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-of-the-art methods should be included.

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)



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

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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

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