

## Molecular Dynamics Analysis of the HIV-1 Protease Enzyme

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The World Health Organization estimates that there are 34 million people living with HIV. In 2010, 2.7 million people were newly infected. The HIV protease is an essential protein that cleaves three previral polyproteins necessary for the maturation of the HIV virus. Because the HIV virus mutates at a rapid pace, it reduces the effectiveness of many inhibitors. This project sought to understand the dynamics of the HIV-1 protease enzyme through the use of long time scale molecular dynamics using the highly efficient DESMOND molecular dynamics package. Conformational results will be presented including the rate at which simulations sampled the “closed,” “semi-open,” “open” and “wide-open” states. These results shed further light on the dynamics of this important protein.