DX platform for target discovery and drug design

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We are working on the research and development of a drug discovery digital transformation (DX) platform aimed at ultra-smartening the drug discovery process through AI and simulation, with the fundamental premise of small teams and low costs. This initiative seeks to enable the Japanese pharmaceutical industry to catch up with and confront global speeds in drug innovation. Specifically, we have been developing AI and simulation technologies for each step of the drug discovery process, from upstream to downstream. These technologies include target discovery, activity prediction (such as efficacy and toxicity), mechanism elucidation, compound design optimized based on these conditions, and the extraction of adverse effect factors from clinical data.

For instance, in a domestic project, we are developing a Graph Convolutional Network (GCN) AI that predicts activity and ADMET properties from chemical structures, by sharing compound data among several pharmaceutical companies. Additionally, we are advancing AI technologies utilizing diverse datasets like multi-omics and clinical data to achieve patient stratification, sample classification, molecular mechanism elucidation, biomarker estimation, and the exploration of drug target molecules. In this lecture, I would like to introduce specific examples of my work and discuss the current state and future prospects of AI in drug discovery.