

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.

Guest Editors

Dr. Guillermin Agüero-Chapin

Dr. Yovani Marrero-Ponce

Prof. Dr. Agostinho Antunes

Deadline for manuscript submissions

31 December 2025



Antibiotics

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.7
Indexed in PubMed



mdpi.com/si/172694

Antibiotics
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
antibiotics@mdpi.com

[mdpi.com/journal/
antibiotics](https://mdpi.com/journal/antibiotics)





Antibiotics

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.7
Indexed in PubMed



[mdpi.com/journal/
antibiotics](https://mdpi.com/journal/antibiotics)



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.

Editor-in-Chief

Prof. Dr. Nicholas Dixon
School of Chemistry and Molecular Bioscience, University of
Wollongong, Wollongong, NSW 2522, Australia

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, PMC, Embase, CAPlus / SciFinder, and other databases.

Journal Rank:

JCR - Q1 (Infectious Diseases) / CiteScore - Q1 (General Pharmacology, Toxicology and Pharmaceutics)