# **Special Issue**

### Chemoinformatics in Drug Design: Achievements and Challenges

### Message from the Guest Editors

Chemoinformatics is a general word implying the massive use of informatics and software engineering in the chemistry field. In particular, in this topic, the focus is on medicinal chemistry and all the methods and their assessment in developing bioactive molecules. Experimental data should always be used to assess the chemoinformatic application, whereas methodology manuscripts will be considered also in absence of experimental data, but deep comparison with state-ofthe-art methods should be included.



## Molecules

an Open Access Journal by MDPI

Impact Factor 4.6 CiteScore 8.6 Indexed in PubMed



mdpi.com/si/70507

Molecules Editorial Office MDPI, Grosspeteranlage 5 4052 Basel, Switzerland Tel: +41 61 683 77 34 molecules@mdpi.com

mdpi.com/journal/

molecules



#### **Guest Editors**

Prof. Dr. Rino Ragno

Rome Center for Molecular Design, Dipartimento di Chimica e Tecnologie del Farmaco, Sapienza Università di Roma, P. le A. Moro 5, 00185 Roma, Italy

#### Dr. Milan Mladenović

Kragujevac Center for Computational Biochemistry, Department of Chemistry, Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, P.O. Box 60, Serbia

### Deadline for manuscript submissions

closed (30 September 2021)



# Molecules

an Open Access Journal by MDPI

Impact Factor 4.6 CiteScore 8.6 Indexed in PubMed



molecules



## About the Journal

### Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

### Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

### **Author Benefits**

### **High Visibility:**

indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Reaxys, CaPlus / SciFinder, MarinLit, AGRIS, and other databases.

### Journal Rank:

JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

### **Rapid Publication:**

manuscripts are peer-reviewed and a first decision is provided to authors approximately 15.1 days after submission; acceptance to publication is undertaken in 2.4 days (median values for papers published in this journal in the second half of 2024).