



## Recent Advances in Virtual Screening 3.0

Guest Editor:

**Dr. Gerard Pujadas**

Departament de Bioquímica i  
Biotecnologia, Universitat Rovira  
i Virgili, Tarragona, Catalonia,  
Spain

Deadline for manuscript  
submissions:

**closed (30 June 2023)**

### Message from the Guest Editor

Dear Colleagues,

This Special Issue is the continuation of our previous special issue "Recent Advances in Virtual Screening".

Finding new leads is an essential step in projects to develop and discover new drugs. There are two alternatives for achieving this goal: (a) experimentally testing compound libraries to find molecules that show any level of the desired bioactivity (a process known as high throughput screening) and (b) a cheaper alternative that aims to computationally predict the bioactivity of interest in files containing molecular databases (known as virtual screening, VS). This Special Issue of IJMS will focus on recent advances in VS with particular emphasis on tools (either local or on-line) or databases that can be used for free for non-profit research or education.

"Novel tools and VS must be either validated in silico or in vitro before first submission."





an Open Access Journal by MDPI

## Editor-in-Chief

### Prof. Dr. Maurizio Battino

Department of  
Odontostomatologic and  
Specialized Clinical Sciences,  
Sez-Biochimica, Faculty of  
Medicine, Università Politecnica  
delle Marche, Via Ranieri 65,  
60100 Ancona, Italy

## Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) 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, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *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.

## 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 (Inorganic Chemistry)

## Contact Us

---

*International Journal of Molecular  
Sciences* Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
www.mdpi.com

mdpi.com/journal/ijms  
ijms@mdpi.com  
X@IJMS\_MDPI