# **Special Issue**

# Recent Advances in Virtual Screening

# Message from the Guest Editor

Dear colleagues, 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.

#### **Guest Editor**

Dr. Gerard Pujadas

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

## **Deadline for manuscript submissions**

closed (15 August 2019)



# International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9 CiteScore 9.0 Indexed in PubMed



mdpi.com/si/22311

International Journal of Molecular Sciences Editorial Office MDPI, Grosspeteranlage 5 4052 Basel, Switzerland Tel: +41 61 683 77 34 ijms@mdpi.com

mdpi.com/journal/ ijms





# International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9 CiteScore 9.0 Indexed in PubMed





# 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.

### **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

### **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)

