

Tentative Outline

Recent Advances in Rational Drug Design for Commonly Occurring Diseases

Guest Editors: Jiwei Hu

• **Scope of the Thematic Issue:** In this special thematic issue of Current Pharmaceutical Design, review articles are planned in the broad field of drug design. Modern drug design has been generally carried out based on genomics/proteomics, bioinformatics, chemoinformatics, quantum mechanics, molecular mechanics, molecular dynamics, computer science, etc. This thematic issue particularly focuses on sophisticated cutting-edge drug design technologies, for example, 2D/3D-quantitative structure activity relationship, molecular docking, virtual screening and artificial intelligence. These technologies have a vast application prospect for the design and development of new chemical entities. This thematic issue is a collection of papers featuring studies on drugs for the coronary heart disease, aging, alzheimer, SARS corona virus, hypertension, HIV, diabetes mellitus, hepatitis and cancers. These are commonly occurring human diseases with high incidence severely threatening the human health and lives, which have attracted tremendous attention and have been broadly studied over the past decades. We plan to invite internationally eminent scholars or distinguished experts to contribute to this special issue concerning recent progress in the field.

Keywords: 2D/3D-quantitative structure-activity relationship; virtual screening; Molecular docking; Principal component analysis; Cross Validation; Bootstrap; Artificial intelligence

The subtopics to be covered within this issue must be provided:

- 2D/3D-quantitative structure-activity relationships in drug design
- Virtual screening in drug design
- Molecular docking in structure-based drug design
- Applications of artificial intelligence in drug design

- ✧ Manuscript submission deadline: March 20, 2020
- ✧ Peer Review Due: May 20, 2020
- ✧ Revision Due: July 30, 2020
- ✧ Announcement of acceptance by the Guest Editors: August 30, 2020
- ✧ Final manuscripts due: September 20, 2020

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