Special Issue

Protein Domains: Structures and Molecular Functions

Message from the Guest Editors

After the completion of human genome projects, it was shown that more than 70% of the genes are encoding multidomain proteins with two or more domains. Understanding of structure–function relationships of the individual domains should lead to interpretations of new physiological functions of unknown genes. We are motivated by this idea to develop methods for high-throughput structure determination, structure prediction, accurate modeling, molecular dynamic simulation, and the prediction of functions. The accumulation of structural, functional and evolutionary knowledge of protein domains is still being continued and is providing an important basis for structure-guided drug discovery, protein therapeutics, genome-based diagnosis, designed proteins, molecular beacons and sensors, and synthetic biology. This Special Issue focuses on recent advances in the domain-centric analysis of proteins in the field of biochemistry, bioinformatics and biophysics. In addition, either the analysis of natural domain pairs (architectures) or the design of artificial multi-domain proteins are in focus. Original research papers, concise reviews, and perspectives are welcome.

Guest Editors

Prof. Dr. Hidekazu Hiroaki

Graduate School of Pharmaceutical Sciences, Nagoya University, Furocho, Chikusa, Nagoya, Aichi 464-8601, Japan

Dr. Kentaro Tomii

Artificial Intelligence Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Tokyo, Japan

Deadline for manuscript submissions

closed (31 March 2020)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/24549

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).