Researchers develop promising molecule in quest to create drug to treat COVID-19

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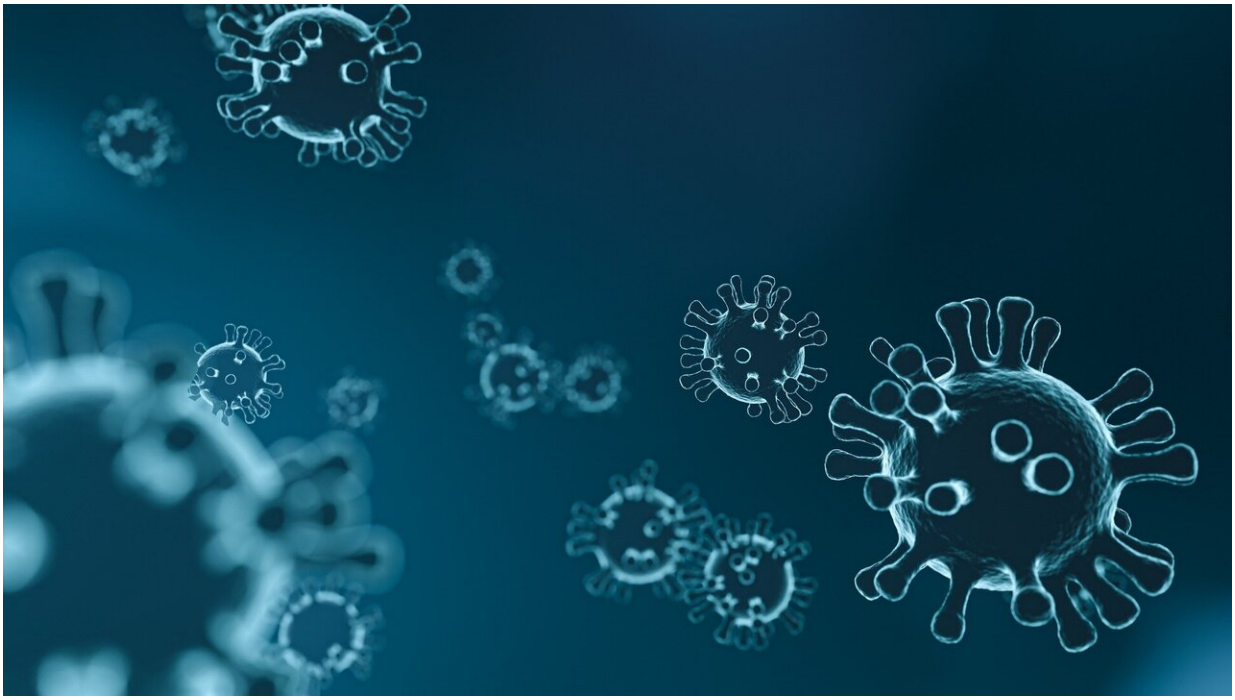

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Uppsala researchers have succeeded in designing a molecule that inhibits the replication of coronaviruses and has great potential for development into a drug suitable for treating COVID-19. The molecule is effective against both the new variant and previously identified coronaviruses. The research article has been published in the *Journal of the American Chemical Society*.

The new coronavirus has caused more than five million deaths. Many lives could have been saved with antiviral drugs, but no treatment of this type has been available to the healthcare system. During the pandemic, researchers around the world have tried to find a pharmaceutical, but the development of new medications often takes a long time.

During the first months of the pandemic, researchers were able to determine the structure of the coronavirus and how it functions at the molecular level. One of the viral enzymes was identified as a promising target for a drug, a strategy that has been successful for other viral diseases, such as AIDS. The idea is to design a molecule with the ability to recognize and bind to the enzyme. This would block its activity and thereby prevent the virus from producing new virus particles, stopping the spread of the virus.

In 2020, researchers at Uppsala University, in collaboration with the Drug Discovery and Development platform at Scilifelab, began to screen for inhibitors of the enzyme. They used computer models to identify molecules that could inhibit the enzyme's activity. This proved to be a fast way to discover starting points for the design of pharmaceuticals. Access to Swedish supercomputers made it possible to evaluate several hundred million different molecules to find those that could bind to the enzyme. The molecules predicted by the models were then synthesized and tested in experiments.

"The most promising molecule shows the same ability to inhibit the replication of the new coronavirus as the active substance in Paxlovid, a combination drug recently approved for treating COVID-19. Our molecule works well on its own, and we have shown that the molecule is also effective against previously identified variants of the coronavirus," says Jens Carlsson, associate professor and the article's lead author.

More information: Andreas Luttens et al, Ultralarge Virtual Screening

Identifies SARS-CoV-2 Main Protease Inhibitors with Broad-Spectrum Activity against Coronaviruses, *Journal of the American Chemical Society* (2022). DOI: 10.1021/jacs.1c08402

Provided by Uppsala University

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