

## Special Issue

# Structural and Computational-Driven Molecule Design in Drug Discovery

### Message from the Guest Editors

Drug development is a complicated, high-risk, expensive, and lengthy process along with several stages such as target identification, lead discovery and lead optimization. In this process, the congruence between computational and experimental outcomes is a mainstay for the exploration of novel compounds. Besides, in the drug development process, many drug candidates could not pass the trials successfully due to the inadequate ADMET properties. Therefore, in silico ADMET analysis is attractive and a cost-saving strategy for a large number of compounds prior to applying expensive and time-consuming in vitro and in vivo ADMET estimation. This Special Issue aims to provide deep mechanistic insights into strategies in structural dynamics studies and computational methods. It is our great pleasure to invite you to submit original research articles and reviews in a Special Issue on "Structural and Computational-Driven Molecule Design in Drug Discovery". Research areas may include (but are not limited to) the following: Structural dynamics studies Computer-aided drug design Molecular dynamics simulations Molecular docking Virtual screening QSAR In silico ADMET.

### Guest Editors

Dr. Halil İbrahim Ciftci  
Dr. Belgin Sever  
Dr. Hasan Demirci

### Deadline for manuscript submissions

closed (26 February 2024)



## 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

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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