

## Special Issue

# Structural Bioinformatics: Molecular Regulation of Drug Design and Targeted Therapy in Human Health

### Message from the Guest Editor

The integration of computers in the drug-discovery process is efficient for analysis of complex biological data, the simulations of drug interactions and the prediction of potential drug efficacy and mechanisms of action. In addition, the use of computer-aided drug design (CADD) methods used for enabling the rational design of compounds with improved pharmacological properties, often considering the structural nature of the target and potential drug molecules. New revolutionizing tools continue to appear, such as AlphaFold and RosettaFold, opening new ways of addressing human health from a structural perspective. This Special Issue will focus on the application of structural bioinformatics to human health, particularly through techniques that emphasize a molecular analysis of the problem. Examples include homology modelling, structure-based drug design and discovery, atomistic molecular dynamics simulations drug-target interactions and other in silico techniques that integrate the structural perspective of molecules and their potential targets in the drug-development process.

[https://www.mdpi.com/journal/ijms/special\\_issues/Bioinformatics-Drug\\_Design](https://www.mdpi.com/journal/ijms/special_issues/Bioinformatics-Drug_Design)

### Guest Editor

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### Deadline for manuscript submissions

closed (25 December 2023)



## International Journal of Molecular Sciences

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CiteScore 9.0  
Indexed in PubMed



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*International Journal of  
Molecular Sciences*  
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### Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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