

Gamers succeed where scientists fail: Molecular structure of retrovirus enzyme solved

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Gamers have solved the structure of a retrovirus enzyme whose configuration had stumped scientists for more than a decade. The gamers achieved their discovery by playing Foldit, an online game that allows players to collaborate and compete in predicting the structure of protein molecules.

After scientists repeatedly failed to piece together the structure of a protein-cutting enzyme from an AIDS-like virus, they called in the Foldit players. The scientists challenged the gamers to produce an accurate model of the enzyme. They did it in only three weeks.

This class of enzymes, called retroviral proteases, has a critical role in how the [AIDS virus](#) matures and proliferates. Intensive research is under way to try to find anti-AIDS drugs that can block these enzymes, but efforts were hampered by not knowing exactly what the retroviral [protease](#) molecule looks like.

"We wanted to see if human intuition could succeed where automated methods had failed," said Dr. Firas Khatib of the University of Washington Department of Biochemistry. Khatib is a researcher in the [protein structure](#) lab of Dr. David Baker, professor of biochemistry.

Remarkably, the gamers generated models good enough for the researchers to refine and, within a few days, determine the enzyme's

structure. Equally amazing, surfaces on the molecule stood out as likely targets for drugs to de-active the enzyme.

"These features provide exciting opportunities for the design of retroviral drugs, including [AIDS drugs](#)," wrote the authors of a paper appearing Sept. 18 in *Nature Structural & Molecular Biology*. The scientists and gamers are listed as co-authors.

This is the first instance that the researchers are aware of in which gamers solved a longstanding scientific problem.

Fold-it was created by computer scientists at the University of Washington Center for Game Science in collaboration with the Baker lab.

"The focus of the UW Center for Game Sciences," said director Dr. Zoran Popovic, associate professor of computer science and engineering, "is to solve hard problems in science and education that currently cannot be solved by either people or computers alone."

The solution of the virus enzyme structure, the researchers said, "indicates the power of online computer games to channel human intuition and three-dimensional pattern matching skills to solve challenging scientific problems."

With names like Foldit Contenders Group and Foldit Void Crushers Group, the gamer teams were fired up for the task of real-world molecule modeling problems. The online protein folding game captivates thousands of avid players worldwide and engages the general public in scientific discovery.

Players come from all walks of life. The game taps into their 3-D spatial abilities to rotate chains of amino acids in cyberspace. New players start

at the basic level, "One Small Clash," proceed to "Swing it Around" and step ahead until reaching "Rubber Band Reversal."

Direct manipulation tools, as well as assistance from a computer program called Rosetta, encourage participants to configure graphics into a workable protein model. Teams send in their answers, and UW researchers constantly improve the design of the game and its puzzles by analyzing the players' problem-solving strategies.

Figuring out the shape and misshape of proteins contributes to research on causes of and cures for cancer, Alzheimer's, immune deficiencies and a host of other disorders, as well as to environmental work on biofuels.

Referring to this week's report of the online gamers' molecule solution opening new avenues for anti-viral drug research, Carter Kimsey, program director, National Science Foundation Division of Biological Infrastructure, observed, "After this discovery, young people might not mind doing their science homework. This is an innovative approach to getting humans and computer models to 'learn from each other' in real-time."

The researchers noted that much attention has been given to the possibilities of crowd-sourcing and game playing in scientific discovery. Their results indicate the potential for integrating online video games into real-world science.

Dr. Seth Cooper, of the UW Department of Computing Science and Engineering, is a co-creator of Foldit and its lead designer and developer. He studies human-computer exploration methods and the co-evolution of games and players.

"People have spatial reasoning skills, something computers are not yet good at," Cooper said. "Games provide a framework for bringing

together the strengths of computers and humans. The results in this week's paper show that gaming, science and computation can be combined to make advances that were not possible before."

Games like Foldit are evolving. To piece together the retrovirus [enzyme](#) structure, Cooper said, gamers used a new Alignment Tool for the first time to copy parts of known [molecules](#) and test their fit in an incomplete model.

"The ingenuity of game players," Khatib said, "is a formidable force that, if properly directed, can be used to solve a wide range of scientific problems.

According to Popovic, "Foldit shows that a game can turn novices into domain experts capable of producing first-class scientific discoveries. We are currently applying the same approach to change the way math and science are taught in school."

Provided by University of Washington

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