HealthManagement
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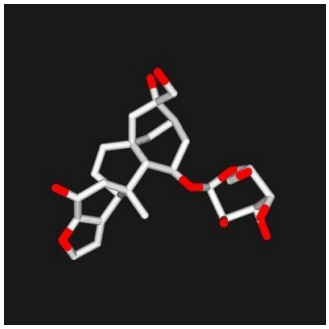
Crowdsourcing COVID-19 Research



An app, easily usable by anyone, allows users to explore molecules that might bind to key proteins on the SARS-CoV-2 and may help in the search for COVID-19 treatments.

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The app, ViDok, has been created by Thanh Truong, University of Utah professor of chemistry, together with colleagues at the Institute for Computational Science and Technology in Vietnam.

With the race continuing to find a COVID-19 vaccine, researchers are also looking for possible treatments. New drug discovery and testing is time-consuming and costly. For COVID-19, researchers try to identify the drug target, a protein on the SARS-CoV-2, and molecules that can bind to that target and halt the virus' reproduction cycles. Professor Truong believes that crowdsourcing this process can make it shorter and cheaper.

The app's design is very simple: the user needs to go through a library of molecules that are likely to bind well to the SARS-CoV-2 protein, determine the binding energy of the molecule and then alter the molecule's structure and test the binding energy again. With each cycle, the app ranks the new molecule against those submitted by other users.

The University's Center for High Performance Computing processes the data and hosts a website with a database of all the app-processed molecules (freely available for download).

So far, the app has been tested by a group of people in Vietnam who have managed to modify 195 of 200 potentially therapeutic molecules from more than 2500 drug candidates. "The beautiful thing is that different people look at things differently. You can improve sequentially," says Professor Truong who hopes to "get a list of the best possible drug leads that experimentalists can actually go into the lab and synthesize it and then perform further studies".

The ViDok app is available on the iOS App Store and on Google Play.

Source and image credit: University of Utah

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