Tea Freedman-Susskind

PI Mentor: Dr. Vanessa Jonsson

PhD Mentor: Natalie Dullerud

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Abstract

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To develop effective strategies to combat the current pandemic caused by the SARS-CoV-2 virus, it will be necessary to have a thorough understanding of possible viral mutations as well as avenues to enhance antibody neutralization. A robust non-experimental technique to evaluate the impact of potential mutations would be a substantial addition to this vital body of knowledge. Here we attempt to predict the effect of mutations on antibody neutralization of SARS-CoV-2 using computational chemistry and machine learning techniques. Mutation stability was calculated using FoldX energy minimization software and analysis developed in Python scripts. Analysis of this data is expected to yield insights into how mutation impacts binding stability as well as support the modeled ΔΔ G with in vivo data. Preliminary results indicate multiple locations of interest where the stability of the bound complex is drastically decreased and could indicate an escape mutation for the RBD from an antibody. These results would inform the search for optimized antibody-based approaches to combating SARS-CoV-2, and validate a relatively fast computational strategy to examine viral fitness after mutations.