Special Issue

Molecular Modeling: Computer-Aided Drug Design

Message from the Guest Editor

Computer-aided Drug Design (CADD) is an approach widely utilized to productively yield hit or lead compounds which possess the potential to be biologically active candidates for further test. We are interested in articles that discuss the current cutting edge CADD methodologies to tackle the ongoing innovation crisis faced by drug discovery. Topics of interest include, but are not limited to, the following:

- Introduction of novel virtual screening method to screen a large compound library for active compounds.
- Study of Quantitative Structure-Activity Relationship (QSAR) to gain insight into structural details of active compounds and to optimize the physicochemical properties of candidate compounds.
- Development of fragment-based approach to form a nucleating site of a molecular entity.
- Application of machine learning to aid the identification of compounds which are promising to be active to target proteins.
- Web-based programs for performing computational drug discovery with freely accessible facility.
- Implementation of network pharmacology-based methods/tools to predict and analyze possible polypharmacology of a test compound.

Guest Editor

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Message from the Editor-in-Chief

You are invited to contribute either a research article or a comprehensive review for consideration and publication in *Processes* (ISSN 2227-9717). *Processes* is published in open access format – research articles, reviews, and other content are released on the internet immediately after acceptance. The scientific community and the general public have unlimited, free access to the content. As an open access journal, *Processes* is supported by the authors and their institutes through the payment of article processing charges (APCs) for accepted papers. We would be pleased to welcome you as one of our authors.

Editor-in-Chief

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