

## **Configuring Glide Docking Algorithms using HIV-1 Protease Inhibitors**

Jeanice Brown and Carol Parish

*Department of Chemistry, University of Richmond*

*Richmond, VA 23173*

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, tests have been run to first identify the specific settings of Glide necessary to accurately simulate the docking of HIV-1 Protease Inhibitors into the HIV-1 Protease. Once Glide has been configured to reproduce experimentally determined binding affinity rankings of the inhibitors, HIV-1 Inhibitors will be docked against the HIV-2 target. Results of G-Score rankings from varying parameters will be compared, along with Superimposition of Glide generated poses and crystal structures of each inhibitor.