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

Guest Editor:

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Deadline for manuscript submissions:
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Message from the Guest Editor

Dear Colleagues,

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.

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Message from the Editor-in-Chief

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