

## Special Issue

# Cheminformatics 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.

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### Guest Editor

Dr. Bono Lučić

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### Deadline for manuscript submissions

closed (30 January 2026)



## International Journal of Molecular Sciences

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### Message from the Editor-in-Chief

The *International Journal of Molecular Sciences (IJMS)* 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, and molecular biophysics. *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.

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