Tentative Outline

Special Thematic Issue for the journal "Medicinal Chemistry"

Title of the Thematic Issue: Advances of anti-cancer medicine based on computational methods

Guest Editor: Chi Zhang
Senior Co-Guest Editor: **Bing Niu**

- **Scope of the Thematic Issue:**

Cancers are chronologic diseases, which are also the main killer of human health. Despite many treatments against cancer have been developed, novel anti-cancer medicines are still demanded. With the quickly development of computational methods combined with huge biological data derived from sequencing technology, the applications of new techniques and approaches have become a very hot topic in drug metabolism, pharmacokinetics, drug disposition and drug design. This special issue will focus on various aspects of the development and application of computational techniques in development of anti-cancer medicine. Potential topics include but are not limited to the following: metabolic pathways; drug-drug interactions and enzyme kinetics; pharmacokinetics, pharmacokinetic-pharmacodynamic modeling, and toxicokinetics; interspecies differences in metabolism or pharmacokinetics, species scaling and extrapolations; drug transporters; target organ toxicity and interindividual variability in drug exposure-response; extrahepatic metabolism; bioactivation, reactive metabolites, and developments for the identification of drug metabolites

Keywords: Machine learning, simulation, artificial intelligence, drug design, big data, QSAR,

Sub-topics:

The sub-topics to be covered within the issue should be provided:

- Discover of hub genes and biomarker
- Discover and validation of potential related drug target
- The development of techniques in prediction biomarker with machine learning
- Clinical data analysis using artificial intelligent techniques
- Drug target discovery by using Molecular Simulation, Multi-spectroscopy and omics Methods
- Targeted drug design based on QSAR
- Computer-based in drug design

Tentative titles of the articles:

1. QSAR Analyses for VEGFR-2 Inhibitors based on bioinformatics
2. Machine learning in drug design in anti-cancer medicine,
3. Current situation, Development and Technological Changes of Antibody-Drug Conjugates
4. Clinical Research and Progress of Anticancer Drugs,
5. Propofol impairs memory consolidation via activating the ubiquitin proteasome system in the hippocampus
6. Application of deep learning techniques in in drug target.

Schedule:

- Thematic issue submission deadline: 2023.1.31

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