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

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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

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