Computer models for 80 potential COVID-19 treatments

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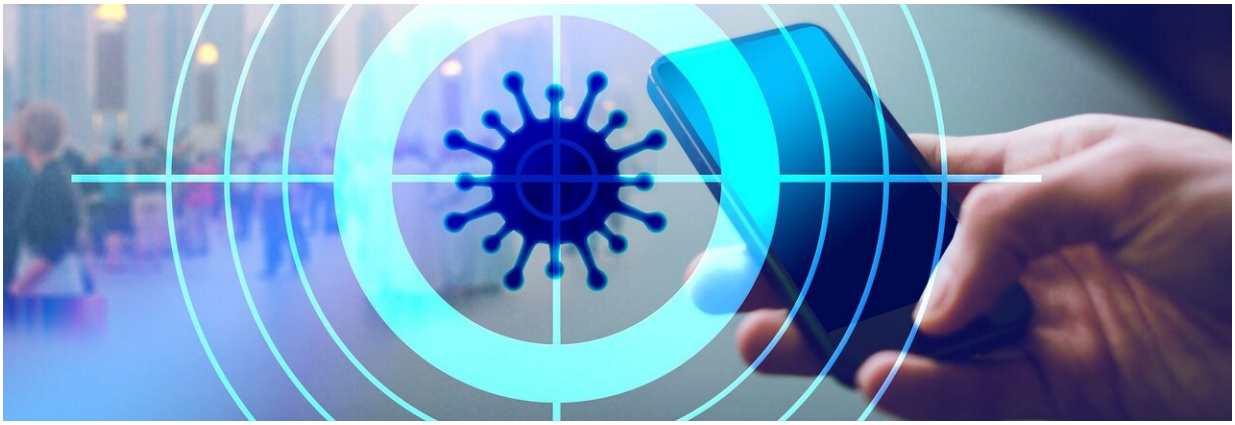

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Australian scientists using cloud-based supercomputer programs have joined forces with biotechnology company Vaxine Pty Ltd to identify up to 80 new potential candidate drugs against the COVID-19 virus.

The team has published their list online on a prepress server to enable other researchers to immediately start further testing of the identified compounds for their ability to safely treat COVID-19 infections.

Using the genetic sequence of COVID-19, the team built three dimensional molecular structures of key COVID-19 proteins that were then used to screen existing drugs and natural remedies for potential

activity against the COVID-19 protease protein.

"We hope that making the results available immediately will enable other research group to use these data to further test the compounds we have identified, thereby enabling the most promising candidates to be rapidly advanced into human clinical trials," says Vaxine Research Director, Flinders University Professor Nikolai Petrovsky.

"This drug discovery work was completed in just months, as compared to the many years normally taken to identify new drugs using more traditional laboratory-based methods,"

The computer-based screening has identified several new targets as well as many of the same antiviral compounds that other research has shown experimentally to have COVID-19 activity.

The team used high performance cloud computing services provided by Oracle Corporation under a research grant to Flinders University that enabled the team to rapidly screen for potential drugs against COVID-19.

Vaxine is working with several other technology and pharmaceutical companies to fast-track its COVID-19 research, including development of a possible COVID-19 vaccine.

"It is exciting to be at the forefront of global COVID-19 science efforts, applying all the latest cutting edge methods including artificial intelligence and high performance cloud computing to create potential pandemic drugs and vaccines as part of the Vaxine team," says first author on the prepress article Dr. Sakshi Piplani, who leads Vaxine's bioinformatics team.

The drug candidate research findings, "Computational screening of

repurposed drugs and natural products against SARS-Cov-2 main protease (Mpro) as potential COVID-19 therapies" can be found online at the arXiv pre-press server ahead of future publication after peer review.

More information: Piplani et al., Computational screening of repurposed drugs and natural products against SARS-Cov-2 main protease (Mpro) as potential COVID-19 therapies. arXiv:2009.00744 [q-bio.BM]. arxiv.org/abs/2009.00744

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