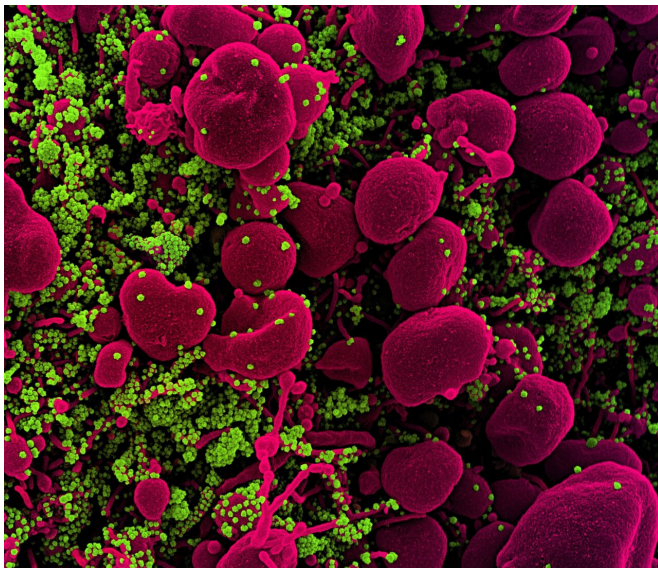


New virtual screening strategy identifies existing drug that inhibits Covid-19 virus

31 December 2020



Colorized scanning electron micrograph of an apoptotic cell (pink) heavily infected with SARS-CoV-2 virus particles (green), isolated from a patient sample. Image captured at the NIAID Integrated Research Facility (IRF) in Fort Detrick, Maryland. Credit: National Institute of Allergy and Infectious Diseases/NIH, 2020 (CC0)

A novel computational drug screening strategy combined with lab experiments suggest that pralatrexate, a chemotherapy medication originally developed to treat lymphoma, could potentially be repurposed to treat Covid-19. Haiping Zhang of the Shenzhen Institutes of Advanced Technology in Shenzhen, China, and colleagues present these findings in the open-access journal *PLoS Computational Biology*.

With the Covid-19 pandemic causing illness and death worldwide, better treatments are urgently needed. One shortcut could be to repurpose existing drugs that were originally developed to treat other conditions. Computational methods can help identify such drugs by simulating how different drugs would interact with SARS-CoV-2, the virus

that causes Covid-19.

To aid virtual screening of existing drugs, Zhang and colleagues combined multiple computational techniques that simulate [drug-virus](#) interactions from different, complimentary perspectives. They used this hybrid approach to screen 1,906 existing drugs for their potential ability to inhibit replication of SARS-CoV-2 by targeting a viral protein called RNA-dependent RNA polymerase (RdRP).

The novel screening approach identified four promising drugs, which were then tested against SARS-CoV-2 in lab experiments. Two of the drugs, pralatrexate and azithromycin, successfully inhibited replication of the virus. Further lab experiments showed that pralatrexate more strongly inhibited [viral replication](#) than did remdesivir, a drug that is currently used to treat some Covid-19 patients.

These findings suggest that pralatrexate could potentially be repurposed to treat Covid-19. However, this chemotherapy drug can prompt significant side effects and is used for people with terminal lymphoma, so immediate use for Covid-19 patients is not guaranteed. Still, the findings support the use of the new screening strategy to identify drugs that could be repurposed.

"We have demonstrated the value of our novel hybrid approach that combines deep-learning technologies with more traditional simulations of molecular dynamics," Zhang says. He and his colleagues are now developing additional [computational methods](#) for generating novel molecular structures that could be developed into new drugs to treat Covid-19.

More information: Zhang H, Yang Y, Li J, Wang M, Saravanan KM, Wei J, et al. (2020) A novel virtual screening procedure identifies Pralatrexate as inhibitor of SARS-CoV-2 RdRp and it reduces viral replication in vitro. *PLoS Comput Biol* 16(12):

e1008489. [DOI: 10.1371/journal.pcbi.1008489](https://doi.org/10.1371/journal.pcbi.1008489)

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APA citation: New virtual screening strategy identifies existing drug that inhibits Covid-19 virus (2020, December 31) retrieved 27 May 2022 from <https://medicalxpress.com/news/2020-12-virtual-screening-strategy-drug-inhibits.html>

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