Collaborative development of a computational tool for coronavirus research

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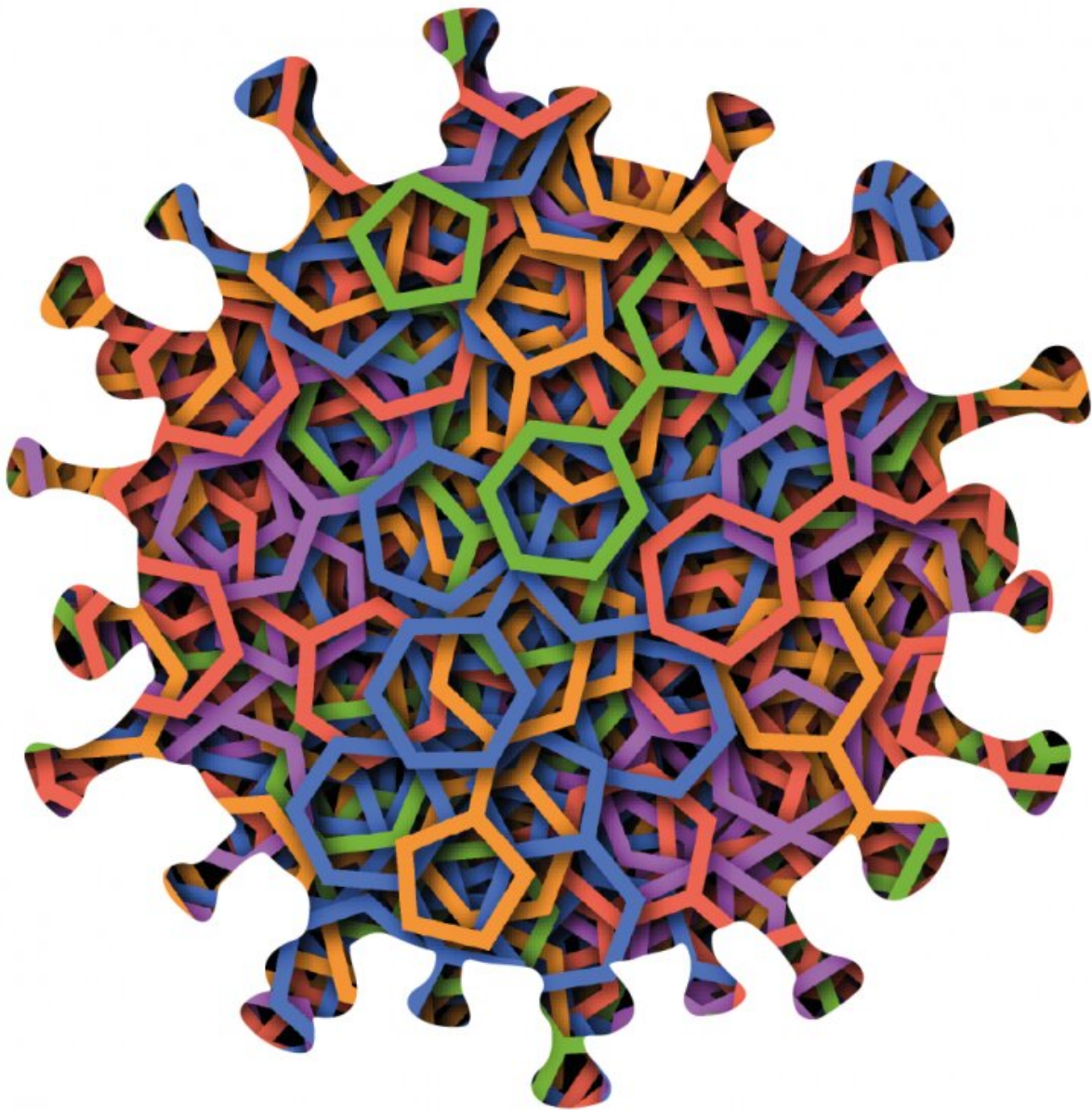
There are currently more than 10,000 scientific articles related to coronavirus infections. In fact, in recent weeks, research to combat COVID-19 has accelerated, and more than 4,000 new academic papers have been published on potential vaccines, therapies, and treatments. Processing this volume of information manually would be unmanageable to be able to advance this urgently needed research fast enough. IRB Barcelona's Structural Bioinformatics and Network Biology Laboratory, led by ICREA researcher Patrick Aloy, has joined forces with Amazon to develop a computational tool that would speed up the process. Using artificial intelligence, this tool will "read" all these articles and extract all relevant information related to the molecules and treatments studied.

Through a limited review of the most relevant scientific literature, researchers at IRB Barcelona have so far identified more than 150 compounds—with different levels of experimental evidence—that are potentially active against COVID-19. The objective is now to find other drugs with characteristics similar to these, thereby expanding the portfolio of molecules of interest and increasing the possibilities of identifying one with high effectiveness. Results are already available at sbnb.irbbarcelona.org/covid19/ .

"What we now need is for research groups working with COVID-19 treatments to introduce their results," explains Aloy. "The new molecules will be incorporated automatically once a day, and thus the entire scientific community will have updated data, which will help to avoid duplication and will generate new hypotheses that would help to find the definitive treatment."

Speedy collaboration for drug discovery

The Chemical Checker is a computational tool that offers information on 1 million molecules with pharmacological potential. "The Chemical Checker aims to process and encode complex data on the effects that different chemical compounds have on living organisms, so that they can be incorporated into new artificial intelligence technologies," says Miquel Duran, researcher of the IRB Barcelona group and first author of the study.

In just over a week, Aloy's laboratory and Amazon have established a collaboration that has enabled to fine-tune this bioinformatics tool. "It has been a pleasure for us to put our artificial intelligence capacity at the service of drug discovery against COVID-19," says Hugo Zaragoza, from the Amazon Search Science and AI group. The experience Amazon has with text-mining, machine learning and natural language understanding has allowed the automatic analysis of scientific articles to be incorporated into the Chemical Checker at a fast pace. "Collaboration with Amazon has been key to get this tool up and running so quickly. Without its AWS cloud computing and text processing capabilities, it would have been impossible," says Aloy.

IRB Barcelona committed to research into COVID-19

The Structural Bioinformatics and Network Biology Lab is also participating in the European project RiPCoN, devoted to the identification of the human proteins that the virus uses for its expansion. This project seeks to identify drugs (already on the market or in clinical trials) that can modulate the activity of the virus and halt its replication.

IRB Barcelona is also working on other projects related to COVID-19. One is devoted to the development of a quick and simple diagnostic test to detect the virus, while another focuses on the development of a spray treatment for COVID-19. Another project centres on reducing the

mortality rate of COVID-19 by finding a treatment for acute respiratory distress syndrome, the main cause of death by this virus.

More information: sbnb.irbbarcelona.org/covid19/

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