

In silico biology and its prospects

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The term “*in silico*”, which is used to differentiate from “*in vitro*” (bench-top) and “*in vivo*” (animals or clinical studies), refers to the original studies conducted on computers using algorithms. Such studies have found vast applications in biological, medical, and pharmaceutical sciences, from genetics to computer-aided drug discovery (CADD), vaccine development, and even clinical trial design and analysis. They enable research with fewer resources and budget by using data obtained from past *in-vitro* and *in-vivo* experiments and can help study complicated cases that may be impossible or very difficult to perform in real life (1). For example, they may assist in developing drugs for rare diseases and pediatrics. *In silico* biology also helps accelerate research conduction. A familiar example is the COVID-19 mRNA vaccine design, performed quickly by bioinformatic tools, as announced by Moderna and Pfizer companies (2).

Keywords: Nanoparticles, Molecular interaction, Biocompatibility, Nanomedicines.

Please cite this article as: Negahdaripour M, Ghasemi Y. *In silico* biology and its prospect. Trends in Pharmaceutical Sciences. 2025;11(1):87-90. doi: 10.30476/tips.2025.105173.1277

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1. Introduction

In silico biology and bioinformatics are closely associated. Bioinformatics, a robust multidisciplinary science, is built on the foundation of multi-omics and big data collected in the biological field, further analyzed, and integrated through computer programming to achieve comprehensive and accurate results. Bioinformatics helps find relationships and patterns in these datasets (for instance, results of high-throughput sequencing studies) that cannot be done manually. It translates the vast data available in databases to new biological insights. Some essential bioinformatics tools include machine learning algorithms, sequence alignment algorithms, and network

analysis tools.

“Computational biology,” which is not exactly the same as bioinformatics (Table 1), refers primarily to computer processes used to study and simulate complex biological systems and processes. Computational biology allows studying and simulating very complex biological systems, including cellular signaling pathways, gene regulation, protein folding, and ligand-receptor interactions. Studying these very complex systems would be almost impossible with experimental approaches. Computational biology is usually used for a broader field encompassing bioinformatics and other research areas involving computational modeling and simulation of biological systems.

Both of these fields are interdisciplinary sciences involving several disciplines, including computer, information technology

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Table 1. A brief comparison of bioinformatics and computational biology.

	Bioinformatics	Computational biology
Subject of study and data used	Large biological datasets, including DNA or RNA sequences	Complex biological systems and processes
Approach	Data analysis	Modeling and simulation
Examples	<ul style="list-style-type: none"> • Sequence alignment tools • Gene expression analysis tools • Network analysis tools • Genomics/ Transcriptome platforms 	<ul style="list-style-type: none"> • Agent-based modeling tools • Machine learning predictive algorithms using biological data • Protein folding and 3D modeling • Cellular signaling pathways • Molecular dynamics simulation tools • Monte Carlo simulation

(IT), mathematics, and statistics, on the one hand, and biology and related natural sciences on the other hand. However, these terms are also often used interchangeably. Moreover, the lines between computational biology and bioinformatics are vanishing, and dealing with biological data usually requires using both to be employed together at various points.

While *in silico* studies may seem straightforward, conducting efficient and rational studies is no easy task. These studies employ various web-based applications, databases, and tools, which replace traditional lab instruments and facilities. To conduct a rational and helpful study, a deep understanding of the field, knowledge of the gaps, and familiarity with available tools are essential. Non-professional use of these tools may lead to invalid results.

In silico studies are based on big data gathered through experiments; considering the complexity of biological systems, there might still be gaps in the rules and models behind the employed computer programs and algorithms. Thus, the predictive ability of such studies is not 100%. In fact, the results of this kind of study should be validated in further experimentation. However, this does not devalue such studies. In biology and medicine, even experimental studies may not always lead to valid data because analyses are based on ob-

servations conducted in samples, and the findings might not always represent the entire population or reality. Multiple examples of the data resulting from clinical trials that have been questioned later, even after several years, can be found in the history of medicine. Along with advancements in science and technology, the accuracy and credibility of *in silico* studies would increase. Moreover, artificial intelligence (AI) has opened a new era in computational biology, bioinformatics, and *in silico* studies. Its emergence is a game-changer, pivotal to the advancement of these fields. With the employment of AI, *in silico* clinical trials have a promising future, with immense benefits if the results can achieve sufficient accuracy and predictive ability (3).

Despite the skeptical view of some academicians and researchers, *in silico* studies are vastly being used by different universities, research, and pharma companies. FDA has also declared that it appreciates the benefits of *in silico* biology and has already used it for some analyses. The 2024 Nobel Prize in Chemistry was awarded to three scientists: David Baker received half of the prize for his work in “computational protein design”, while Demis Hassabis and John Jumper shared the other half for their contributions to “protein structure prediction”. All these show that the role of computational studies in biological sci-

ences is getting more important, especially since AI has accelerated these advancements. While the future role of these technologies in biological research and medical practice may not be fully defined yet, a revolution in the

field is anticipated.

Conflict of Interest

The authors declare that they have no conflict of interest.

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