Special Issue

Deep Learning for Modeling the Structure, Dynamics, and Function of Small and Large Molecules

Message from the Guest Editor

The rising algorithmic sophistication of deep learning frameworks is allowing us to make increasingly rapid discoveries and real headways in many long-standing, hallmark problems in computational biology and bioinformatics. Integrating such knowledge is leading to novel deep learning methods that are situated in molecular biology and biophysics and are leading to prediction of tertiary structure and structure ensembles, modeling of structural dynamics, design of novel proteins, optimization, and in-silico generation of small molecules for novel therapeutics and biotechnology applications, design of novel energy functions, prediction of variant effects on structure, stability, and function, prediction of function at varying levels of granularity, prediction and design of binding sites, and much more. The purpose of this special issue is to bring together the increasingly diverse and growing community of researchers across artificial intelligence, machine deep learning, bioinformatics, biophysics, and molecular biology.

Guest Editor

Prof. Dr. Amarda Shehu

Department of Computer Science, College of Engineering and Computing, George Mason University, Fairfax Campus, Fairfax, VA 22030, USA

Deadline for manuscript submissions

closed (20 March 2025)

International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/si/145702

International Journal of Molecular Sciences
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
ijms@mdpi.com

mdpi.com/journal/ijms

MDPI

International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/journal/ijms

MDPI

About the Journal

Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

Editor-in-Chief

Prof. Dr. Maurizio Battino
Department of Odontostomatologic and Specialized Clinical Sciences, Sez-Biochimica, Faculty of Medicine, Università Politecnica delle Marche, Via Ranieri 65, 60100 Ancona, Italy

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, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

Journal Rank:

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