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AI-driven Precision Medicine and Drug Discovery

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AI plays an increasingly important role in precision medicine and drug discovery. In this talk, I will introduce some of our recent efforts in AI-driven precision medicine and drug discovery, primarily in the context of our experiences in competing in international precision medicine competitions called DREAM Challenges. DREAM Challenges are a series of competitions, aiming to solve challenging problems in precision medicine, through a collaborative community effort. The first challenge we participated was the Astra-Zeneca Sanger Drug Combination DREAM challenge. The participants were expected to design a machine learning model to predict the synergistic combination of cancer drugs for each individual patient. We used the genomic and transcriptional features of patients and the chemical properties of drugs to predict the synergy. Our model was ranked at the second place in the competition. The second competition we participated was the NCI-CPTAC Proteogenomics DREAM Challenge. In the challenge, the participants were asked to build a machine learning model to predict the protein abundance using the abundances of other proteins or the copy number and the expression level of the given protein. We built a prediction model based on a collaborative filtering algorithm. Our model achieved the first place in the competition. Finally, I will introduce the Multi-targeting Drug DREAM Challenge. The challenge asked the participants to submit a list of drug candidates that can bind to a given set of targets and at the same time can avoid a given set of non-targets. We built Siamese Neural Networks called ReSimNet to predict the transcriptional response phenotype similarities between drugs. The drug candidates selected using our ReSimNet was determined as the winner of the competition.