

## Special Issue

# Molecular Simulations Applications in Biochemistry and Molecular Biology

### Message from the Guest Editors

This Special Issue will include research articles that describe the development of novel molecular simulation approaches and the applications of current methods to unexplained aspects of biochemical mechanisms, with the opportunity to present purely computational studies, as well as computational studies with experimental validations. The Special Issue will include also articles from the 15th edition of the Bioinformatics and Computational Biology Conference ([www.bbcc-meetings.it](http://www.bbcc-meetings.it)), Naples, Italy, November 16–18th, 2020.

### Guest Editors

Prof. Dr. Angelo Facchiano

National Research Council, Institute of Food Science, Via Roma 64,  
83110 Avellino, Italy

Dr. Anna Marabotti

Department of Chemistry and Biology “A. Zambelli”, Università di  
Salerno, Salerno, Italy

### Deadline for manuscript submissions

closed (31 May 2022)



## Molecules

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*Molecules*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[molecules@mdpi.com](mailto:molecules@mdpi.com)

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## About the Journal

### Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th 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 all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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### 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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#### Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).