

Special Issue

Application of Computational Studies for Elucidation of Protein Structure and Function

Message from the Guest Editor

Nowadays, computational techniques are widely applied to various problems including biological systems. In particular, many computer simulation techniques are applied to protein dynamics and folding. Bioinformatics techniques are also applied to extract various information from amino acid sequences and evolutionary results. Artificial intelligence techniques have been developed in the field of protein structure prediction. Thus, we are planning this Special Issue regarding new applications of various computational techniques to solve problems related to protein structures and functions. It should be noted that pure theoretical works are important to solve protein problems. We are also interested in very complicated protein systems and drug discovery.

Guest Editor

Dr. Takeshi Kikuchi

College of Life Sciences, Ritsumeikan University, 1-1-1 Nojihigashi, Kusatsu 525-8577, Shiga, Japan

Deadline for manuscript submissions

30 September 2025



Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



mdpi.com/si/196846

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

[mdpi.com/journal/
molecules](https://mdpi.com/journal/molecules)





Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



[mdpi.com/journal/
molecules](https://mdpi.com/journal/molecules)



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 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

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).