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Japan-based Fujitsu and RIKEN develop AI drug discovery technology utilising generative AI

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New technology uses AI with electron microscope images to reduce development time and cost of drug discovery



Fujitsu Limited and the High Performance Computing (HPC)- and AI-driven Drug Development Platform Division of the RIKEN Center for Computational Science, in Japan, have developed an artificial intelligence (AI) drug discovery technology that can predict structural changes of proteins from electron microscope images as a 3D density map in wide range by utilising generative AI.

In conjunction with this announcement, Fujitsu also plans to make its prediction technology for protein structural changes available as an AI innovation component of the Fujitsu Kozuchi (code name) - Fujitsu AI Platform, an AI platform that allows users to quickly test out advanced technologies.

As part of a joint research project launched in May 2022, Fujitsu and RIKEN developed a generative AI technology that accurately estimates the various forms of a target protein's conformation and their possible proportions from a large number of projection images taken by electron microscopy, as well as a technology that predicts conformational changes in the target protein from the estimated proportions.

Based on these two technologies, the two parties developed an AI drug discovery technology that can predict structural changes of a protein in a wide range, with the aim of developing next-generation IT drug discovery technology that significantly reduces the development time and cost of drug discovery.

Moving forward, Fujitsu and RIKEN will use the newly developed generative AI technology as one of the core technologies for realising next-generation IT drug discovery technology that can analyse the complex relationships between target proteins and antibodies, and predict global structural changes of molecules with high accuracy and speed.