Abstract Submitted
for the OSF20 Meeting of
The American Physical Society

Study on Antiviral Agents Using Theoretical and Computational Simulations: Potential of Synthetic and Non-synthetic Drugs to Treat Virus Infection RICHARD KYUNG, MAXIMILLIAN CHEVAL, CRG-NJ — In this project, we assessed the thermodynamical and stereochemical properties of several types of drugs that can be used for virus treatment. An open-source molecular editing program equipped with an auto-optimization feature was used for the analysis. Commercial synthetic drugs and antibiotics produced in nature by plants were studied to model, optimize, and compare the resulting molecular optimization energies of the derivatives. To define the efficiencies of the antibiotics, this research focused on calculating the optimized energy, finding the dipole moment which is caused by different values of electronegativity of different atoms in a molecule and obtaining electrostatic potential map diagram that shows any charge-related details of a molecule. Optimization configurations were collected in order to compare each chemical compound's stability. This research focused on the antiviral effects of synthetic and non-synthetic drugs to treat virus infection and their therapeutic potential against severe acute respiratory syndrome using theoretical and computational simulations.

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Date submitted: 25 Sep 2020 Electronic form version 1.4