Special Issue

Computer-Aided Drug Design Strategies

Message from the Guest Editor

Computer-aided drug design is nowadays a widespread research field that is continuously taking ground, raising more and more interest in the scientific community. This is undoubtedly due to the increasing use of machine learning (ML) and other artificial intelligence (AI) approaches in drug design and discovery. AI models demonstrated their reliability in a plethora of applications, including the prediction of physical-chemical properties and biological activities of small molecules, in silico evaluation of ADME and toxicological profiles of chemicals, as well as protein structures and ligand–protein complex prediction. Nevertheless, thanks to the constant improvement of computation power and efficiency, classic ligand-based and receptor-based in silico strategies still provide invaluable help in drug discovery, design and optimization. Long molecular dynamics (MD) simulations, allowing us to evaluate complex protein motions are now becoming more affordable, and MD studies for evaluating stability and potential binding affinity of predicted ligand–protein complexes are now commonly performed in hit finding, hit-to-lead and lead optimization campaigns.

Guest Editor

Dr. Giulio Poli

Department of Pharmacy, University of Pisa, Via Bonanno 6, 56126 Pisa, Italy

Deadline for manuscript submissions

closed (31 May 2024)

About the Journal

Message from the Editor-in-Chief

The *International Journal of Molecular Sciences* (*IJMS*) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, and molecular biophysics. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

Editor-in-Chief

Prof. Dr. José L. Quiles
Department of Physiology, Institute of Nutrition and Food Technology "Jose Mataix", Biomedical Research Center, University of Granada, Avda. Conocimiento s/n, 18100 Armilla, Granada, Spain

Author Benefits

Open Access:
free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:
indexed within Scopus, SCIE (Web of Science), PubMed, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

Journal Rank:
JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)