Drug-Design Investigations using POSS as a Potential HIV Protease Inhibitor

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During the HIV life cycle, HIV Protease cleaves the Gag-Pol polyprotein in order to form new HIV virions. This discovery has led to a great impetus for drug discovery in order to prevent the replication of the HIV retrovirus. Throughout the past decades, 11 FDA protease inhibitor drugs have been approved for public use. This project examines the applications of Polyhedral Oligomeric Silsesquioxane (POSS) - a synthetic nanostructured hybrid chemical comprised of Oxygen, Silicon, and Hydrogen atoms - as a potential inhibitor by using computational methods to study binding affinity. POSS provides a novel approach to Protease Inhibitors due to its unique structure and solubility. Various R group side chains were attached to POSS in order to determine the structural efficacy it has with binding to the active site. Molecular Dynamic simulations were performed to run calculations using AMBER14 with the AMBERffSB force field on the HIV Protease. Gaussian was used to derive values to parameterize POSS.