



Inaugural Editorial for *Computational Biomedicine*

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Received: November 19, 2025 **Accepted:** November 19, 2025 **Published:** November 20, 2025

Cite this article: Huang D. Inaugural Editorial for *Computational Biomedicine*. *Comput Biomed.* 2026;1:202524. <https://doi.org/10.70401/cbm.2025.0002>

1. Introduction

The growing intersection between computational technology and biomedicine marks one of the most profound transformations in contemporary science. The rapid development of artificial intelligence (AI), machine learning (ML), and high-performance computing has created unprecedented opportunities to decode the complexity of biological systems. By integrating quantitative modeling, multi-omics analytics, and clinical informatics, computation now permeates all levels of biomedical research—from molecular structures and cellular networks to patient records and population health. This convergence not only enables large-scale pattern discovery but also drives a paradigm shift toward predictive, data-centric, and mechanism-aware medicine.

Computational Biomedicine is founded to advance this transformation by providing an interdisciplinary forum where algorithmic reasoning meets biological understanding. The journal emphasizes integrative studies that combine computational methods, experimental data, and clinical validation to generate actionable insights and translational outcomes. It welcomes contributions spanning AI-driven diagnostics, computational drug design, digital-twin modeling, and large-language-model applications in healthcare. Through its commitment to scientific transparency, reproducibility, and collaboration across disciplines, *Computational Biomedicine* seeks to accelerate the evolution of intelligent biomedical systems and promote a new era of computationally empowered precision medicine.

2. Artificial Intelligence and Machine Learning in Biology and Medicine

AI and ML have redefined the landscape of biomedical research, enabling predictive, interpretable, and data-driven medicine. Deep learning models outperform conventional statistical methods in disease classification, medical imaging, and molecular prediction tasks^[1]. Multi-modal architectures integrating genomics, imaging, and electronic health records provide unprecedented insight into complex disease mechanisms^[2]. Recent progress in explainable AI improves clinical interpretability, supporting trustworthy deployment in diagnostics, oncology, and personalized treatment^[3]. As healthcare systems increasingly rely on AI, the integration of human expertise and computational intelligence remains the central challenge for future biomedical innovation.

3. AI-Driven Biomedical Data Analysis

The explosion of biomedical data has generated new demands for scalable, intelligent analysis frameworks. AI-driven analytical pipelines have been developed to integrate omics, pathology, and clinical data, enabling the discovery of disease subtypes and patient stratification^[4]. Self-supervised and federated learning now allow cross-institutional collaboration while protecting data privacy^[5]. These approaches facilitate early diagnosis, longitudinal health monitoring, and precision therapeutics, transforming data into actionable medical knowledge^[6]. The journal highlights works that combine methodological rigor with real-world biomedical applications, particularly in integrative multi-omics analytics and clinical data harmonization.

4. Computational Platforms, Models, and Algorithms for Biomedicine

Advances in computational infrastructures and algorithm design underpin all modern biomedical simulation and modeling. Recent works leverage graph neural networks, Bayesian inference, and physics-informed learning to represent multi-scale biological systems^[7]. Cloud-native bioinformatics platforms such as Nextflow and DeepBioSim enhance reproducibility and computational efficiency^[8]. Hybrid algorithms linking stochastic biological modeling and AI prediction engines have improved simulation accuracy for immune, metabolic, and signaling systems^[9]. As complexity in biomedical datasets grows, the development of adaptive, scalable, and explainable algorithms will remain a fundamental mission of computational biomedicine.



5. Natural Language Processing and Data Mining in Healthcare

Biomedical literature, clinical notes, and patient records represent vast repositories of latent knowledge. Natural language processing (NLP) transforms these unstructured texts into computable data for reasoning and discovery. Domain-specific large language models such as BioGPT, Med-PaLM 2, and PubMedBERT have achieved state-of-the-art results in biomedical question answering and evidence summarization^[10]. Knowledge-graph-augmented retrieval systems further enhance interpretability and factual grounding^[11]. Recent studies illustrate that NLP models can synthesize mechanistic insights across millions of biomedical papers, supporting hypothesis generation, clinical documentation, and translational research^[12].

6. Intelligent and Process-Aware Information Systems in Medical Practice

Process-aware intelligent systems are reshaping the modern clinical environment. By integrating workflow mining, sensor data, and real-time decision support, these systems optimize patient management and reduce medical errors^[13]. AI-enabled hospital information architectures allow predictive scheduling, adaptive triage, and automated protocol recommendations^[14]. Beyond operational efficiency, process-aware computing contributes to safety, quality assurance, and the standardization of complex clinical pathways^[15]. The journal encourages research that bridges AI-based informatics with clinical process modeling to advance evidence-based, patient-centric healthcare.

7. Software and Algorithms for Bioinformatics and Computational Biology

Reproducible and open software ecosystems are essential for progress in computational biomedicine. Workflow managers such as Snakemake, Galaxy, and Nextflow have become standard for scalable bioinformatics pipelines^[16]. New algorithms in protein-structure prediction, network inference, and single-cell data analysis have accelerated biological discovery^[17]. The field increasingly emphasizes transparency and interoperability, adhering to FAIR principles (Findable, Accessible, Interoperable, Reusable)^[18]. *Computational Biomedicine* welcomes contributions that deliver methodological innovation with tangible impact on biomedical research, from genome analysis to molecular simulation.

8. AI-Assisted Drug Design and Development

AI has dramatically shortened the drug-discovery cycle through deep generative chemistry and molecular simulation. Graph neural networks and transformer models accurately predict molecular properties, docking affinities, and toxicity profiles^[19]. Diffusion models and reinforcement-learning based molecule generators demonstrate strong potential for de novo compound design^[20]. Integration of AI with wet-lab automation, as shown by the synergy between AlphaFold and generative screening, establishes a feedback loop between computation and experiment^[21]. This section invites works that bridge computational modeling, medicinal chemistry, and translational pharmacology.

9. Mathematical Modeling, Simulation, and Studies in Proteomics and Genomics

Mathematical modeling provides a rigorous framework to connect molecular interactions to cellular- and organism-level behaviors. Multi-scale models have been successfully used to simulate tumor growth, immune response, and metabolic dynamics^[22]. In proteomics and genomics, deep generative and Bayesian models reveal regulatory networks underlying disease heterogeneity^[23]. Simulation studies enhance understanding of biological complexity and inform therapeutic interventions. The journal supports works combining theoretical modeling with experimental validation to advance precision systems biology^[24].

10. AI Algorithms for Electronic Medical Record Analysis

Electronic medical records (EMRs) offer an unparalleled source of real-world clinical data. Machine learning algorithms detect comorbidities, predict patient outcomes, and optimize hospital workflows^[25]. Transformer-based clinical language models, such as GatorTron and ClinicalBERT, have advanced risk prediction and automated coding^[26]. Federated frameworks further ensure privacy-preserving learning across hospitals^[27]. The integration of EMR-derived intelligence into daily clinical practice exemplifies the transition toward learning health systems that continuously improve through data.

11. Digital Twin Visualization for Health Data

Digital-twin technologies construct personalized virtual models of patients by integrating genomic, physiological, and behavioral data. These dynamic representations enable real-time monitoring and predictive simulation of disease progression^[28]. Applications range from cardiology to neurorehabilitation, allowing physicians to test interventions in silico before clinical implementation. Visualization platforms powered by AI and IoT devices provide interactive dashboards for precision health management. This emerging field exemplifies the fusion of computational modeling and human-centered medicine^[29].

12. Large Language Models for Biomedicine and Health Data

Large language models (LLMs) represent a paradigm shift in computational biomedicine. Biomedical LLMs such as BioMedGPT,

PMC-LLaMA, and Med-Gemini integrate multimodal inputs, text, image, and molecular data, to generate biologically grounded reasoning^[30]. They enhance hypothesis generation, literature mining, and molecular property prediction^[31]. Integration with retrieval-augmented databases improves factual accuracy and interpretability^[32]. As models evolve toward domain-specific, trustworthy AI assistants, they are poised to become core components of biomedical research and healthcare delivery.

13. Conclusion

As computational technologies continue to reshape the foundations of modern biomedicine, the need for a unified forum that bridges algorithmic innovation, biological insight, and clinical translation has never been more urgent. *Computational Biomedicine* has been established to meet this demand. By integrating artificial intelligence, multi-omics analytics, mathematical modeling, and digital-twin technologies, the field is transitioning toward a data-centric, mechanism-informed, and prediction-driven paradigm of medical science. This journal aims to accelerate that shift by promoting rigorous methodological development, reproducible computational workflows, and interdisciplinary collaboration among researchers, clinicians, and engineers.

Declarations

Authors contribution

The author contributed solely to the article.

Conflicts of interest

De-Shuang Huang is the Editor-in-Chief of *Computational Biomedicine*. No other conflicts of interest to declare.

Ethical approval

Not applicable.

Consent to participate

Not applicable.

Consent for publication

Not applicable.

Availability of data and materials

Not applicable.

Funding

None.

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