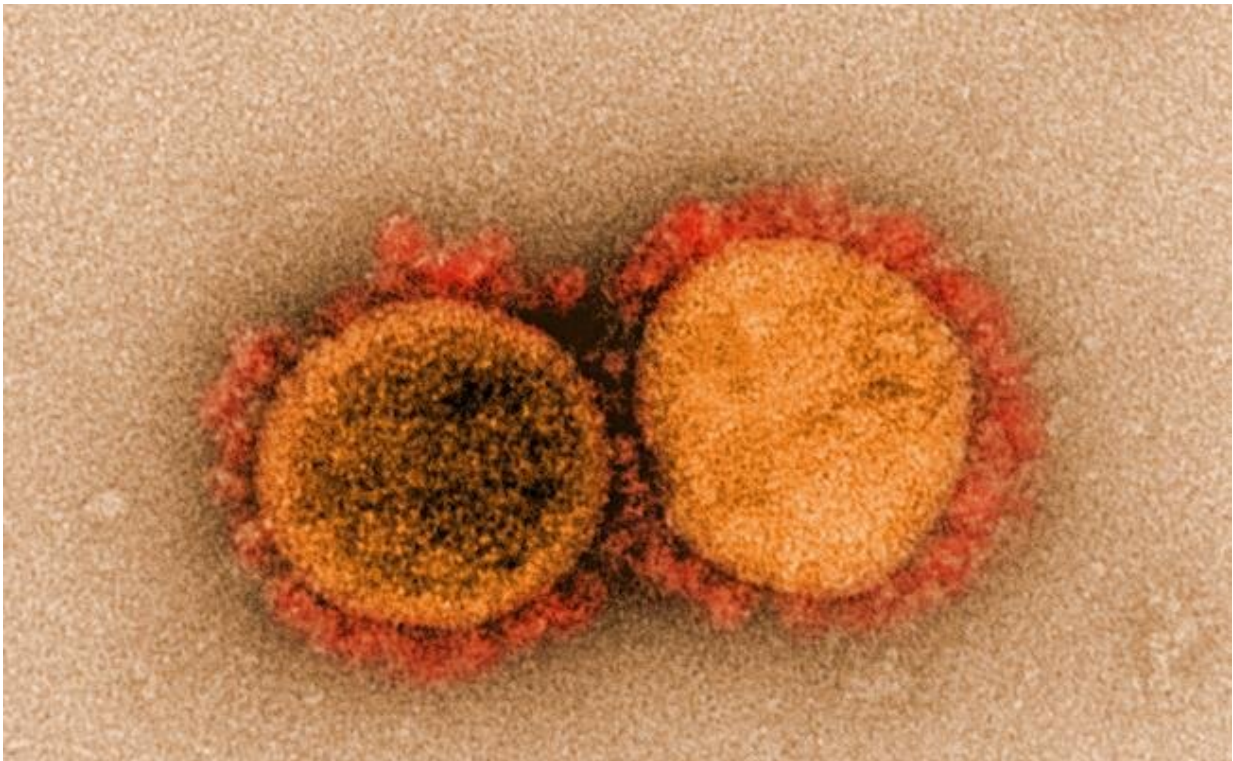


Study finds repurposed drug inhibits enzyme related to COVID-19

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Transmission electron micrograph of SARS-CoV-2 virus particles, isolated from a patient. Image captured and color-enhanced at the NIAID Integrated Research Facility (IRF) in Fort Detrick, Maryland. Credit: NIAID

With the end of the pandemic seemingly nowhere in sight, scientists are still very focused on finding new or alternative drugs to treat and stop the spread of COVID-19. In a first-of-its-kind study, researchers at the

University of New Hampshire have found that using an already existing drug compound in a new way, known as drug repurposing, could be successful in blocking the activity of a key enzyme of the coronavirus, or SARS-CoV-2, which causes COVID-19.

"The goal was to slow or prevent the spread of the virus by using a strategic therapeutic that could possibly disrupt key steps in the viral life cycle at the [molecular level](#), like the first contact with a healthy cell or the first step in replicating within an [infected cell](#)," said Harish Vashisth, associate professor of chemical engineering.

In their study, recently published in the journal *Proteins: Structure, Function, and Bioinformatics*, researchers set out to target a key enzyme responsible for COVID-19, called the main protease enzyme Mpro, which has become a primary target of intense research and therapeutic development because it is essential for the virus to replicate. In this case, they explored the inhibiting properties of a derivative of the potent chemical compound known as Thiadiazolidinones, or TDZD, which are already being studied as a potential treatment for neurological disorders like Parkinson's Disease. Researchers used a specific TDZD compound, known as CCG-50014, to target Mpro which acts like a molecular scissor by cutting up long chains of polypeptide proteins of the virus into smaller component proteins. These smaller segments can fold and mature to form new virus particles. Using [molecular dynamics simulations](#) combined with laboratory experiments, the researchers determined that TDZD compound was able to inhibit the Mpro enzyme.

"Coronaviruses, like COVID-19, are a notorious group of infectious agents that include a large class of viruses with RNA genomes, similar to the human DNA genome, that depend on well-organized protein structures crucial for viral growth and replication," said Vashisth. "These viruses can develop rapid defenses at the [cellular level](#) by orchestrating these layers, or folding mechanisms, in [viral proteins](#) so the key is to find

a way to shut them down."

RNA viruses are known for causing seasonal epidemics, like influenza, and can appear as novel [virus](#) strains with high fatality rates (COVID-19, SARS, Zika and Ebola). Researchers say the need for an alternative [drug](#) development pipeline, instead of the intensive process of introducing new drugs to market, is illustrated by the high infection rate of COVID-19 (compared to previous coronaviruses) and is important for a long-term effective response to new and reoccurring outbreaks.

More information: Jacob Andrzejczyk et al, Molecular interactions and inhibition of the SARS-CoV-2 main protease by a thiadiazolidinone derivative, *Proteins: Structure, Function, and Bioinformatics* (2022). [DOI: 10.1002/prot.26385](#)

Provided by University of New Hampshire

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