Relationship between Drug Side-Effects and Therapeutic Indications

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DESCRIPTION

Drug discovery is a time-consuming and laborious process. Today's conservative estimate is that it will take at least 10 to 15 years, $ 500 billion to $ 2 billion to bring a single drug to market. In addition, the productivity gap is widening. R and D costs continue to rise, but the number of new therapeutic chemicals and biologics approved by the US FDA has declined since the late 1990s. Lack of efficacy and adverse side-effects are two of the main reasons drugs fail in clinical trials, each accounting for about 30% of failures. Therefore, the development of tools that can predict therapeutic indications and side effects is very promising for reducing attrition rate and improving the drug discovery process.

Inferring potential therapeutic indications (i.e., drug repositioning) for new or approved drugs is an important approach to drug development. The beginning of a known connection with a well-characterized pharmacology and safety profiles was able to reduce the risk of attrition at the clinical phases. There were several successful examples of drug repositioning (e.g., thalidomide for the treatment of leprosy or Finasteride to prevent baldness). But they were the results of all serendipitous discoveries, not well-thought strategies. Recently, several computational methods have been developed to predict drug indications. Drug positioning has five typical computational strategies: (1) Preparation of new drug applications based on shared treatment profiles using network-based guilt-by-association method (2) Prediction of drug indications based on chemical structure of drug. (3) Inferring drug indications from a protein target interaction network. (4) Identifying the relationship between drugs based on their phenotypic profile similarity. (5) Integration of multiple properties (e.g., chemical, biological or phenotype information) of drugs and diseases for predicting drug indications. With the exception of these strategies are primarily focused on the use of preclinical information. However, clinical therapeutic effects are not always consistent with preclinical results.

At the same time, side effects of drugs and adverse drug reactions are of great concern to healthcare. To explain the extent of this problem, serious drug side effects are estimated to be the fourth leading cause of death in the United States, death rate up to 100,000 people each year. Identifying potentially serious adverse side-effects is a challenge at many stages of the drug development process. Experimental detection of drug side effects is cost-effective, while a useful experimental approach for predicting side effects is to test the compound in preclinical in vitro safety profiling, biomedical and cellular assays is still a big challenge. Therefore, several computational methods have been proposed for analyzing or predicting the side effects of drugs. This method can be divided into three types: (1) According to the spirit of QSAR (Quantitative Structure-Activity Relationship), the side effects of drugs are associated with the chemical structure. (2) Relating drug side effects with their protein targets because drugs with similar in vitro protein binding profiles tend to exhibit similar side effects. (3) Prediction of drug side effects by integrating multiple data sources (chemical, biological, phenotypic properties, etc.).

Both therapeutic indications (i.e., drug’s indicated diseases) and side effects are measurable behavioral or physiological changes in response to treatment. Intuitively, if the drug that treats the disease has the same side effects, this may be a manifestation of the underlying Mechanism of Action (MOA) that links the indicated disease to the side effects. In other words, the expression of the side effect phenotype can correlate with the expression of the disease phenotype. In addition, there are few translation issues, as both therapeutic indications and side effects are human observations at the clinical stage. This forms the basis for relate a disease with side effects (and vice versa) even if the exact pharmacological mechanism is unknown.

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