# The impact of hypothesis and prediction in data-driven pharmacological studies

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Recent pharmacological studies have been developed based on the finding of new disease-related gene, which is accompanied with the production of gene-manipulated disease model animals and high-affinity ligands for the target protein. However, emergence of the gene-based strategy has led to the rapid deprivation of drug target molecules. To overcome this situation, we have been trying to utilize clinical big data to explore a novel and unexpected hypothesis of drug-drug interaction that leads to the drug repositioning. Here, we introduce our data-driven approach in which adverse self-reports, JMDC claims database and University hospital health records are analyzed and compared to find and validate new drug targets. We also present our recent effort to predict the binding affinity of theoretically any chemical ligands to a target protein by deep learning of chemical structures and their measured affinity to the target with graph convolutional neural network. The hypothesis and prediction provided by data-driven approaches will impact on the style of pharmacological study.