Special Issue

Computational Analysis for Protein Structure and Interaction

Message from the Guest Editor

Protein structure analysis is a hot topic and key issue in organic chemistry and molecular biology research. Several essential protein molecules were rebuilt with Cryo-EM (Cryo-Electron Microscopy) and their structures were published in *Nature* and *Science*. Computational structure analysis and prediction is a key process for the 3D structure reconstruction. Machine learning techniques have been employed for protein secondary and tertiary structure prediction for a long time, and it seemed to have reached a bottleneck. However, the development of the Cryo-EM technique brings new challenges and requirements to computer science. Additionally, deep learning in machine learning also seems to be powerful. Therefore, there is considerable and increasing interest in developing computational methods for protein structure analysis and prediction. Moreover, new techniques on structure could also facilitate protein–protein interaction research.

Guest Editor

Prof. Dr. Quan Zou

Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, Chengdu 610054, China

Deadline for manuscript submissions

closed (31 December 2018)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/9059

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

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

MDPI

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).