

Special Issue

Drug Target Exploration and Drug Design & Development Based on Small Molecule: 2nd Edition

Message from the Guest Editors

The recent advancements in medicinal chemistry have facilitated the identification and development of small molecules by using classical and green methods. Moreover, the application of computational approaches such as docking and molecular dynamics has been crucial in the exploration of potential targets, including those that are traditionally considered 'undruggable' or orphans (<https://doi.org/10.3390/books978-3-0365-2778-9>). This Special Issue aims to provide a comprehensive overview of the latest advances in the research on drug target exploration as well as drug design and development based on small molecules. We welcome submissions from researchers in the field of drug discovery and design, including original research and review articles related to pharmaceutical sciences, pharmacology, chemical biology, and bioinformatics. The first edition of our Special Issue, titled "Drug Target Exploration and Drug Design & Development Based on Small Molecule," garnered significant scholarly interest. Building upon this success, we are pleased to announce the release of its second edition "Drug Target Exploration and Drug Design & Development Based on Small Molecule: 2nd Edition".

Guest Editors

Dr. Marco Tutone

Dipartimento di Scienze e Tecnologie Biologiche Chimiche e Farmaceutiche (STEBICEF), Università degli Studi di Palermo, Via Archirafi 32, 90123 Palermo, Italy

Dr. Giulia Culetta

Department of Biological, Chemical and Pharmaceutical Sciences and Technologies (STEBICEF), University of Palermo, 90123 Palermo, Italy

Deadline for manuscript submissions

25 July 2026



Pharmaceuticals

an Open Access Journal
by MDPI

Impact Factor 4.8
CiteScore 7.7
Indexed in PubMed



mdpi.com/si/266822

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

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





Pharmaceuticals

an Open Access Journal
by MDPI

Impact Factor 4.8
CiteScore 7.7
Indexed in PubMed



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



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.

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

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 (Pharmacology and Pharmacy) / CiteScore - Q1 (Pharmaceutical Science)