

Special Issue

Computational Methods for Drug Discovery and Biological Big Data Analysis

Message from the Guest Editor

This Special Issue presents research at the intersection of mathematical theory, computational methods, and intelligent systems for drug discovery and large-scale biological data analysis. Advances in AI, mathematical algorithms, and high-throughput technologies are creating new opportunities to address major challenges in pharmaceutical research and complex biological systems. We welcome submissions on drug target prediction, drug response modeling, drug combination analysis, and drug repurposing, as well as studies using biological big data—multi-omics integration, sequence analysis, and large biological networks—to generate new insights. Research on non-coding RNAs, biomarker discovery, and computational or machine-learning models supporting biological interpretation and clinical applications is also encouraged. Interdisciplinary works combining applied mathematics—optimization, probabilistic modeling, network analysis—with modern computational frameworks are particularly welcome. This Special Issue aims to promote methodological innovation and collaborations that advance intelligent, efficient, and interpretable solutions for biomedical challenges.

Guest Editor

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About the Journal

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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