Aims & Scope:

Computational techniques have been successfully applied in the field of pharmacy and medicine. Specially, computer-aided drug design, computational drug repositioning, drug-target interactions prediction and synergistic drug combinations prediction based on heterogeneous biological data have become critical topics in the search for novel drugs and therapeutic targets for various human complex diseases. The study of these topics is not only to provide better understandings of the mechanisms of disease progression and drug therapy, but is also critical to the development of new drugs and the improvement of treatments. As is well-known, the processes for drug discovery and development are still time consuming, expensive and limited to small-scale research even nowadays. With the development of new experimental techniques, vast amounts of datasets now flow through the different stages of drug development and disease treatment, and there is a major requirement to extract knowledge from these datasets and employ it to improve these processes in all respects. There is therefore a strong incentive to develop powerful computational methods capable of mining these datasets efficiently in order to provide new predictions for experimental scientists and narrow the scope of candidates to accelerate drug discovery. For the potential prediction results with higher scores, biological experiments could be implemented for validation. Recently, the applicability of computational techniques has been extended and broadly applied to nearly every stage in the drug discovery and development workflow.

Keywords: Drug discovery, drug-drug interaction, synergistic drug combinations, side-effect.

Subtopics

- Computer-aided drug design
- Drug effect and side-effect prediction
- Computational drug repositioning
- Drug–target interactions prediction
- Drug-drug interaction prediction
- Synergistic drug combinations prediction
- Adverse drug reactions prediction

Tentative Publication Date: June 2018