

Gamers helping in Ebola research

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Months before the recent Ebola outbreak erupted in Western Africa, killing more than a thousand people, scientists at the University of Washington's Institute for Protein Design were looking for a way to stop the deadly virus.

For inspiration, they turned to an unlikely source: gamers.

Specifically, they asked thousands of computer game enthusiasts worldwide to tackle an Ebola puzzle on the interactive game Foldit, a 6-year-old project that encourages people to solve puzzles for science.

Some of those solutions were so promising that researchers have started to investigate them.

The collaborative work between scientists and game players could as easily be a dead end as a breakthrough. But one thing is clear: The three-dimensional insights by Foldit players helped jump-start an effort to design proteins that could one day help neutralize the deadly disease.

"We actually noticed that the scientists don't know where to start" when beginning to design a protein to counter Ebola, said Zoran Popovic, director of the Center for Game Science at the UW, which runs Foldit. "What Foldit is doing is creating three, four, five possible places to start from."

Designing proteins from scratch in the laboratory to block emerging diseases is a new idea, more science fiction than reality. Scientists think

it could one day be used to quickly create treatments for dangerous new diseases, or even block old ones, such as influenza.

Six months ago - by coincidence, around the time the current Ebola virus outbreak was identified in southeastern Guinea - biochemistry senior fellow Vikram Mulligan, with the UW's Institute for Protein Design, put up an Ebola puzzle on Foldit.

Mulligan could have written a computer algorithm from scratch to find weaknesses in the Ebola virus protein, or he could have adapted an already-written algorithm. Instead, he opted to try to use the expertise of Foldit players.

He asked them to identify possible entry points in the virus that could be used to "gum up the Ebola machinery," jamming the virus's ability to replicate and sicken humans.

If a protein could be designed to stick to the virus, altering or disrupting its function, that protein could be made into a treatment.

For several weeks, about 500 of the more than 300,000 registered Foldit players tried their hand at the Ebola puzzle, looking for a place where a short chain of amino acids could fit into the virus.

Foldit players manipulated protein models online, taking advantage of human puzzle-solving intuition. They used their cursors to move, bend and twist color-coded protein chains.

And several players came up with top-scoring solutions - "hot spots," or places where a protein could bind to the virus.

"It turned out human intuition could solve this problem very, very well," Mulligan said.

Now, Mulligan and other UW researchers are using the results in the lab, designing peptides that could eventually become the basis of an Ebola-fighting drug.

Mulligan emphasized that the lab is not using live Ebola cultures. The UW lab is using an Ebola protein that cannot replicate itself, nor can it infect humans. It is made with a harmless strain of bacteria using recombinant DNA technology, and the peptides are made with yeast, using genetic-engineering techniques.

The two are mixed together to see which peptides specifically stick to the Ebola protein. If some promising candidates result from the work, the results could be given to outside collaborators who work with live Ebola virus strains.

Researchers at the Institute for Protein Design hope that one day, treatments for emerging diseases will be designed in weeks or months - by researchers using computer algorithms to design specific proteins. "The hope is we'll have a very rapid pipeline one day, from disease threat to candidate treatment," Mulligan said.

That comes back to the Foldit players. How important are they?

Even a small protein can fold into a tremendous number of different shapes, and knowing the structure of a protein is the key to understanding how it works. As it turns out, "humans can think in 3-D much more easily than computers can," said Brian Koepnick, a graduate student at the Institute for Protein Design who worked on the Ebola puzzle.

Human Foldit players seem to be better than computers at finding things like virus hot spots, Koepnick said. And researchers may be able to teach those human strategies to computers, making protein-folding solutions

even faster and more efficient.

Vijay Pande, a professor of chemistry at Stanford University and director of the Pande Lab, is skeptical about the contribution human gamers can make.

"In this particular case, it seems to me that computation (not gamers) would be more successful" at designing a drug, Pande said by email.

His lab has used computational methods to recombine existing drugs into a potential Ebola treatment. A company, Globavir Biosciences, plans to develop the drug and seek approval for it.

The drug does not use human-designed proteins, and Pande said repurposed drugs are easier to administer and manufacture. "From a drug-design perspective, there are numerous benefits to the repurposing drug strategy, especially when we need to move quickly," he said.

The UW's Institute for Protein Design points to some successes, Mulligan said, including a protein that effectively binds some of the peptides in wheat gluten that cause irritation in those who suffer from celiac disease. The drug is going into clinical trials.

And the lab has also designed a protein that protected mice against a lethal dose of the influenza virus. Foldit players contributed to that research, which is still in the early stages.

Protein design is "science fiction now, but we hope it will be science fact one day," Mulligan said.

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