Computational and Mathematical Methods in Medicine

Hindawi

Special Issue on

Computerized Techniques for Accelerating Discovery of Natural and Natural-Based Drug Candidates

CALL FOR PAPERS

Natural and natural-based medicines constitute at least one-third of the approved drugs. Although computational methods are well established in drug discovery and molecular design, their application in the field of natural products is still in its infancy. Only few works reported application of *in silico* techniques in research projects of natural-based drug discovery. Aiming to accelerate identification of bioactive natural-based drug candidates and to optimize drugs in clinical use by maximizing their efficacy and minimizing their potential side effects, we need to intensify the application of computerized techniques and modeling approaches in this field.

Natural products are considered as chemicals that have been optimized to interact with biological systems through a long natural selection process, and the utility of mathematical/statistical-based modeling approaches could provide insights into the physicochemical properties associated with their drug-likeness at the molecular level. Therefore, scientific works that analyze natural product databases for their "drug-like" properties and pharmacokinetic profiles are of high importance.

This special issue aims to collect original research and review articles focused on the *in silico* infrastructure for accelerating the discovery of natural and natural-based drugs and computerized tools and modeling approaches, in addition to mathematical, computational, methodological, and good practices for the discovery of natural-based drug candidates. We anticipate that papers will address issues of data analysis, optimization methods, computerized tools, modeling approaches, and models for accelerating natural and natural-based drug discovery process.

Potential topics include but are not limited to the following:

- Methodologies and tools for modeling and data analysis that are applied to accelerate drug discovery process
- Optimization and machine learning methods in drug discovery
- Good practices for discovery of drug candidates via application of modeling techniques
- Application of *in silico* techniques in the discovery of bioactive natural products
- Application of structural-based and/or ligand-based modeling techniques in discovery of bioactive natural products
- Mathematical modeling approaches in natural-based drug development, safety, and efficacy studies
- Application of modeling techniques to predict natural likeness of chemicals and its application in drug design
- Natural products and synthetic chemicals: data analysis and application of modeling tools to make synthetic chemicals more natural-like
- Application of modeling tools to prove the safety of natural products

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Papers are published upon acceptance, regardless of the Special Issue publication date.

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