Network-based and data-driven drug discovery by machine learning

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Drug repositioning, or the identification of new indications of drugs (i.e., new applicable diseases), is an efficient strategy for drug discovery, and it has received remarkable attention in medical and pharmaceutical science. The drug repositioning approach can increase the success rate of drug discovery and to reduce the cost in terms of time, risk, and expenditure. In this study, we developed novel machine learning methods for automatic drug repositioning in order to predict unknown therapeutic indications of known drugs or drug candidate compounds. We also proposed to use molecular pathways as the therapeutic targets and develop a novel computational approach for screening drug candidate compounds. The prediction is performed based on the analysis of various large-scale omics data and molecular interaction networks of drugs, compounds, genes, proteins, and diseases in a framework of supervised network inference. Our results show that the proposed method outperforms previous methods in terms of accuracy and applicability. We performed a comprehensive prediction of new indications of all approved drugs and bioactive compounds for a wide range of diseases defined in the International Classification of Diseases. We show clinically and biologically meaningful examples of newly predicted drug indications for cancers and neurodegenerative diseases. The proposed methods are expected to be useful for various pharmaceutical applications in drug discovery.