Comparing the Molecular Properties of HIV-1 Protease Inhibitors Drugs

Kendra Cunningham and Carol Parish
Department of Chemistry, University of Richmond
Richmond, VA 23173

Computer modeling was used to understand the molecular properties of eleven potent HIV protease inhibitors: Amprenavir, Atazanavir, Indinavir, Lopinavir, Nelfinavir, Saquinavir, Ritonavir, JE-2147, Tipranavir, TMC-126 and Darunavir. Low energy structures for each inhibitor were identified by exhaustive conformation scans of the OPLS2550/GBSA(water) surface and subsequently subjected to further geometry optimization using B3LYP/6-31G*. The volume, solvent accessible surface area (SASA) and electrostatic potential energy maps were calcuated for each inhibitor and compared.