Special Issue

Molecular Docking and Dynamics in Drug Discovery

Message from the Guest Editor

Molecular docking and molecular dynamics simulations are foundational pillars of modern structure-based drug discovery. These computational techniques provide critical insights into ligand–receptor interactions, accelerating the identification and optimization of novel therapeutic candidates. Despite significant progress, challenges remain in areas such as scoring function accuracy, the comprehensive treatment of protein flexibility, and the predictive power of simulations. This Special Issue invites original research, methodological advancements, and critical reviews addressing the forefront of this dynamic field. We seek submissions detailing new methodologies, innovative applications showcasing SBDD campaigns, and insightful critical reviews on the strengths and limitations of current computational tools. For original research articles, in vitro experimental validation of key computational findings is required, and this requirement should be clearly emphasized in the manuscript summary. This will ensure alignment with the scope of the Special Issue and prevent potential misunderstandings regarding purely in silico studies.

Guest Editor

Dr. Črtomir Podlipnik
Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia

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Biomolecules
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
biomolecules@mdpi.com

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Department of Cellular and Molecular Medicine, Faculty of Health and Medical Sciences, University of Copenhagen, Blegdamsvej 3C, DK-2200 Copenhagen, Denmark

Prof. Dr. Lukasz Kurgan
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