Special Issue

Chemoinformatics and Bioinformatics Tools in Structure-Activity Modelling in Molecular Sciences: 3rd Edition

Message from the Guest Editor

At a time of universal digitization of data in various fields of research, including molecular sciences, there are more and more studies modeling the continuous or classification endpoints (activities/properties) of molecules. In doing so, the endpoints of molecules are most often classified (digitized) into two classes—active or inactive, and the classification is often carried out by grouping data into three or more classes.

This Special Issue aims to collect relevant contributions (papers) relating to one or more of the topics listed above (and those related to them), which are important for the acceleration of structure–activity research in molecular sciences. Applications aimed at modeling a broad spectrum of chemical, biological, pharmaceutical, biochemical, and environmentally relevant activities and properties of molecules are also welcome.

All forms of scientific articles covering the mentioned or related topics are welcome, i.e., original papers, reviews, and communications.

Guest Editor

Dr. Bono Lučić

The Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, Croatia

Deadline for manuscript submissions

closed (20 July 2025)

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

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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

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