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Application of Artificial Intelligence in Biochemistry

Raghda M.A. Al-Ani
Department of Chemistry/ University of Sakarya/ Institute of Natural Sciences/ Türkiye,

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corresponding author:
Raghda M.A. Al-Ani
raghda.alani996@gmail.com

ABSTRACT

The adaptation artificial intelligence (AI) to biochemistry has become more suited to many areas of this field. AI adoption as a powerful tool that boosts creativity and innovation has become prevalent in today's world by chemists in all its branches, including biochemistry. Artificial intelligence applications have become diverse in biochemistry which has led to the detection of modern capabilities addressing complex genetic issues, developing new paths in pharmaceutical fields, and drug discovery. AI, as significant tool, has helped to enhance understanding main concept of basic processes of life. Many AI algorithms have been used today to achieve chemical activity forecasting. Digitization and automation combined with algorithms, become necessary to discover new compounds, recognize the biological activity molecules, and analyze their features .

The scientists have reached important results through the use of artificial intelligence applications and algorithms. For example, predicting protein structures, and categorizing, predicting various chemical phenomena .

Due increasing importance of using artificial intelligence in biochemistry, in this paper, I will illustrate the most important applications used in biochemistry and explain the results achieved via them.

Keywords: Biochemistry, artificial intelligence, chemoinformatics, laboratory information management system.

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INTRODUCTION

By using AI applications many ancient traditional practices have modified in biochemistry and biotechnology. This change in practices brought about the ability to analize big data which is characterized by complexity, generate appropriate predictions, and uncover hidden patterns. We also find that artificial intelligence techniques and new algorithms have helped in predicting protein structure, genome operations with the existence of modern high-speed computing technology have developed new methods to analyze big data quickly, accurately, and more cost-effectively (Praveen *et al*., 2024).

Biochemists consider AI an important, essential, and valuable tool in the path of pattern analysis and proactive data analysis, as AI has enabled them to abandon traditional methods in biochemistry despite the benefits achieved through it, but it is considered time-consuming and requires a lot of labor when compared to AI applications**.**

It can be said that artificial intelligence has become an influential factor in the development of AI capabilities have helped drive innovation. At the same time, it can be asserted that until now, the full potential of artificial intelligence which is developing day by day, has not been fully exploited. Current applications of AI in biochemistry are diverse and offer a glance into the future of convoluted molecular and genetic research, pointing the path for a future affluent with capabilities (Cain, 2023).

Biochemistry (biological)

The main goal of biochemistry is to ensure the survival of living organisms. It encompasses both the biological and chemical materials present in the body, as well as the internal balance and communication between these components. This intricate interplay can be analyzed through laboratory and biological experiments. The importance of biochemistry lies in its study of how life is maintained and preserved (Komoda and Matsunaga, 2015).

Biochemistry refers to the chemistry of living cells, as life is fundamentally based on various biochemical reactions. This connection has established biochemistry as a foundational concept in all biological sciences. Biochemistry primarily focuses on the structures and functions of cellular components, including proteins, carbohydrates, lipids, nucleic acids, and other bimolecular and their transformations (Petushok *et al*., 2019).

Biochemistry focuses on the molecular functions of the body. In addition to water, the normal human body primarily comprises proteins and triglycerides, with triglycerides being the most abundant. Triglycerides are the main form of metabolic energy storage and are mainly found in adipose tissue. On the other hand, proteins are critically important as they form the structural backbone of cells and tissues, and they play essential roles in enzymatic catalysis, membrane transport, and cell movement. Carbohydrates, including glucose and the polysaccharide glycogen, are also vital as they serve as substrates for generating metabolic energy, it is important to mention that the term biochemistry is synonymous with two phrases: the first is physiological chemistry, and the second is biological chemistry (Stotz and Vennesland, 2025).

Artificial intelligence (AI)

Artificial intelligence refers to technology that enables computers and machines to replicate human capabilities such as learning, understanding, problem-solving, decision-making, and creativity. Through various applications and devices equipped with artificial intelligence, these systems and applications will be able to see and identify things. Artificial intelligence allows for understanding and responding to human language. In addition, it can learn from new information and experiences. This technology can provide personalized recommendations to users and experts, all of which contribute to the optimal decision-making process (Cole and Kavlakoglu, 2024).

AI is created by developing algorithms and models that allow machines to learn from data and make decisions based on that learning. The choice of programming language used in AI development depends on the type of machine learning being implemented.

Also, it has a wide range of applications across various fields. For instance, in healthcare, AI has enabled drags development, enhanced the analysis of medical images, and assisted in diagnosing diseases.

Additionally, machine learning algorithms have been trained to detect cancer in mammograms with high accuracy (Słapczyński, 2022).

Artificial intelligence has become deeply integrated into biochemistry, particularly in healthcare as well as drug discovery and development. Its applications have greatly advanced the ability to study and understand molecular structures, which helps in determining various molecular properties (Choudhary *et al*., 2022).

Chemoinformatics

One of the concepts that emerged in the late 1990s is the concept of cheminformatics. This includes various methods of digitization and automation as well as artificial intelligence technology. Deep learning applications in chemistry and biochemistry have helped scientists accurately model the chemical structures of different atoms and molecules in structural chemistry and biochemistry. This advancement allows researchers to replicate numerous chemical reactions in both general and organic chemistry, with a primary focus on biochemistry for foundational, pharmaceutical, and medical applications.

The AI algorithms developed have enhanced the automation of chemical systems. A superior understanding has been achieved in interpreting the glucose metabolism in cells, oxidation-reduction reactions, as well as the structures of atoms and molecules. The use of AI algorithms has helped in finding solutions to issues related to missing values or poor-quality data collected from chemical reactions and experiments (El-Feghali and Kahura, 2023). This is illustrated in Fig. (1).

Rapid advances in cheminformatics and machine learning technologies for generating, processing, storing, and transmitting data across different environments, as cheminformatics, and artificial intelligence have played a crucial role in enhancing the design and development of new, more sustainable agents as well as creating predictive modeling algorithms (Djoumbou-Feunang *et al*., 2023).

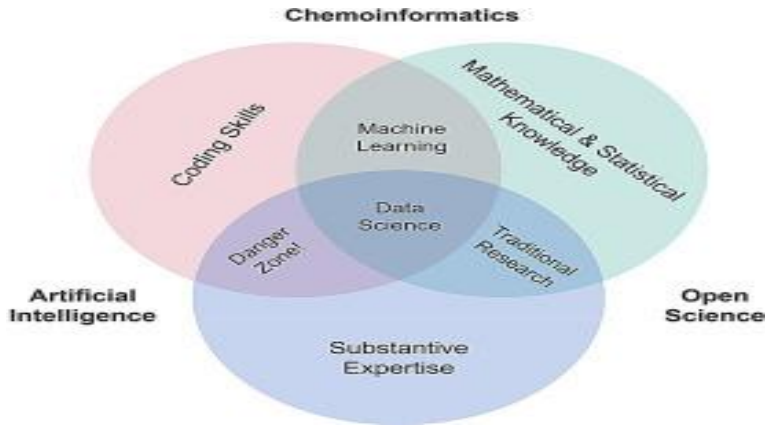

Fig. 1: Artificial intelligence-open science collaboration in chemoinformatics (Miljković and Medina-Franco, 2024).

Big data with its duplicate information poses a significant challenge in the field of cheminformatics as this duplication negatively affects the accuracy of similarity measurements. By developing advanced algorithms and leveraging the capabilities of artificial intelligence, the efficiency and accuracy of similarity assessments in drug design have been improved and important discoveries have been made, especially when cheminformatics and bioinformatics are combined with artificial intelligence. For instance, machine learning and deep learning techniques are now

combined with established bioinformatics methods, molecular evolution, and protein structure analysis to enhance the drug design and discovery process (Raslan *et al*., 2023).

EXPERİMENTAL

Artificial intelligence has become an important tool in the pharmaceutical industry. The application of artificial intelligence algorithms to drug discovery presents significant opportunities and challenges. Machine learning and deep learning techniques are relied upon in drug screening and design, and accelerating the drug discovery process. AI models improve prediction of expected biological responses to a molecule that has not yet been tested, and sometimes has not yet been manufactured (Han *et al*., 2023).

Supervised learning is one category of machine learning, where data is carefully selected, and algorithms are trained using this data. The goal is to associate each input sample with its corresponding output. By leveraging these input-output pairs, the algorithm learns to create a model to make accurate predictions on new, unseen data. Various algorithms fall under this category, one of which is support vector regression (SVR). This algorithm addresses regression problems by optimizing functions to identify a region that closely approximates a continuous-valued function while minimizing prediction errors (Comito and Pizzuti, 2022).

RESULTS AND DISCUSSION

The integration of artificial intelligence (AI) models into bioinformatics has greatly enhanced the analysis and interpretation of biological data. Significant advancements have occurred in various AI methodologies, including machine learning (ML), deep learning (DL), and natural language processing (NLP). These methodologies have been applied in numerous areas within the field, such as genome sequencing, protein structure prediction, and drug discovery. As a result, AI algorithms have demonstrated effectiveness in addressing complex biological challenges (Jamialahmadi *et al*., 2024).

In experiments of integrating AI algorithms into different biochemical sensors, the results indicated improved performance, accurate analysis, and diagnostic assistance.

AI has accelerated discoveries in biochemistry, and the current applications of AI are expected to further enhance this pace. Below, we briefly discuss some examples of artificial intelligence applications in biochemistry research.

Applications related to drug discovery and development

The process of discovering and developing new drugs is lengthy, complex, and costly. Recently, artificial intelligence (AI) techniques have been integrated into this process, facilitating the design and enhancement of candidate drug molecules. The efficiency of clinical trials has been improved when generative models are used to repurpose existing therapies and predict protein targets. In addition, these models provide initial predictions of drug safety and toxicity, helping to reduce failure rates (Jada *et al*., 2023).

Protein structure prediction

Conventional techniques for determining the three-dimensional structures of proteins require complex and expensive experimental methods such as X-ray crystallography and nuclear magnetic resonance. These techniques are important and valuable; however, it faces limitations in speed and cost and can only be used on specific types of protein structures (Qiu *et al*., 2024).

One of the AI systems developed and produced by google is AlphaFold, this application is considered one of the most popular applications in the field of protein structure prediction. This application enables the prediction of the three-dimensional structures of proteins based on their amino acid sequences and achieves accuracy comparable to that of experienced researchers, this is illustrated in Fig. (2). AlphaFold is known as the highest-rated method for protein structure prediction, this application allows users to download data for human proteins in addition to proteins from 47 other important organisms relevant to global health and scientific research (Hassabis, 2022).

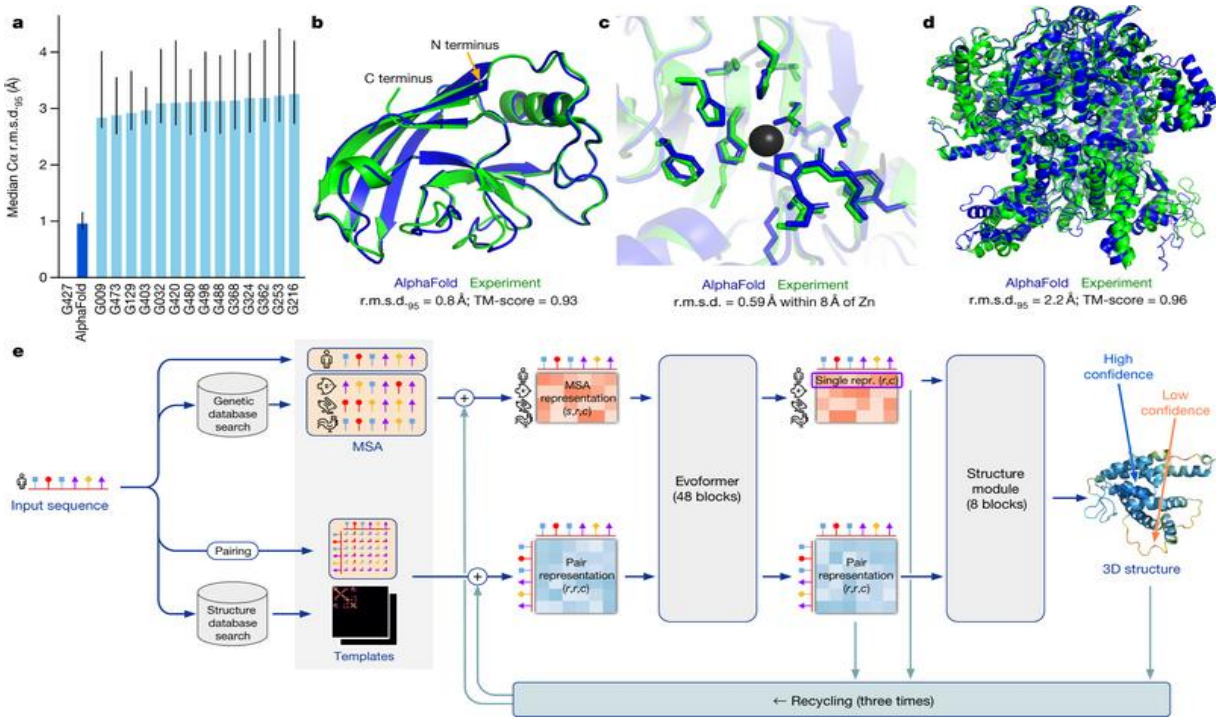

Fig. 2: AlphaFold application produces deeply accurate structures (Jumper *et al*., 2021).

Laboratory information management systems (LIMS)

Laboratory information systems are digital systems that are decisive to many processes and functions within clinical laboratories. The flow and transmission of information within all parts of the laboratory, it's the job these systems perform, facilitating, and discloseing the reporting of outcomes, and facilitating the implementation of rules and guidelines that reduce the need for twin tests (McCudden *et al*., 2020).

A laboratory information management system (LIMS) is a software programming package designed to help sophisticated laboratories perform and conduct more efficiently. This is achieved via tracking samples, experiments, laboratory procedures, and equipment data, the system boosts laboratory productivity. Through laboratory information management system (LIMS), the technical staff and scientists can monitor samples and variety all through the analytical process, including performing tests, reviewing test results, and overseeing control limits and quality control values. In chemical laboratories, a laboratory information management system (LIMS) has become essential for managing sample registration, recording information about users and equipment used, and automating workflows. The system plays an important role in the reporting process (McCudden and Henderson, 2017).

A laboratory information management system (LIMS) as software has a master database that contains data collected in laboratories. The use of AI solutions to extract data allows decision-makers to gain important insights. For example, in the tasks of predictive maintenance where algorithms can forecast equipment failure or provide indications, allowing correct timely prevention (Yuewei, 2023).

Deep neural network (DNN)

They described deep neural network (DNN) as an artificial neural network with considerable layers of interconnected nodes, which are known as neurons. The layers encompass an input layer, multiple hidden layers, and an output layer. Each neuron processes the input data via weights application, biases, and an activation function to generate an output (Jamialahmadi, 2024).

Deep multilayer neural networks can utilize basic descriptors and transform them into outstanding forecasting target characteristics. These networks are also able to retrieve descriptors directly from raw descriptions of chemical structures, which can then be used to predict the properties of chemical compounds.

In addition, possibly can generate inverse descriptions by deep autoencoders possibly can generate inverse descriptions, and thus enabling the reconstruction of chemical structures (Baskin, 2020).

The amazing results of deep learning models have been studied previously, especially those in classification tasks, the efficacy of the DNN model was displayed using a standard dataset for predicting 5hmC sites. This was accomplished by employing the DNN model with input and output layers, along with three hidden layers. The output from the first hidden layer served as the input to the subsequent hidden layer (Khan *et al*., 2024).

Simulation-based learning

In the realm of biochemistry education, AI has become a dynamic tool by modeling more interactive educational applications. AI has upgraded critical thinking skills by allowing students to compare different solutions. Simulation is the provision of practical experiments that convincingly mimic real events or scenarios. This approach has given students the ability to communicate and interact within a virtual environment. This approach has provided a cost-effective and authentic learning experience that promotes deep learning, inquiry, and problem-solving. In general, the integration of AI into biochemistry education has improved learning experiences by making harsh concepts more accessible and engaging, ultimately leading to deeper understanding among students (Dai and Ke, 2022).

CONCLUSIONS

One of the masterpieces of human achievements, the unity and integration between AI and biochemistry is considered to be such achievements. AI has been strongly distinctive for its ability to diagnose patterns, perform predictive analysis, and process big data. AI is becoming increasingly important in the field of biochemistry. While traditional biochemical methods are important, they are time-consuming, labor-intensive, and expensive. AI's ability to process and analyze data quickly greatly enhances the efficiency and accuracy of the field. It is a beacon of progress, paving the way for a future that will grant for a better understanding of the elementary processes of life.

The likelihood of AI in serving biochemistry is enormous, although it has not yet been perfectly realized and is expected to revolutionize many aspects of this discipline.

Interrelation and integration between biochemistry and AI have approved the power of association between differing disciplines, but this does not mean that there are no challenges facing the use of AI in biochemistry. Most famous challenges include data collection, organization, accuracy, and reliability, with technical obstacles in comparing molecules and how to indicate molecular structures mathematically to understand the relationships between them.

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تطبيق الذكاء الاصطناعي في الكيمياء الحيوية

رغده محمود عبد الغفور العاني

قسم الكيمياء/ جامعة سكاريا/ معهد العلوم الطبيعية/ تركيا

الملخص

لقد أصبح تكييف الذكاء الاصطناعي مع الكيمياء الحيوية أكثر ملاءمة في العديد من مجالات هذا المجال. أصبح تبني الذكاء الاصطناعي كأداة قوية تعزز الإبداع والابتكار أمرًا شائعًا في عالم اليوم من قبل الكيميائيين في جميع فروعه، بما في ذلك الكيمياء الحيوية. أصبحت تطبيقات الذكاء الاصطناعي متنوعة في الكيمياء الحيوية مما أدى إلى اكتشاف قدرات حديثة في معالجة القضايا الوراثية المعقدة، وتطوير مسارات جديدة في المجالات الصيدلانية، واكتشاف الأدوية. ساعد الذكاء الاصطناعي كأداة مهمة في تعزيز فهم المفهوم الرئيسي للعمليات الأساسية للحياة. أصبحت العديد من خوارزميات الذكاء الاصطناعي مستخدمة اليوم لتحقيق التنبؤ بالنشاط الكيميائي. تصبح الرقمنة والأتمتة عند دمجها مع الخوارزميات ضرورية لاكتشاف مركبات جديدة، والتعرف على جزيئات النشاط البيولوجي، وتحليل ميزاتها.

لقد توصل العلماء إلى نتائج مهمة من خلال استخدام تطبيقات وخوارزميات الذكاء الاصطناعي. على سبيل المثال، التنبؤ بهياكل البروتين، وتصنيفها، والتنبؤ بالظواهر الكيميائية المختلفة.

نظرًا للأهمية المتزايدة لاستخدام الذكاء الاصطناعي في الكيمياء الحيوية، سأوضح في هذه الورقة أهم التطبيقات المستخدمة في الكيمياء الحيوية وأشرح النتائج التي تم تحقيقها من خلالها.

الكلمات الدالة: الكيمياء الحيوية، الذكاء الاصطناعي، المعلوماتية الكيميائية، نظام إدارة معلومات المختبرات.