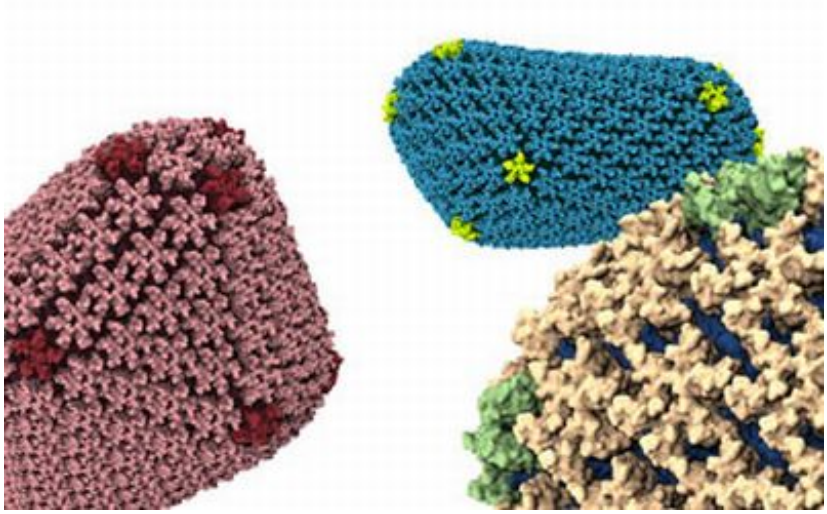
Scientists Crack the Code of HIV, Provide an Up-Close View



Three different renderings of the HIV capsid, with multiple colors. Image courtesy of the Theoretical and Computational Biophysics Group, Beckman Institute for Advanced Science and Technology, UIUC

Researchers have determined the precise chemical structure of the HIV capsid, a protein shell that protects the virus's genetic material and is a key to its ability to infect and debilitate the human body's defense mechanism. Detailed simulations were achieved with the use of a supercomputer on a 64 million atom sample. The capsid has become an attractive target for the development of new antiretroviral drugs that suppress the HIV virus and stop the progression of AIDS. The research paper describing these results is the cover story of this week's journal Nature (May 30, 2013).

This discovery was enabled by a recently-dedicated, new supercomputer called Blue Waters, one of the world's most powerful computers. Until the arrival of petascale supercomputers, scientists were unable to decipher in atomic-level detail the entire HIV capsid--an assemblage of more than 1,300 identical proteins forming a cone-shaped structure. The simulations that added the missing pieces to the puzzle were conducted during testing of Blue Waters at the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign (UIUC).

"The sustained petascale performance of Blue Waters is precisely what enabled these talented researchers to explore new methods combined with structural and electron microscopy data to reliably model the chemical structure of the HIV capsid in great detail," says Irene Qualters, NSF program manager for advanced cyberinfrastructure. "This knowledge will allow researchers to infiltrate that membrane with HIV-fighting drugs."

Source: National Science Foundation