

## Special Issue

# Innovative Computational and Experimental Strategies in Antimicrobial Drug Discovery

### Message from the Guest Editors

Our Special Issue aims to highlight cutting-edge research and reviews integrating experimental and computational approaches in the discovery and development of next-generation antimicrobial agents. The combination of *in silico* tools, such as virtual screening, molecular modeling, and artificial intelligence, with *in vitro* and *in vivo* screening platforms, is reshaping antimicrobial research, accelerating drug discovery, and providing key mechanistic insights for rational design. Topics of interest include drug repurposing, structural optimization of existing agents, and emerging paradigms such as photopharmacology, polypharmacology, and hybrid strategies merging synthetic chemistry with computational methods.

We warmly invite researchers from academia and industry to contribute their innovative works on novel antimicrobial entities, computational investigations, and experimental validation, fostering collaboration and inspiring new directions in the global fight against antimicrobial resistance.

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### Guest Editors

Dr. Domiziana Masci

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### Deadline for manuscript submissions

closed (10 May 2026)



## Pharmaceuticals

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## About the Journal

### Message from the Editor-in-Chief

Because of your expertise in the field of drug sciences, I kindly invite you to consider publishing your current work, in the form of a research article or a review, in the open access electronic journal *Pharmaceuticals*.

*Pharmaceuticals* is characterized by an active editorial board and a dynamic editorial staff. Manuscripts are peer-reviewed and a final decision is provided to authors within 4–6 weeks after submission. Papers are published on the web immediately after acceptance. For details on the submission process or any other matter, please do not hesitate to contact us.

We hope to handle your contribution to *Pharmaceuticals* soon.

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### Editor-in-Chief

Prof. Dr. Amélia Pilar Rauter

Departamento de Química e Bioquímica (DQB) e Centro de Química Estrutural (CQE), Institute of Molecular Sciences, Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal

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