Editorial

Application of Computational Biology in Bio-Pharmacy

With the development of high throughput screening methods, a large number of chemicals have been discovered or designed. On the other hand, numerous properties of the newly found chemicals have also been mined and stored in public databases. Traditional computational methods cannot effectively deal with these large-scale data, inducing high failure rates of candidate chemicals in drug discovery. It is urgent to develop a series of computational methods, which can integrate current known data, to investigate important drug-related or chemical-related problems. This special issue collects seven outstanding studies in this regard.

Huang et al. gave a review on computational drug repositioning approaches. Four main strategies: the target-based, the gene-expression-based, the phenome-based and the multi-omics-based, were summarized in their paper. Furthermore, the developing trends of computational drug repositioning were discussed. An ensemble approach was proposed by Lu et al. to predict hepatotoxicity of drug metabolites. A total of 270 descriptors were used to encode each drug compound, and a strategy similar to boosting was adopted to tackle the data imbalance. Lu et al. presented a novel computation method to infer novel candidate drugs for breast cancer. Several types of information, such as chemical-chemical interactions, chemical-protein interactions, and the EM clustering algorithm were integrated in the method. Fifteen candidates evaluated by the method were confirmed to be effective for breast cancer. Ding and Zhang gave a computational analysis on carcinogenic and non-carcinogenic chemicals using gene ontology terms and KEGG pathways. The enrichment theory of GO and KEGG was adopted to encode each chemical and the minimal redundancy maximal relevance (mRMR) method was used to analyze these GO and KEGG features, thereby extracting important GO terms and KEGG pathways that are helpful for discriminating carcinogenic and non-carcinogenic chemicals. A review on the pharmacological action, pharmacology network, including mutation of signaling receptor and modulation of intracellular signaling pathway, and combination treatment strategy of Epigallocatechin-3-gallate (EGCG) was given by Song et al. The possible targets and combinatorial applications based on the characteristics of EGCG were also summarized and sorted out in their study. Wang et al. proposed a random forest-based prediction model for distinguishing three post-translational modifications (PTMs), including lysine acetylation, sumoylation, and ubiquitination. The mRMR method and incremental feature selection (IFS) method were adopted to build an optimal prediction model and extract key features, which are helpful to describe the differences between these three PTMs. The last study presented by Kong et al. gave a method for identifying dysregulated pathways related to Alzheimer’s disease (AD). The proposed method took into account the internal correlations not only between genes but also pathways. Mutual information (MI) was used to measure interdependencies between genes, and by integrating the topology information from KEGG, the significant pathways involved in the feature genes were identified. Then, the distance correlation (DC) was applied to measure the pairwise pathway crosstalk between normal and AD samples to discover the dysregulated pathways. Such molecular biology analysis shows that it can help to find new effective target genes for drug design.

It is my great honor to organize this special issue that contains seven outstanding studies. It is expected that the new proposed methods would give novel ways for tackling different types of data and novel findings yielded by these methods would provide new insights to biologists and medical scientists. Finally, I must express my great thanks to the Editor-in-Chief of Combinatorial Chemistry & High Throughput Screening, Prof. Gerald H. Lushington, for giving me an opportunity to bring this special issue.

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(Guest Editor)

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