Tentative Outline

Special Thematic Issue for Combinatorial Chemistry & High Throughput Screening

Novel Bioinformatics and Systems Biology approaches and techniques in Pharmaceutical and Biochemical Sciences

Guest Editor: Prof. Yudong Cai

Aims & Scope:

With the development of Next-Generation Sequencing (NGS) and high throughput omics technologies, the whole picture of complex diseases and biochemical processes can be revealed. But analyzing these big data and integrating various omics data is a great challenge for pharmacologists and biologists. Take the TARGET (Therapeutically Applicable Research to Generate Effective Treatments) project as example, it provides a comprehensive genomic big data of childhood cancers, including Acute lymphoblastic leukemia (ALL), Acute myeloid leukemia (AML), Kidney Tumors, Neuroblastoma (NBL) and Osteosarcoma (OS). It is very difficult to determine the key molecular changes that drive tumorgenesis from millions of transcriptome profiling, nucleotide variation, copy number variation and clinical data.

Meanwhile, the development of Artificial Intelligence (AI) technologies, such as deep learning methods, is also rapidly. Unfortunate, the AI scientists which focus on machine learning and graph theory, are not familiar with the biological context of the great challenges the pharmacologists and biologists are facing. IBM Watson is a good start for introducing AI to analyze clinical information and medical literature. But we need more and more such inter-discipline studies or projects to overcome the barrier between computational scientists and pharmacologists/biologists. Together, novel Bioinformatics and Systems Biology methods and software may be developed to solve the big data analysis and the heterogeneous data integration problem. Until then, the science community may find the cause of complex diseases and the compound that may cure the diseases. The goal of this special issue is to create a dialogue of both fields, computational scientists and pharmacologists/biologists, and to explore advances in NGS and omics data analysis and integration as well as a breadth of other topics.

Keywords: Next-Generation Sequencing (NGS), Omics Profiling, Artificial Intelligence (AI), Machine Learning, Graph Theory, Key Driver, Drug Target.

Subtopics:

The subtopics to be covered within this issue are listed below:

➢ Prediction of nitrated tyrosine residues in protein sequences by extreme learning machine and feature selection methods.

➢ An integrated multi-label classifier with chemical-chemical interactions for prediction of chemical toxicity effects.

➢ Random Walk with Restart Algorithm for the Identification and Analysis of Novel Genes Associated with Colorectal Cancer.

➢ Oscillatory Dynamics of P53 Network With Time Delays.
Hybrid Feature Selection Algorithm mRMR-ICA for Cancer Classification from Microarray Gene Expression Data.

➢ Dynamic effects of two time delays on a model for tumor growth.

➢ A Six-Gene Signature Predicts Clinical Outcome of Gastric Adenocarcinoma

Schedule:

✧ Manuscript submission deadline: <u>November 3, 2017</u>
✧ Peer review due: <u>January 30, 2018</u>

- ✧ Revision due: May 20, 2018
- ✧ Notification of acceptance by the Guest Editor: May 30, 2018
- ✧ Final manuscripts due: August 01, 2018

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