# Special Issue

# Computational Biophysics: Advances in Molecular Dynamics

## Message from the Guest Editor

Recent advancements in computational chemistry and computer-aided drug design (CADD) have significantly accelerated the discovery and optimization of novel therapeutic agents. By integrating molecular modeling, ligand- and structure-based drug design, cheminformatics, and artificial intelligence, these approaches reduce both time and cost compared to traditional pipelines. This Special Issue aims to showcase cutting-edge research and methodologies in molecular docking, molecular dynamics simulations, QSAR/QSPR modeling, ADME-Tox predictions, and machine learning applications in drug discovery. We welcome original research articles, reviews, and perspectives that highlight innovative computational strategies and their successful application to the design and development of new drugs.

## Guest Editor

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## Deadline for manuscript submissions

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