

**Analyzing Conformational Search Results of HIV-1 Protease Inhibitors:
Force Field Analysis**

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The ultimate goal of a conformational search process is to extract all low energy structures from the Potential Energy Surface (PES) generated by specific force fields. A force field is a collection of molecular mechanics equations and parameters that conceptually account for molecular motion. An accurate force field is the key to generating a good PES and, therefore, is the root to acquiring good conformational search results. However, only through further analysis and examination of the results obtained do numbers become meaningful. This particular analysis seeks to focus on the validity of the newly developed OPLS_2005 force field using conformational search results of selected HIV-1 protease inhibitors. The conditions of conformational searching were as follows: 50:50 Monte Carlo/Low Mode sampling, GB/SA water as solvent, and OPLS_2005 force field employed. The resulting low-energy conformations were then compared and analyzed by superimposition of ensembles with experimental crystal structures along with quantum mechanical minimization validation.