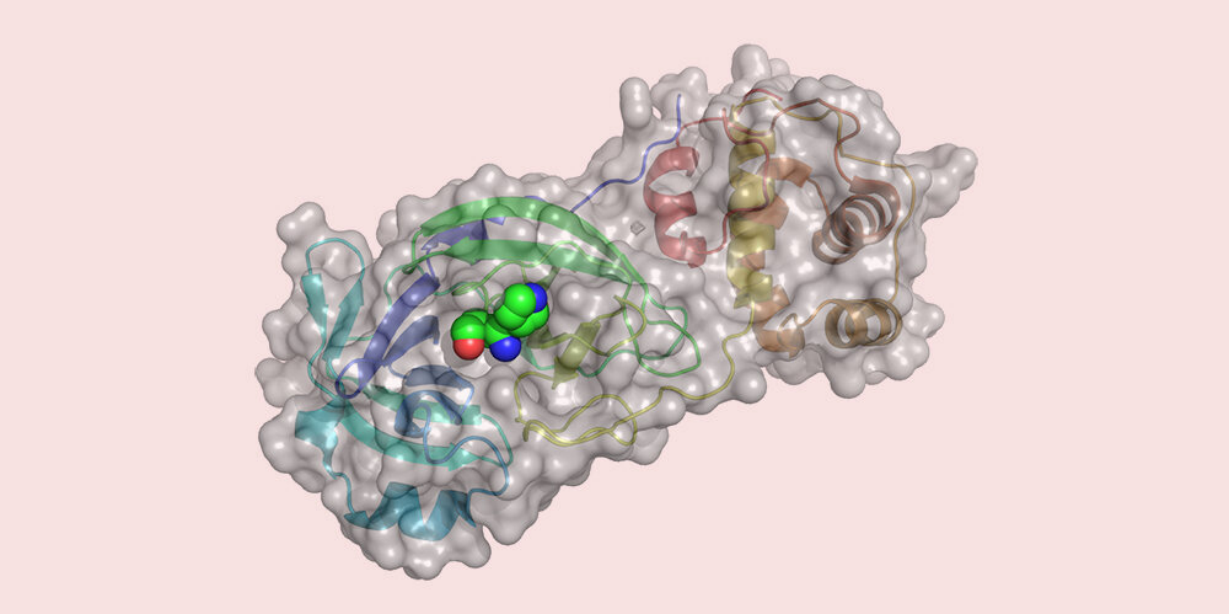
Virtual screening for active substances against the coronavirus

March 10 2020



Researchers have tested more than 680 million substances on the computer to virtually test one of the virus' important proteins, the central protease. Credit: University of Basel, Computational Pharmacy

The University of Basel is part of the global search for a drug to fight the rampant coronavirus. Researchers in the Computational Pharmacy group have so far virtually tested almost 700 million substances, targeting a specific site on the virus—with the aim of inhibiting its multiplication. Due to the current emergency, the first results of the tests will be made

available to other research groups immediately.

Over the past few weeks, the research group in the Department of Pharmaceutical Sciences, led by Professor Markus Lill, has been working with computer-aided methods to identify possible new drugs to combat the current coronavirus outbreak and similar epidemics in the future. In the process, the researchers have tested, albeit virtually, more than 680 substances on one of the virus's key proteins: its central protease.

This "virtual screening" has already identified several interesting substances that have the potential to inhibit the virus's critical enzyme—and thus its further multiplication. "Even if the complete development of a drug to fight this particular coronavirus is likely to exceed the duration of the current epidemic, it is important to develop drugs for future coronaviruses. This will make it possible to nip health crises like this one in the bud in the future," says Lill.

Test results made public

In light of the current crisis, the group took an unusual decision by immediately making the test results publicly available in the form of an open-source preprint. The publication was consulted more than 3,000 times during the first 48 hours alone.

The Basel researchers hope that a larger number of research groups worldwide will test their proposals on the virus and initiate further trials. Normally, when it comes to drug design, the molecules of interest would be experimentally tested with other groups before the results were patented and published. The main focus of other ongoing coronavirus trials is currently on the usability of existing antiviral drugs or the realignment of other drugs.

More information: Inhibitors for Novel Coronavirus Protease Identified by Virtual Screening of 687 Million Compounds: chemrxiv.org/articles/Inhibito … Compounds/11923239/1

Provided by University of Basel