Tentative Outline

Special Thematic Issue for Combinatorial Chemistry & High Throughput Screening

CADD and Molecular Dynamic Simulations: Potential Impacts to Conventional Medicines

Guest Editors: Dr. Muhammad Rizwan Javed, Dr. Dong-Qing Wei and Dr. Aman Chandra Kaushik

Aims & Scope:

Computer Aided Drug Designing (CADD) and Molecular Dynamic (MD) Simulations are extensively utilized for high-quality research related to drug screening and discovery based on artificial intelligence approaches. Machine Learning Approaches in CADD and MD simulations is an emerging field of study concerned with the drug design and testing of its molecular properties, behavior and interactions in order to assemble better materials, systems, and processes for specific functions. Molecular Docking and MD Simulation advancements in parallel with the rapid progress in drug design methods are the areas of current research Worldwide. These techniques are becoming a powerful tool in medicinal chemistry to identify the starting points as hit molecules, opening up new avenues for drug discovery. These approaches also help out to reduce the time and cost taken for drug research and their development.

This thematic issue aims to publish the leading-innovative research on Computer Aided Drug Designing, Molecular Dynamic Simulations, Molecular Docking and Machine Learning Approaches based on Artificial Intelligence, to process and analyze high throughput data of biomedicine. It will provide an excellent collection of the latest research on bioinformatics and health informatics, serving as a forum to bring together interdisciplinary scientists from molecular biology, computer science, chemistry, physics, medicine, mathematics and statistics.

Keywords: CADD, Molecular Dynamic Simulations, Molecular Docking, Artificial Intelligence, Machine Learning, Bioinformatics, Health Informatics, High Throughput Screening, Drug Chemistry.

Subtopics:

The subtopics include but are not limited to the following:

- Computer aided drug discovery and target identification
- Implications for machine learning in modulating drug targets
- Influence of compounds in the era of machine learning
- Molecular dynamics simulations and molecular docking
- Novel breakthroughs towards mechanism-based and machine learning-based precision medicines
- Machine learning approaches for new sampling techniques in molecular/quantum simulations
- Interdisciplinary technologies and applications for biomedical informatics

Schedule:

- **Manuscript Submission Deadline:** 15 October, 2020
- **Peer Review Due:** 30 November, 2020
- **Revision Due:** 15 December, 2020
- **Announcement of Acceptance by the Guest Editors:** 30 December, 2020
- **Final Manuscripts Due:** 15 January, 2021

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