

## Special Issue

# In Silico and In Vitro Screening of Small Molecule Inhibitors

### Message from the Guest Editors

This Special Issue aims to highlight the latest advances, challenges and applications of in silico tools and in vitro screening in the field of drug discovery of SMIs. We welcome the submission of research and review articles on advances in the drug discovery, design and development of biological target inhibitors against different disease models. Scientists from both academia and industry are invited to submit their manuscripts covering relevant topics, including the design and synthesis of novel chemical entities (NCEs), repurposing of approved drugs, cell-based or animal experiments and in silico computational approaches to elucidate future directions in drug discovery.

The main objective of this Special Issue is to provide a comprehensive overview of cutting-edge in silico and in vitro screening methodologies for the design and development of bioactive NCEs with therapeutic relevance across various disease contexts, with a specific focus on the elucidation of SMI–biological target interaction mechanisms by employing the synergistic strategy of combining computational with experimental approaches.

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### Guest Editors

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### Deadline for manuscript submissions

closed (10 June 2025)



## 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*.

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

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### Editor-in-Chief

Prof. Dr. Amélia Pilar Rauter

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