



Computational Analysis for Protein Structure and Interaction

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)

Message from the Guest Editor

Dear Colleagues,

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.

Prof. Dr. Quan Zou

Guest Editor





an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical
Biology and Phytochemistry,
University of Münster,
Corrensstrasse 48, D-48149
Münster, Germany

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.

Author Benefits

Open Access: free for readers, with [article processing charges \(APC\)](#) paid by authors or their institutions.

High Visibility: indexed within [Scopus](#), [SCIE \(Web of Science\)](#), [PubMed](#), [MEDLINE](#), [PMC](#), [Reaxys](#), [CaPlus / SciFinder](#), [MarinLit](#), [AGRIS](#), and [other databases](#).

Journal Rank: JCR - Q2 (Chemistry, Multidisciplinary) / CiteScore - Q1 (Chemistry (miscellaneous))

Contact Us

Molecules Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/molecules
molecules@mdpi.com
[X@Molecules_MDPI](#)