Tentative Outline

Special Thematic Issue for the journal "Current Cancer Drug Targets"

Title: Natural products-based drug discovery using informatics and computational methods

Guest Editor: Jincheng Wang

Co-Guest Editor: Chunjie Jiang

• **Scope of the Thematic Issue:**

Natural products, including their primary and secondary metabolites, are small molecules and complex structures derived from any organism. Over the past decades, natural products have enlightened the advent of modern medical science, and natural products-based drug discovery has contributed to one of the most remarkable achievements in pharmaceutical science. Pharmacotherapy for many diseases (especially for cancer, metabolic disorders, and aging-related diseases) has substantially improved owing to natural products. The significant achievements further inspire drug discovery based on natural products, and a fast-growing is observed in the natural product sciences. However, further identification of natural products with higher efficiency remains challenging.

As new research technologies, informatics and computational methods can get useful information by integrating massive data. Compared with traditional laboratory methods, informatics and computational methods can effectively increase research efficiency and guide the research direction. Recently, informatics and computational technology have provided a systematical and efficient tool to investigate natural products and thus extended drug discovery. Many informatics and computational methods have been applied to screen natural products and analyze the underlying mechanisms of their pharmacological effects, such as data mining, big data processing, molecular docking, network pharmacology, cheminformatics, etc. For example, network pharmacology is a data-driven computational method for drug investigation that encompasses systems biology, network analysis, and connectivity. Computational methods can also monitor drug efficacy, assess drug metabolism, and predict treatment response. Importantly, artificial intelligence (deep learning-based computational techniques) also contributed to drug discovery from a higher dimension.

This Special Issue aims to focus on the investigation of natural products for clinical disease management. Various informatics and computational methods, such as data mining, big data processing and machine learning techniques, are warmly welcomed. We invite scientists to submit clinical studies, experimental research, or review articles for this issue.

Keywords: natural products, network pharmacology analysis, drug discovery, bioinformatics, drug target mining, machine learning, drug–disease interaction targets

Sub-topics:

➢ Informatics and computational methods to discover novel drugs based on natural products.

➢ Informatics and computational methods to identify drug-disease interaction targets.

➢ Network pharmacology analysis for the detection of potential treatment strategies.

➢ Network pharmacology analysis to investigate the mechanisms underlying their pharmacological effects.

➢ Clinical studies for investigating the effect of natural products in cancer treatment.

➢ Clinical validation on natural products as adjuvant therapy in cancer treatment strategies.

➢ Natural products-based drug discovery targeting COVID-19.

➢ Informatics and computational methods to predict the interaction between natural products.

➢ Digital online database recoding putative or validated natural products target.

➢ Software tools or online web servers to assistant natural products-based drug discovery.

➢ Underlying factors affecting the sensitivity of drugs based on natural products.

➢ Review article to summarize the recent technological developments in natural products-based drug discovery.

Schedule:

- ✧ Thematic issue submission deadline: 30 August 2023

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