# Tentative Outline

*Sectional Editor: Dr. Mariangela Agamennone*

**Title: Recent advances in the application of computational approaches to drug design**

**Scope of the Thematic Issue:**
The scope of the Thematic Issue is to provide an updated view of the computational approaches that can be applied in the drug discovery field. The issue will cover both ligand-based and structure-based methods, with a special attention to the increasing application of machine learning methods.

**Keywords:** docking; QSAR; pharmacophore; machine learning; in silico; virtual screening; chemoinformatics; bioinformatics; molecular dynamics

## Sub-topics:

➢ Machine learning methods in drug discovery
➢ Structure-based approaches
➢ Ligand-based approaches
➢ Virtual screening
➢ Emerging strategies in computer-aided drug design

## Schedule:

✧ Thematic issue submission deadline: **March 31st 2024**

## Contacts:

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