

## Special Issue

# Computational Approaches in Discovery and Design of Antimicrobial Peptides—2nd Edition

### Message from the Guest Editors

Bacterial resistance to antibiotics is still a serious concern worldwide, especially when dealing with bacterial infections associated with COVID-19. Because of the potential of the naturally occurring antimicrobial peptides when facing multi-resistant problems, many computational approaches have been developed to assist the search and design of antibiotic peptides within the AMPs chemical space. Currently, classical alignment-based and alignment-free prediction algorithms and non-conventional approaches such as complex similarity networks are being applied for AMPs detection. On the other hand, the design and optimization of AMPs are also computationally assisted by the *in silico* generation of both random and rationally oriented peptide libraries. Finally, with the improvement of high-throughput screening (HTS) techniques applied to the discovery of AMPs in biological samples, the associated computational approaches have also evolved to assist this biodiscovery process. This Special Issue invites authors to publish original research including *in silico* approaches used for the rational search/discovery and design of AMPs. Review papers on this topic are welcome too.

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### Guest Editors

Dr. Guillermin Agüero-Chapin

Dr. Yovani Marrero-Ponce

Prof. Dr. Agostinho Antunes

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### Deadline for manuscript submissions

30 June 2025



## Antibiotics

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## About the Journal

### 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 disciplines 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.

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### Editor-in-Chief

Prof. Dr. Nicholas Dixon  
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