Drug-Target Relationship Analysis

Drug targets refer to biological macromolecules that have pharmacodynamic functions in the body and can be acted upon by drugs, such as certain proteins and nucleic acids. They have targeted structures and target molecules related to specific diseases. The analysis of drug targets can reflect which structures of drugs can interact with the target molecules and produce curative effects, so as to achieve the purpose of curing diseases.



Figure 1 Drug target structure



Drug research and development is the driving force of the pharmaceutical industry, and it has also caused a research boom in the academic community. Computer-aided drug design is a supplement to traditional experimental drug discovery. It accelerates the development of new drugs, shortens drug development time, and reduces the cost of drug R & D projects. Physics-based calculation methods used in CADD improve the success rate of drug development.

In the process of drug research, it is very important to understand the <u>drug-target</u> relationship. Drug-target interaction prediction is an important auxiliary method for drug development. Network pharmacology and drug repositioning subvert the traditional drug development concepts, improve the theoretical basis of drug-target

Drug Relationship

Michael Levi, Petrus C. van Duyne

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