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# THE ROLE OF ARTIFICIAL INTELLIGENCE IN BIOCHEMICAL RESEARCH

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**Abstract**

Artificial intelligence (AI) has become an increasingly important tool in modern biochemical research. The rapid development of genomics, proteomics, metabolomics, structural biology, and high-throughput experimental technologies has generated large and complex datasets that are difficult to analyze using conventional approaches alone. AI-based methods, particularly machine learning and deep learning, provide new possibilities for identifying molecular patterns, predicting protein structures, analyzing enzyme properties, integrating multi-omics data, and supporting drug discovery. This review examines the current applications of AI in biochemical research and evaluates its potential advantages and limitations. The analysis shows that AI can accelerate data interpretation, assist in the prediction of molecular properties, support enzyme engineering, identify potential therapeutic targets, and improve the selection of compounds for experimental testing. At the same time, problems related to data quality, model interpretability, reproducibility, and experimental validation remain important challenges. Therefore, AI should not replace experimental biochemistry but should be integrated with laboratory approaches to improve the efficiency and precision of scientific research. The combination of artificial intelligence and experimental biochemistry may provide new opportunities for understanding complex molecular processes and developing innovative biomedical applications.

**Keywords:** artificial intelligence, machine learning, biochemistry, protein structure prediction, enzyme engineering, multi-omics, metabolomics, drug discovery

## Introduction

Biochemistry plays a central role in understanding the molecular mechanisms that maintain life. Proteins, enzymes, nucleic acids, metabolites, lipids, and carbohydrates participate in highly interconnected processes, and changes in one molecular component may influence multiple biochemical pathways. The development of modern experimental technologies has allowed researchers to obtain enormous amounts of biological information. However, the increasing volume and complexity of these data have created a new challenge: extracting biologically meaningful information from large datasets.

Artificial intelligence has emerged as one of the technologies capable of addressing this challenge. Machine learning algorithms can learn relationships from previously collected data and use these relationships to make predictions about new biological samples or molecules. Deep learning methods can analyze particularly complex datasets and have become increasingly important in structural biology, molecular modeling, and drug discovery.

The role of AI in biochemical research has expanded significantly in recent years. One of the most influential developments has been the use of AI for protein structure and molecular interaction prediction. Current AI methods can predict protein structures and complexes with increasing accuracy, providing researchers with information that may be difficult or time-consuming to obtain experimentally.

AI is also being applied to enzyme engineering. Recent research shows that protein language models and generative approaches can assist in exploring enzyme sequence space, predicting protein properties, and designing potentially useful enzyme variants.

Another important area is the integration of AI with multi-omics data. Genomics, transcriptomics, proteomics, and metabolomics provide complementary information about biological systems, and AI can help identify relationships between these molecular layers.

The aim of this review is to describe the major applications of artificial intelligence in biochemical research, evaluate its potential benefits and limitations, and discuss the importance of combining computational predictions with experimental validation.

**Materials and Methods**

This article was prepared as a narrative review of scientific literature concerning the application of artificial intelligence in biochemical and biomedical research. Relevant peer-reviewed publications and scientific reviews addressing artificial intelligence, machine learning, protein structure prediction, enzyme engineering, metabolomics, multi-omics analysis, molecular modeling, and drug discovery were examined.

Recent publications from 2025 and 2026 were given particular attention in order to reflect the current development of the field. Established publications were also considered where they provided important methodological or conceptual background.

The selected literature was analyzed according to several major themes, including AI-assisted protein structure prediction, enzyme engineering, metabolic and multi-omics analysis, molecular interaction prediction, and drug discovery. Particular attention was given to the practical advantages of AI, its limitations, and the relationship between computational predictions and experimental biochemical evidence.

Because this work is a literature-based review, no human participants, animals, or biological samples were directly involved.

**Results**

The reviewed literature demonstrates that artificial intelligence is being incorporated into several important areas of biochemical research. The most prominent applications include protein structure prediction, enzyme engineering, multi-omics analysis, metabolic research, and drug discovery.

AI-based protein structure prediction has become an important resource for structural and molecular biology. Modern computational models can estimate three-dimensional protein structures and predict interactions between proteins and other biomolecules. These approaches can provide researchers with structural hypotheses before experimental studies are performed. However, current methods still have challenges involving protein dynamics, ligand interactions, nucleic-acid complexes, and the evaluation of prediction accuracy.

Enzyme research is another rapidly developing area. Machine learning and protein language models can analyze relationships between amino acid sequences and enzyme properties. This may help researchers select promising mutations or protein variants for experimental testing. Recent research also indicates that generative AI can contribute to the design of new protein structures and potentially improve enzyme performance.

The combination of AI and metabolic engineering is particularly promising. AI models can integrate information about protein sequences, metabolic pathways, and cellular phenotypes. This creates opportunities to design more efficient microbial systems and investigate complex metabolic processes. The development of AI-powered biofoundries may further connect computational prediction with automated laboratory experimentation.

AI can also assist in the interpretation of metabolomic and other omics datasets. Large-scale molecular measurements often contain patterns that are difficult to identify through conventional statistical analysis. Machine learning can support classification, biomarker identification, and prediction of biochemical states. The integration of several omics layers may provide a more comprehensive representation of disease-associated molecular changes.

Drug discovery represents another major application. AI can support target identification, virtual screening, molecular property prediction, lead optimization, and safety assessment. Recent reviews describe the increasing use of AI across different stages of the drug discovery process.

At the same time, the reviewed evidence indicates that computational performance does not automatically translate into clinical success. Biological data are highly dependent on experimental conditions, genetic background, environmental factors, and other variables. Consequently, a model that performs well on a computational benchmark may not necessarily produce the same level of benefit in real-world drug development.

**Discussion**

The results demonstrate that AI has the potential to significantly influence the methodology of biochemical research. Its main advantage is the ability to process large and heterogeneous datasets and identify relationships that may be difficult to detect through conventional approaches.

In protein research, AI can provide structural predictions that assist scientists in developing hypotheses about protein function, molecular interactions, and potential therapeutic targets. This is particularly useful when experimental structural information is unavailable. However, predicted structures should be interpreted as computational models rather than unquestionable experimental evidence.

The application of AI to enzyme engineering is also highly significant. Traditional protein engineering may require the experimental examination of a large number of variants. AI can reduce this search space by identifying candidates that are predicted to possess desirable properties. Recent developments are moving beyond simple prediction toward generative and multimodal approaches capable of integrating sequence, structure, and functional information.

The integration of AI with multi-omics data may provide an additional advantage. Biological systems are not composed of isolated molecular pathways. Genes, proteins, metabolites, and signaling processes continuously interact. AI may help researchers analyze

these interactions at a systems level and identify molecular patterns associated with disease or altered metabolism.

Nevertheless, several limitations must be considered. The performance of an AI model strongly depends on the quality of its training data. Incomplete or biased datasets may result in predictions that do not generalize to different biological populations or experimental conditions.

Interpretability is another major concern. Some deep-learning models can generate highly accurate predictions while providing limited information about the biological reasoning behind them. In biochemical research, understanding the mechanism is often as important as obtaining the prediction itself.

Experimental validation therefore remains essential. AI can suggest that a particular protein mutation may increase enzyme activity or that a compound may interact with a molecular target, but these hypotheses must be tested under appropriate laboratory conditions. Recent work on AI-driven protein design emphasizes the importance of a complete pipeline involving data curation, computational design, candidate selection, and experimental validation.

A similar issue exists in drug discovery. Although AI has produced considerable technological progress, current evidence does not yet demonstrate that AI alone consistently produces faster or more successful clinical development. Recent critical assessments emphasize the gap between computational performance and clinically meaningful outcomes.

Therefore, the most promising future model is not one in which AI replaces biochemical scientists. Instead, AI should function as a complementary tool within an iterative research process. Computational models can generate hypotheses, prioritize experiments, and analyze experimental results, while laboratory research provides the biological evidence required to confirm or reject those predictions.

**Conclusion**

Artificial intelligence is becoming an important component of modern biochemical research. Its applications now extend from protein structure prediction and enzyme engineering to multi-omics analysis, metabolic engineering, molecular interaction prediction, and drug discovery.

The reviewed literature indicates that AI can improve the speed and scale of biochemical data analysis and help researchers identify promising molecular candidates and biological relationships. In enzyme engineering and protein design, AI may reduce the experimental search space, while in drug discovery it can support target identification and molecular screening.

Despite these advantages, AI has important limitations related to data quality, interpretability, reproducibility, and biological validation. Computational predictions should therefore be considered hypotheses that require appropriate experimental investigation.

The future of biochemical research will likely depend on closer integration between artificial intelligence, computational biology, and experimental science. The combination of machine-based prediction with laboratory validation may provide a more efficient approach to understanding molecular mechanisms and developing new therapeutic and biotechnological applications.

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