Special Issue

Discovery of Novel Antimicrobial Peptides Using Machine Learning and Molecular Dynamic Simulations

Message from the Guest Editors

Antimicrobial peptides are a class of small molecules composed of peptides with antimicrobial activity, possessing unique mechanisms against various pathogens, and are considered one of the important directions in future antimicrobial drug research. Through data-driven machine learning methods, researchers can utilize large-scale biological data for pattern recognition and prediction, thereby accelerating the process of discovering antimicrobial peptides. Additionally, molecular dynamics simulation techniques can simulate the interactions between antimicrobial peptides and target molecules, revealing their structural and functional features at the molecular level and providing crucial insights for designing antimicrobial peptides with enhanced selectivity and efficacy. This Special Issue aims to explore the acceleration of the discovery of novel antimicrobial peptides and their antimicrobial mechanism research using machine learning and molecular dynamics simulation.

Guest Editors

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Message from the Editor-in-Chief

There are very few fields that attract as much attention as scientific endeavor related to antibiotic discovery, use and preservation. The public, patients, scientists, clinicians, policy-makers, NGOs, governments, and supra-governmental organizations are all focusing intensively on it: all are concerned that we use our existing agents more effectively, and develop and evaluate new interventions in time to face emerging challenges for the benefit of present and future generations. We need every discipline to contribute and collaborate: molecular, microbiological, clinical, epidemiological, geographic, economic, social scientific and policy disciples are all key. *Antibiotics* is a nimble, inclusive and rigorous indexed journal as an enabling platform for all who can contribute to solving the greatest broad concerns of the modern world.

Editor-in-Chief

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