Molecular Dynamics Analysis of Potential Inhibitors of HIV-1 Protease

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C_{60} fullerene has been shown to inhibit the HIV-1 protease through interactions with its active site. However, the low solubility of Buckminister fullerene in water limits the ability of C_{60} to act as viable protease inhibitors in the human body. This work utilizes the MMFF force field along with the GBSA solvent model for water to perform stochastic dynamics simulations to model the energetics and interactions of potential HIV-1 protease inhibitors that are similar to C_{60} fullerene, but more soluble in water. In addition, the program Maestro was utilized to determine and compare the physical characteristics, such as surface area, of C_{60} and the potential inhibitors.