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J-BHI Special Issue on "Application of computational techniques in drug discovery and disease treatment"

Computational techniques have been successfully applied in the field of drug discovery and disease treatment. 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 of drugs and therapeutic targets for various 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 them to improve these processes in all respects. Therefore, there is 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.

The proposed special issue will focus on novel computational techniques in drug discovery and disease treatment. We will invite investigators to contribute research article and reviews of describing recent findings which use computational techniques for the research of drug discovery and disease treatment.

Potential topics include, but are not limited to

- Drug-target interaction prediction
- Drug-drug interaction prediction
- Synergistic drug combination prediction
- Computer-aided drug design
- Computational drug repositioning
- Drug effect and side-effect prediction
- Adverse drug reactions prediction
- Anti-cancer drug response prediction
- Microbe-drug association prediction
- Small molecule drug-ncRNA interaction prediction
- Drug network analysis

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Key Dates

Deadline for Submission: 30 September, 2023 First Reviews Due: 30 October, 2023 Revised Manuscript Due: 30 November, 2023 Final Decision: 30 December, 2023



