

عنوان مقاله:

Polypharmacology in Drug Discovery

محل انتشار:

پانزدهمین همایش بیوشیمی فیزیک ایران (سال: 1397)

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خلاصه مقاله:

Traditional approaches for the identification of bioactive compounds use a chemical library, a single target protein, and an assay, which allows us to measure the activity of these compounds against one target. Therefore, one target, one drug, one disease model has long been the standard strategy for discovering new drugs in pharmaceutical research. Computational drug discovery techniques such as quantitative structure-activity relationships (QSARs) have been carried out to design potent inhibitors against the selected target. Unfortunately, the QSAR model cannot consider the information of the target and in many studies has a minimal ability to predict selective inhibitors. Therefore, recently a meaningful decrease in the rate of discovery of new drug candidates has been observed. Because of complex physiological processes in the body, considering only one target in drug discovery projects is not rational. The main reason for this is that, the multiple activities of drugs against several targets might lead to dramatic side effects and toxicity. Nowadays, increasing evidence that several drugs exert their biological effects through interactions with multiple targets is boosting the development of new research such as chemogenomics, polypharmacology and proteochemometrics. Therefore, the purpose of drug discovery has changed from one drug, one target strategy to a multi drug, multi target. In this lecture, I will describe the current state of drug discovery and the concepts of QSAR, polypharmacology and proteochemometrics.

کلمات کلیدی:

Drug discovery, Polypharmacology, Proteochemometrics, QSAR

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