

## Special Issue

# Accelerating Therapeutic Innovation: Advances in Computer-Aided Drug Discovery

### Message from the Guest Editors

This Special Issue on Computer-Aided Drug Discovery and Design (CADD) aims to present the latest advances and applications of computational methods in modern drug discovery, considering the continuous improvement of high-performance computing technologies. The goal of CADD methods is to improve and accelerate the drug discovery process. This issue will cover a wide range of CADD techniques, including traditional structure- and ligand-based drug design, possibly complemented by innovative machine learning approaches. We invite submissions that explore the application of CADD to address new challenges in drug discovery, such as the identification of novel therapeutic agents. Emphasis will be placed on innovative strategies that have undergone experimental (in vitro) validation, effectively linking computational predictions to practical outcomes.

### Guest Editors

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### Deadline for manuscript submissions

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