



an Open Access Journal by MDPI

Contribution of Computational Tools for Drug Development against Pathogens

Guest Editors:

Dr. Edson Roberto da Silva

Laboratório de Farmacologia e Bioquímica (LFBq), Departamento de Medicina Veterinária, Universidade de São Paulo Faculdade de Zootecnia e Engenharia de Alimentos, Pirassununga, SP 13635-900, Brazil

Dr. Simone Brogi

Department of Pharmacy, University of Pisa, Via Bonanno 6, 56126 Pisa, Italy

Deadline for manuscript submissions: closed (20 January 2024)

Message from the Guest Editors

This Special Issue "Contribution of Computational Tools for Drug Development against Pathogens" welcomes submissions of review and research articles related to the contribution of computational tools for drug development against human and/or animal pathogens, as well as plant pathogens.

In silico studies can accelerate and guide drug discovery and therapeutic approaches. In this manner, we invite submissions of manuscripts that highlight and/or improve the use of tools such as docking analysis; in silico studies of pharmacokinetics parameters of absorption, distribution, metabolism, and excretion (ADME); and use of electronic tools to analyze data and/or Big Data related to animals and plants pathogens. Furthermore, studies on molecular modeling are also welcome.

In summary, this Special Issue plans to highlight the latest research on the use of in silico tools against pathogens. This Special Issues will be a guide for tools related to drug development and future collaborative research studies.



mdpi.com/si/106743







an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Hinh Ly

Department of Veterinary & Biomedical Sciences, University of Minnesota, Twin Cities, MN, USA

Message from the Editor-in-Chief

The worldwide impact of infectious disease is incalculable. The consequences for human health in terms of morbidity and mortality are obvious and vast but, when infections of animals and plants are also taken into account, it is hard to imagine any other disease that has such a significant impact on our lives—on healthcare systems, on agriculture and on world economics. *Pathogens* is proud to continue to serve the international community by publishing high quality studies that further our understanding of infection and have meaningful consequences for disease intervention.

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, PubAg, CaPlus / SciFinder, AGRIS, and other databases.

Journal Rank: JCR - Q2 (*Microbiology*) / CiteScore - Q2 (*General Immunology and Microbiology*)

Contact Us

Pathogens Editorial Office MDPI, Grosspeteranlage 5 4052 Basel, Switzerland Tel: +41 61 683 77 34 www.mdpi.com mdpi.com/journal/pathogens pathogens@mdpi.com X@Pathogens_MDPI