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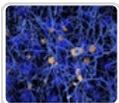
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First atomic-scale view of inte capsid and host protein cyclo

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A new study offers the first atomic-scale view of an the protein coat that shepherds HIV into the nucleu known as cyclophilin A. This interaction is key to HI

A paper describing the research appears in the jour

Cyclophilin A is found in most tissues of the human inflammatory response, immunity and the folding a it fails to work properly or is overproduced in cells, diseases such as rheumatoid arthritis, asthma, can facilitates some viral infections, including HIV.

"We have known for some time that cyclophilin A p University of Illinois physics professor Klaus Schulte postdoctoral researcher Juan R. Perilla and Universi Zhang and postdoctoral researcher Chuang Liu.

The HIV capsid somehow tricks this cellular protein transits through the cell and makes its way to the r capsid interacts with a nuclear pore that offers an e virus uses the pore as a channel to inject its geneti commander the cell.

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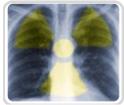
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Studies in cell culture have found that the virus can disguise itself as cyclophilin. Drugs that interfere with cyclophilin cannot be used in human HIV treatment because they would suppress the immune response.

In the new study, the researchers used a massive computer simulation which they developed in a 2013 study. Building this model of the interactions of 64 million atoms, a feat that required a supercomputer at the National Center for Supercomputing Research Center.

For the new study, the team used Blue Waters as well as the Ridge National Laboratory to simulate the interaction between the virus and cyclophilin. The 3-D structure of cyclophilin A was known from X-ray crystallography studies.

"We knew every atom of the underlying capsid, and then we put the cyclophilin on top of that, of which we also knew every atom," Schulten said.

The simulations revealed that cyclophilin A binds to the capsid in two ways. First, there is the "classic" binding site, one revealed decades earlier in crystallography studies. But in some places, a single cyclophilin A protein also bound the capsid at a second site, forming a bridge between two hexamers. (The HIV capsid is made up of a lattice of pentamers.) Cyclophilin's bridging behavior occurred only when the capsid was fully occupied, the researchers found.

Further research with NMR spectroscopy, which can corroborate the existence of a second binding site.

By varying the amount of cyclophilin A added to the simulation, the researchers also saw that cyclophilin did not compete for binding sites at high concentrations, individual cyclophilin molecules attached to the capsid, disrupting their ability to bind.

Laboratory experiments also showed that having too much cyclophilin interfered with the virus's ability to infect cells.

"What we think is happening is, where there is no cell, the virus can't recognize it and trigger a process that destroys the cell. If the capsid is fully occupied by cyclophilin A, it prevents the virus from forming a complex. So there is an optimal amount of cyclophilin that allows the virus to infect cells."

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allows the HIV infection to go forward."

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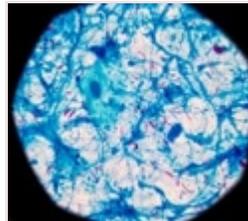
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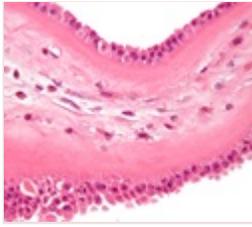


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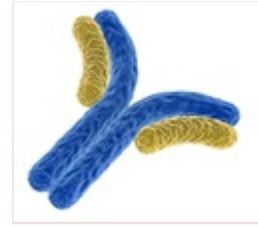
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