The Efficacy of HIV-1 Protease Inhibitors on HIV-2 Protease

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There are two types of HIV: HIV-1, which is responsible for majority of the infections globally occurring, and HIV-2, which is accounts for a smaller fraction of infections, and is more so confined within West Africa. Due to its predominance, antiviral drug design has generally focused on the inhibition of HIV-1, whereas only a limited number of studies consider HIV-2. Here we use computational methods to investigate the relative effectiveness of HIV protease inhibitors, all designed and tested against HIV-1, on both HIV-1 and HIV-2 proteases. In addition, we are using molecular dynamics (MD) and computational docking to compare relative calculated affinities of the eleven FDA-approved HIV protease inhibitors for HIV-1 with HIV-2. From this project, we hope to gain insight of the receptor-ligand interactions that differentiate HIV-2 from HIV-1 protease inhibition. Our long-term goal is to optimize the FDA approved inhibitors for HIV-2.