Docking HIV-1 Protease Inhibitors into the HIV-2 Protease

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A significant effort has been expended understanding the behavior of HIV-1; however, studies of HIV-2, isolated from AIDS patients in Africa, are far more limited. A series of drugs have been designed to inhibit the cleavage of polypeptide chains within the protease of the HIV-1 retrovirus but very little has been published describing small molecules that inhibit the HIV-2 protease. This work attempts to answer questions such as "Do inhibitors designed for HIV-1 bind similarly to HIV-2?" "Can HIV-1 drugs be modified so as to more effectively inhibit HIV-2?" To this end, we have performed docking studies of small molecule drugs, developed to inhibit the HIV-1 protease, against the HIV-2 protease target. The docking algorithm, as implemented in Glide, allows rigid and flexible docking as well as a variety of scoring schemes. Results with these different protocols will be compared.