Advances in Pharmacological and Pharmaceutical Sciences

Hindawi

Special Issue on

Computational and Synthetic Approaches in Drug Discovery of Bioactive Compounds for Metabolic Disorders

CALL FOR PAPERS

Drug discovery is a complex and time-consuming process that involves identifying and developing new therapeutic agents for treating diseases. The identification of new natural bioactive compounds is an essential aspect of modern medicine, allowing for improved efficacy in the treatment of a wide range of diseases. In recent years, the use of synthetic and computational approaches has revolutionized drug discovery and enabled the rapid discovery and optimization of new bioactive compounds. Synthetic approaches involve the creation of new compounds, while computational approaches use computer-based tools to design and optimize potential drug candidates.

The field of drug discovery for the treatment of metabolic disorders faces several pressing challenges. These include the need for novel, effective targets for diabetes treatment, addressing the growing problem of drug resistance, minimizing adverse side effects, and improving the bioavailability of potential drug candidates. Additionally, the complex nature of diabetes, with its multiple subtypes, further complicates the development of tailored therapies. Meeting these challenges is crucial in the quest for more efficient and safer antidiabetic agents.

This Special Issue aims to provide a platform for researchers to present their findings, showcasing the latest advances in the use of computational and synthetic approaches to in the discovery of natural bioactive compounds. We hope to highlight new developments, challenges, and future directions in both synthetic and computational approaches for the treatment of metabolic disorders using bioactive compounds. We welcome both original research and review articles.

Potential topics include but are not limited to the following:

- Molecular docking and virtual screening in drug design of bioactive compounds
- Molecular dynamics simulations in drug development
- Computational approaches for targeting protein-protein interactions
- Pharmacophore modeling and feature-based screening
- Structure-based design of antibiotics and antivirals
- In silico adsorption, distribution, metabolism, elimination, and toxicity (ADMET) prediction and assessment
- Network pharmacology and systems biology in drug discovery
- Drug repurposing and polypharmacology
- Machine learning and artificial intelligence in drug discovery of bioactive compounds
- Chemoinformatic and bioinformatic applications in drug discovery
- Structural bioinformatics for target identification and validation
- Quantum computing in drug discovery

Authors can submit their manuscripts through the Manuscript Tracking System at https://review.wiley.com/submit?specialIssue=723495.

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

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