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Japanese firms initiate joint research on next-gen IT drug discovery technology

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Using the supercomputer Fugaku and simulation integrated artificial intelligence (AI)



Japan-based Fujitsu and RIKEN have launched a joint research project on next-generation IT drug discovery technology utilizing the supercomputer Fugaku. The collaboration aims to accelerate DX (digital transformation) in drug discovery to explore promising new areas in this process. The effort can dramatically reduce development periods and costs for new drug development.

The joint research project will leverage high-performance computing technologies. The supercomputer Fugaku will accelerate simulation integrated AI that combines Fujitsu's DeepTwin AI technology. The process accurately acquires quantitative features from complex data by unsupervised learning, with molecular dynamics simulation using RIKEN's AI drug discovery simulation technology.

The approach is expected to improve the accuracy and speed of molecular simulation and establish innovative technologies that can predict changes in the structure of target proteins over a wide range.

Based on this research, the two parties aim to develop a next-generation IT drug discovery technology with world-leading capabilities by the end of fiscal 2026. Fujitsu and RIKEN anticipate that this technology will perform an analysis of the target protein and drug candidate molecule complex. It can also predict large-scale structural changes of molecules with high speed and high accuracy contributing to the development of middle-molecular drugs and large-molecular drugs, which are expected to have high efficacy and low side effects.