Speeding up the search for an effective COVID-19 cure

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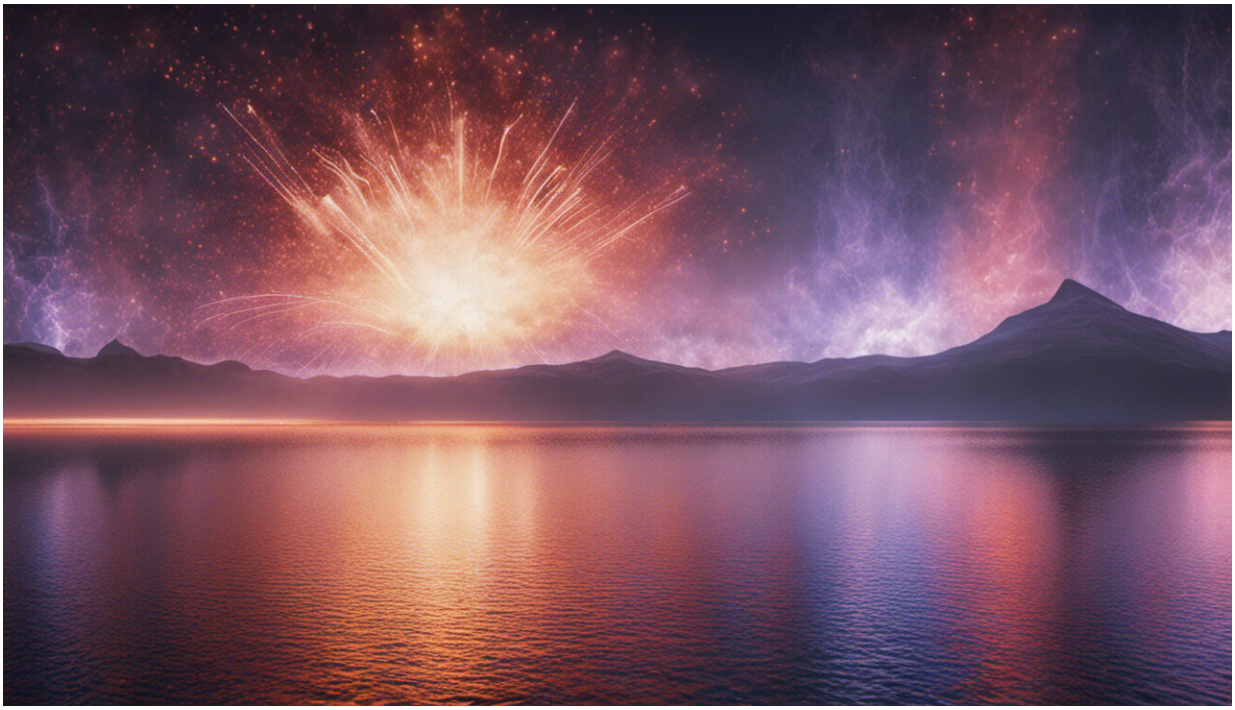

Credit: AI-generated image (disclaimer)

As the race against time to find a drug for COVID-19 continues, a team of experts is using a supercomputing platform to combat the current outbreak and efficiently counter future pandemics. At the core of these efforts is the Exscalate (EXaSCale smArt pLatform Against paThogEns) supercomputing platform, an outcome of the EU-funded ANTAREX

project. The platform "leverages a 'chemical library' of 500 billion molecules, thanks to a processing capacity of more than 3 million molecules per second," as noted in a press release.

The Exscalate4CoV (E4C) public-private consortium is coordinated by ANTAREX project partner Dompé Farmaceutici. The same press release states: "The aim of E4C is twofold, identify molecules capable of targeting the coronavirus (2019-nCoV) and develop a tool effective for countering future pandemics to be consolidated over time." The E4C's HPC platform will build 3-D molecule structures that can be used by scientists to mimic how the pathogen's proteins interact with specific drugs. "This activity has already started," the press release adds. "The supercomputing component of the project will be then exploited to model future mutations of the virus. These activities will allow to identify candidate molecules (either from repurposing libraries or from proprietary or commercial compound libraries) which will then be provided and/or synthetized to be tested. In parallel, E4C partners shall start the protein production for some of the identified sequences."

Zika virus and beyond

The Exscalate platform will also be available "to external partners willing to cooperate in the drug hunting exercise, as previously with the Zika virus. This considerable effort to test roughly more than 25,000 compounds will ensure E4C doesn't lose any active candidate molecules and will evaluate other possible mechanisms previously underestimated," according to the press release. "The project will also use inverse genomic screening to identify host factors associated with virus infection and connectivity mapping analysis to predict relevant host-specific compounds for testing." The platform will also be used as a "sustainable resource for an emergency engine for compound identification to be deployed in all future pandemic emergencies," the Dompé press release notes. The virtual screening activities of the Exscalate platform will be

supported and empowered by three of the most powerful computer centres in Europe, namely CINECA, the host of the Marconi supercomputer, Barcelona Supercomputing Center and Jülich Research Centre, as noted on the E4C website.

The ANTAREX (AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems) project, which ran between September 2015 and November 2018, used the Marconi supercomputer to accelerate drug discovery. Focusing on the real-life case of the Zika pandemic crisis that was triggered by the 2015 outbreak in Brazil and quickly spread to other parts of South America, North America and various regions worldwide, ANTAREX partners identified 26 binding sites from the crystal structures of five Zika proteins. They tested a total of 1.2 billion molecules via computer simulation on 1 million computational threads available through the Marconi supercomputer.

More information: ANTAREX project website: www.antarex-project.eu/

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