HIV Capsid Structure Defined

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For the first time, scientists have identified the precise atomic structure of the HIV capsid, which is the container of genes the virus inserts into human immune cells. This discovery, which was aided by the powerful Blue Waters supercomputer at the University of Illinois at Urbana-Champaign, may help in the development of new HIV therapies that would attack the capsid. Since this would be a novel approach to fighting HIV, such therapies would hold promise for people resistant to other classes of drugs.

After using Blue Waters' computational power to aid in defining the atomic structure of the capsid, the researchers ran a simulation through the computer of how the capsid would behave in organic situations.

"When you know the chemical nature of [the capsid] you can [attack it] in a more rational, guided way," says Klaus Schulten, PhD, a physics professor at the university, who headed up the study. "Now we can guide the development of new drugs."

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http://beta.docker.poz.com/article/hiv-capsid-structure-24346-1817