Special Issue

Application of Computational Methods in Drug Design

Message from the Guest Editors

The proposed workshop, entitled "*DesignIT-TO-LEAD: 1st Computational Medicinal Chemistry WorkShop*" is intended as a first trial to establish regular workshops in drug design on a biennual based frequency. The *DesignIT-TO-LEAD* will be organized at the Faculty of Science, University of Kragujevac, Republic of Serbia, from June 11 to June 15, 2018. The contribution of computational methodologies to drug discovery is no longer a matter of dispute, and all major world pharmaceutical and biotechnology companies use computational design tools. Computer-aided drug design encompasses computational methods and resources that are used to facilitate the design and discovery of new bioactive chemical entities. This workshop "*DesignIT-TO-LEAD: 1st Computational Medicinal Chemistry WorkShop*" will cover the main computational techniques currently used in the drug discovery process, supplying a basic level of knowledge of this field. Prof. Milan Mladenović

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 Mladenovic

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 (15 November 2018)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.2
CiteScore 7.4
Indexed in PubMed

mdpi.com/si/14474

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

mdpi.com/journal/molecules

Molecules

an Open Access Journal by MDPI

Impact Factor 4.2
CiteScore 7.4
Indexed in PubMed

mdpi.com/journal/molecules

MDPI

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 (Chemistry, Multidisciplinary) / CiteScore - Q1 (Chemistry (miscellaneous))

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).