

Researchers Just 'Hacked' HIV with Supercomputer Help

Figure this: in 1928, the biologist Alexander Fleming took a vacation, leaving behind a petri dish full of staph bacteria. When he returned, Fleming found a dish full of not bacteria, but blue-green mold secreting what he later identified as penicillin. The penicillin had killed off the staph, and, soon after, the world was a very different place.

That's an oversimplification, of course, but the point is that Fleming more or less stumbled into a drug that would eliminate one of the biggest killers on Earth: bacterial infections. Contrast this with HIV, a disease so advanced there should be another word for it beyond "disease." Some three decades later, with research capabilities Fleming couldn't have dreamed of, we've managed only to minimize the disease's risk.

That minimization (through highly active antiretroviral therapy) is actually a massive accomplishment that's saved many, many lives, but it isn't a cure. And the contrast between one guy's luck and the research army of the post-industrial world is kinda fascinating. And it might even be the case that it took a supercomputer to unlock HIV (not kill it, just decode its armor), according to [a report](#) in last week's edition of *Nature*. Given that the problem of finding a way through the HIV virus' protein shell involves a sampling of 64 million atoms, it shouldn't be too surprising that the resources of the [Blue Waters](#) supercomputer, one of the world's most powerful, were called upon for the National Science Foundation-led research.

That research was indeed successful and we now have a map of the precise chemical structure of HIV's protein shell (aka its capsid). This is crucial. "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, in a statement. "This knowledge will allow researchers to infiltrate that membrane with HIV-fighting drugs."

The research also involved cryo-electron microscopy; Blue Waters is hardly the only technological marvel at work. Actually, with the technology available in 1928, it's doubtful Fleming or anyone else would have actually identified HIV at all. It took two years, 1981 to 1983, to make it from generic/unknown immuno-deficiency to "some kind" of virus, and that was in the relative science-fiction of modern medicine.

Reach this writer at michaelb@motherboard.tv.