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Molecular Modeling: Computer-Aided Drug Design

Guest Editor:

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Deadline for manuscript submissions:
closed (31 July 2022)

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.

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Message from the Editor-in-Chief

Processes (ISSN 2227-9717) provides an advanced forum for process/system-related research in chemistry, biology, material, energy, environment, food, pharmaceutical, manufacturing and allied engineering fields. The journal publishes regular research papers, communications, letters, short notes and reviews. Our aim is to encourage researchers to publish their experimental, theoretical and computational results in as much detail as necessary. There is no restriction on paper length or number of figures and tables.

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