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Fujitsu Japan deploys world's fastest supercomputer for COVID-19 therapies

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Explores novel molecular mechanisms for infection inhibition aiming the development of new COVID-19 Treatments



Fujitsu Japan has announced that it will initiate a new research project with a research team led by Japan's Research Center for Advanced Science and Technology (RCAST) at University of Tokyo.

The research utilizes the world's fastest supercomputer, Fugaku, which was jointly developed by RIKEN and Fujitsu. The research will leverage Fugaku to identify small molecule inhibitory compounds that can be used as potential drugs in treatments for COVID-19 as well as clarifying the molecular mechanism by which COVID-19 infections are inhibited, leading to the eventual development of small molecule therapeutic drugs. Full-scale research begins on June 22nd, 2021, and will continue until March of 2022.

In their joint research, Fujitsu and RCAST will leverage IT drug discovery technology with a focus on inhibitory compound creation technology and molecular simulation technology that precisely represents the state of molecules, performing calculations on Fugaku to identify inhibitory compounds based on the dynamic behavior of viral proteins and to predict the properties of future mutations.

By utilizing Fugaku, molecular simulations for viral proteins and inhibitory compounds formulation can be accelerated, clarifying the complexity of binding states and interactions between viral proteins and inhibitory compounds, with the aim of identifying inhibitory compounds that can lead to therapeutic drugs at an early stage.

Going forward, Fujitsu will continue harnessing the power of supercomputers and molecular simulation technologies as it strives to quickly deliver on the promise of potential therapies for COVID-19 with its joint research alongside RCAST Project Associate Professor Yamashita, contributing to the realization of a society in which all people can live with peace of mind.