Special Issue

Machine Learning Methods for Bioinformatics

Message from the Guest Editor

Machine learning is transforming molecular informatics by enabling breakthroughs in predicting, designing, and optimizing small molecules and proteins. Yet challenges such as sparse biological data, combinatorial complexity, and interpretability demand methods that balance innovation with biophysical realism. This Special Issue invites methodological advances in ML for bioinformatics, focusing on rigorous solutions in areas like prediction (e.g., geometric deep learning for 3D protein–ligand dynamics), design (e.g., diffusion models for synthesizable molecules), and screening (e.g., federated learning across chemical libraries). We particularly welcome approaches addressing cryptic binding sites, ADMET optimization, or functional protein engineering, especially those integrating domain knowledge—e.g., physics-based priors or pharmacophoric rules. We also encourage submissions in ML for genomics, proteomics, or biomedical imaging. Manuscripts should demonstrate methodological novelty and in silico validation, including robustness, scalability, or consistency with structural principles. Open-source and reproducible contributions are highly encouraged.

Guest Editor

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Message from the Editor-in-Chief

The journal *Mathematics* publishes high-quality, refereed papers that treat both pure and applied mathematics. The journal highlights articles devoted to the mathematical treatment of questions arising in physics, chemistry, biology, statistics, finance, computer science, engineering and sociology, particularly those that stress analytical/algebraic aspects and novel problems and their solutions. One of the missions of the journal is to serve mathematicians and scientists through the prompt publication of significant advances in any branch of science and technology, and to provide a forum for the discussion of new scientific developments.

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