate the dynamics and antibody evasion behavior by the B.1.617.2 (delta) variant of SARS-CoV-2. I found that the receptor-binding β-loop-β motif in the spike protein adopts an altered conformation that causes binding difficulty for some of the neutralizing antibodies that were generated against the original corona virus strain. This study reflects the possible mechanism for the immune evasion exhibited by the delta variant.

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