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Review Article

Redefining Biomolecular Frontiers: The Impact of Artificial Intelligence in Biochemistry and Medicine

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Abstract

Artificial Intelligence (AI) is redefining the frontiers of biochemistry and medicine by enhancing molecular understanding, diagnostic precision and therapeutic discovery. This review examines the transformative roles of AI across key biomedical domains, including medical imaging, disease prediction, protein structure modeling, drug development, enzyme engineering and multiomics integration. Deep learning architectures, such as convolutional neural networks and transformers, now surpass traditional diagnostic approaches in accuracy and efficiency, particularly in neuroimaging for conditions like Alzheimer's disease. Tools like AlphaFold2 and generative models (e.g., ChemBERTa, MolGPT) have revolutionized protein structure prediction and de novo drug design. AI-driven strategies also empower personalized medicine through real-time health monitoring, wearable integration and omics-based systems biology. Despite these advances, challenges remain including data heterogeneity, model interpretability, ethical concerns and global disparities in AI access. This manuscript addresses these barriers by highlighting solutions such as explainable AI, open-source platforms and international collaboration. Furthermore, emerging applications, including AI-enhanced microplastic toxicology, sleep biochemistry, herbal compound modeling and gut microbiota host interaction mapping, illustrate the interdisciplinary breadth and future potential of AI in biochemistry. By synthesizing foundational developments with next-generation innovations, this review affirms AI's role as a catalyst for accelerating discovery, improving healthcare equity and reshaping the molecular sciences for the next era of research and clinical translation.

Key words: Artificial intelligence, deep learning, biochemistry, protein structure prediction, drug discovery, multi-omics integration

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INTRODUCTION

Artificial Intelligence (AI) has emerged as a transformative force across scientific disciplines, with its profound impact increasingly evident in biochemistry and medicine. Leveraging computational power, AI, particularly deep learning models, has significantly enhanced the analysis, interpretation and prediction of complex biological data. Its applications now span from medical imaging and diagnostics to drug discovery and molecular biology, redefining the paradigms of biomedical research and clinical practice.

One of the earliest and most notable breakthroughs of AI in healthcare is in the field of medical image analysis. Convolutional Neural Networks (CNNs), a subclass of deep learning algorithms, have demonstrated exceptional performance in tasks such as tumor detection, segmentation and classification across various imaging modalities, including MRI, CT and ultrasound. Foundational surveys by Litjens *et al.*¹ and Shen *et al.*² comprehensively chart the evolution of deep learning in medical imaging, highlighting key breakthroughs and practical implementations that underpin current AI-assisted diagnostics^{1,2}.

A landmark study by McKinney *et al.*³ revealed the capability of AI systems to outperform radiologists in breast cancer screening, emphasizing not just accuracy but also consistency and efficiency in diagnostics³. Similarly, AI-driven solutions in radiology are now streamlining workflows and improving patient outcomes, as evidenced by significant reductions in diagnostic errors and turnaround times⁴. These developments underscore a paradigm shift in radiological practices, where AI serves not as a replacement but as an augmentation to human expertise.

Transformer-based architectures have further expanded these capabilities by enhancing segmentation precision through global context integration. Models like TransUNet exemplify this shift by combining convolutional layers with transformer modules to better capture anatomical features⁵. These advancements, along with newer transformer-based models, surpass CNN methods in handling complex biomedical imaging tasks by modeling long-range dependencies and spatial hierarchies⁶.

As AI continues to evolve, its integration into the fabric of biochemistry and medicine opens new avenues for scientific inquiry and clinical innovation. This article explores the multifaceted contributions of AI to the bimolecular sciences, with particular focus on its role in medical diagnostics, protein structure prediction, drug development, genomic analysis and ethical considerations.

Artificial intelligence in biomedical sciences

AI in medical imaging and diagnostics: Artificial Intelligence (AI) has profoundly transformed medical imaging by enhancing image interpretation, increasing diagnostic accuracy and reducing human error. The AI-powered deep learning models, particularly Convolutional Neural Networks (CNNs), are now integral in detecting pathologies from imaging modalities such as CT, MRI and X-rays. Esteva *et al.*⁷ emphasized that AI systems rival expert-level performance in detecting skin cancer and diabetic retinopathy, offering rapid, scalable diagnostic support across healthcare settings⁷. Harmon *et al.*⁸ demonstrated that AI algorithms can detect COVID-19 pneumonia from chest CT scans with high sensitivity across multinational datasets, thus accelerating pandemic response efforts⁸.

Furthermore, transformer-based architectures are emerging as a powerful tool in neuroimaging. A recent scoping review by Iratni *et al.*⁹ highlighted the expanding role of transformers in segmenting complex brain structures, thus facilitating early diagnosis of neurological conditions⁹. In Alzheimer's disease, 3D CNNs applied to structural MRI scans have enabled automated classification with high precision¹⁰.

Figure 1 visually represents the AI-driven medical imaging workflow. It demonstrates how deep learning models, such as Convolutional Neural Networks (CNNs) and transformer-based architectures, process medical scans to perform segmentation, classification and automated diagnosis. As shown by Esteva *et al.*⁷ and Harmon *et al.*⁸, AI models trained on large-scale datasets can detect complex patterns with higher sensitivity than traditional methods. Moreover, Iratni *et al.*⁹ and Basaia *et al.*¹⁰ describe the integration of these models into clinical pipelines, enhancing the detection of diseases like COVID-19 and Alzheimer's through automated analysis of CT and MRI scans.

Figure 1 outlines the sequential stages of AI-assisted diagnostic imaging, from image acquisition via MRI/CT, through AI-powered segmentation and classification, to the generation of a diagnostic report.

AI in disease prediction and monitoring: Beyond diagnostics, AI is now employed for predictive modeling and real-time monitoring of disease progression. In neurodegenerative disorders like Alzheimer's disease, AI models analyze longitudinal imaging and EEG data to predict cognitive decline trajectories. Dauwels *et al.*¹¹ reviewed how EEG signals, combined with machine learning, offer non-invasive, cost-effective avenues for Alzheimer's diagnosis and monitoring.

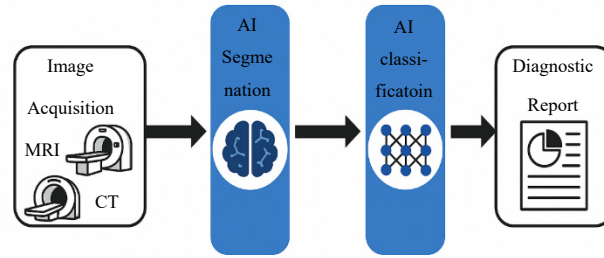


Fig. 1: AI-powered medical imaging workflow: From acquisition to diagnostic report (self-generated)

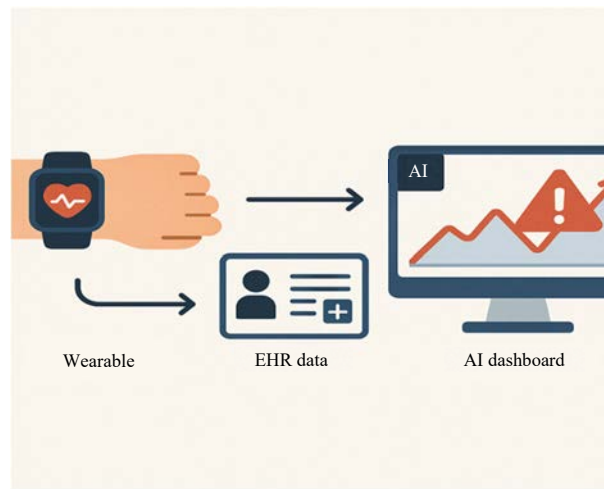


Fig. 2: AI in disease prediction and monitoring (self-generated)

Liu and Brown¹² provided baseline methodologies for ASL imaging, upon which recent AI-driven quantification tools have improved sensitivity to early vascular dysfunction.

In medical image segmentation, Chen *et al.*¹³ introduced a cross-fusion network combining attention mechanisms and transformer layers, further refining diagnostic precision across scales. These approaches help clinicians not only detect diseases earlier but also track their evolution, leading to more personalized treatments. The flow of data from wearable health devices to AI-powered dashboards through the integration of Electronic Health Records (EHR) is shown in Fig. 2. The AI systems utilize continuous data streams from smart wearables and patient EHRs to predict disease trajectories and support real-time monitoring. The AI dashboard in the image highlights how these inputs are processed to generate early warnings, enabling more proactive and personalized healthcare interventions.

An illustration showing the integration of wearable devices, Electronic Health Records (EHR) and AI dashboards. Fig.2 demonstrates how AI processes real-time health data for personalized disease prediction and continuous patient monitoring.

Case example-Alzheimer's diagnosis using deep learning:

Alzheimer's disease (AD) is a progressive neurodegenerative disorder that presents a major diagnostic challenge due to its complex pathology and often subtle early symptoms. Deep learning has emerged as a promising tool for improving diagnostic precision in AD through the analysis of neuroimaging data.

Recent advancements in protein structure prediction have contributed to a better understanding of AD at the molecular level. The success of AlphaFold, an AI system developed by DeepMind, has enabled researchers to model amyloid precursor protein (APP) and tau protein structures with remarkable accuracy, facilitating the exploration of their roles in neurodegeneration¹⁴. This structural insight complements imaging approaches, enhancing molecular diagnosis and therapeutic targeting.

The complementary role of AI in both clinical diagnostics and molecular research on Alzheimer's disease was illustrated in Fig. 3. The left panel displays a stylized neuroimaging heatmap representing brain regions affected by Alzheimer's, while the right panel features AlphaFold-predicted structures of the amyloid precursor protein (APP) and tau protein. Deep learning

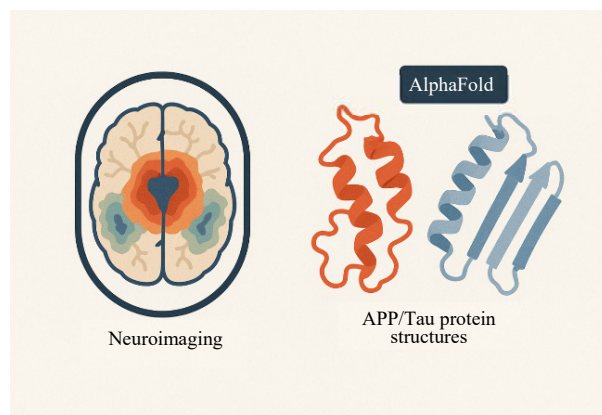


Fig. 3: Molecular insights into Alzheimer's disease using AI (self-generated)

models are employed to classify MRI and EEG data for early diagnosis, while AlphaFold enables accurate 3D prediction of key neurodegenerative proteins. This integrative approach underscores how AI facilitates a multi-dimensional understanding of Alzheimer's disease, linking imaging biomarkers to protein-level insights essential for diagnosis and therapy development.

A dual-pane illustration combining neuroimaging data with AlphaFold-predicted structures of amyloid precursor protein (APP) and tau protein, highlighting how AI bridges clinical diagnostics and molecular understanding in Alzheimer's disease, shown in Fig. 3.

The critical assessment of protein structure prediction (CASP) community has validated AlphaFold's superior performance, highlighting its ability to predict highly accurate protein structures, including those relevant to neurodegenerative diseases like AD¹⁵. These predictions aid researchers in understanding protein misfolding and aggregation mechanisms, key features of Alzheimer's pathology.

Additionally, the AlphaFold Protein Structure Database has vastly expanded the accessible structural landscape, providing detailed 3D models of proteins involved in AD pathophysiology¹⁶. The availability of these models has enhanced the interpretability of biomarker-related studies and accelerated drug development targeting protein misfolding. By integrating deep learning for both neuroimaging and molecular modeling, AI is providing a multi-dimensional approach to Alzheimer's diagnosis and treatment design.

Artificial intelligence in biochemistry

Protein structure prediction-AlphaFold2 and beyond:

Protein structure prediction has traditionally been one of the most difficult challenges in computational biology due to the complexity of folding patterns and the sheer variability in

amino acid sequences. However, recent breakthroughs in AI have dramatically improved structural prediction accuracy and accessibility. Generative AI models are now being used to explore protein folding landscapes by predicting possible conformations and modeling atomic interactions. Walters and Murcko highlighted how generative methods are reshaping the design process in medicinal chemistry by enabling de novo exploration of protein configurations and ligand docking¹⁷.

In parallel, transformer-based models have been introduced to predict molecular properties and folding outcomes using large-scale sequence data. Tran and Eze¹⁸ demonstrated that these models accurately estimate physicochemical features of biomolecules, helping prioritize folding candidates for deeper analysis.

A major milestone came with the application of deep learning to real-world drug discovery. Zhavoronkov *et al.*¹⁹ employed an end-to-end deep learning pipeline that led to the rapid identification of DDR1 kinase inhibitors, marking one of the first successful uses of AI in practical therapeutic design. These methods also leverage protein structure predictions as inputs, reinforcing the value of structural insights from models like AlphaFold in guiding AI-powered discovery¹⁹.

Figure 4 illustrates the AI-driven pipeline for predicting 3D protein structures, beginning with an amino acid sequence, processed through transformer layers and resulting in a predicted protein conformation. Generative AI models like AlphaFold2 employ deep learning architectures, particularly transformers, to model spatial and physicochemical relationships between amino acid residues. This process has revolutionized protein structure prediction, achieved near-experimental accuracy and accelerated research in molecular biology, drug design and enzymology. The visual encapsulates how sequence-based input is transformed by AI into actionable molecular insights.

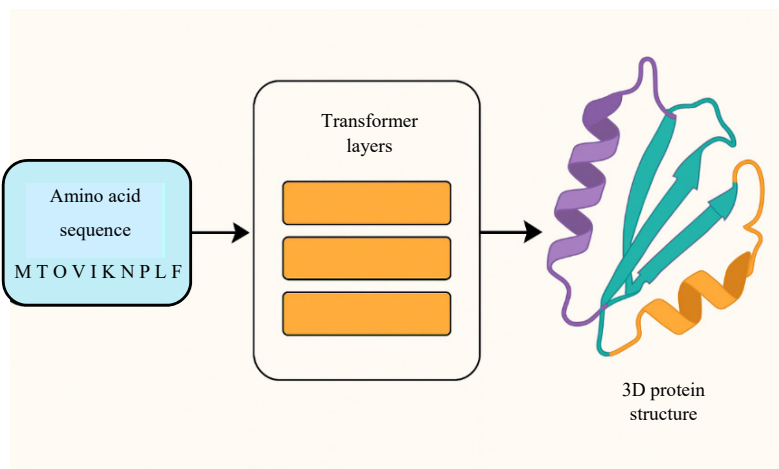


Fig. 4: Protein structure prediction with generative AI (self-generated)

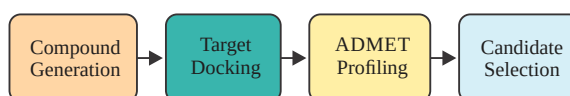


Fig. 5: AI pipeline for drug discovery (self-generated)

A schematic representation of a generative AI pipeline that predicts protein structure from an amino acid sequence input through transformer-based layers to produce a 3D protein model. Figure 4 highlights the core mechanism behind AI-driven structural biology tools like AlphaFold2.

The convergence of these technologies is pushing the boundaries of protein science and setting the stage for real-time, AI-assisted structural biology.

AI in drug discovery and development: Artificial intelligence has become a cornerstone in modern drug discovery, enabling faster and more cost-effective identification of drug candidates. One striking example of AI's real-world impact was the repurposing of Baricitinib as a treatment option during the COVID-19 pandemic. Richardson *et al.*²⁰ demonstrated how AI-guided molecular modeling identified this anti-inflammatory agent as a potential therapeutic, illustrating the power of computational reasoning in urgent medical contexts.

In enzyme-targeted drug discovery, machine learning has been applied to streamline the design and optimization of bioactive compounds. Mazurenko *et al.*²¹ showcased how supervised learning algorithms, trained on enzyme-ligand interaction datasets, improve substrate specificity prediction and support rational inhibitor design²¹. AI has also been instrumental in expanding our understanding of noncoding

genetic variants, which play crucial roles in drug response and disease susceptibility. Zhou and Troyanskaya²² developed a deep learning model that accurately predicts the regulatory effects of noncoding mutations, thereby enabling more targeted therapy development²². Furthermore, in transcriptomics, deep neural networks have been applied to predict splicing outcomes from primary sequences. Jaganathan *et al.*²³ illustrated how such models enhance our ability to interpret pathogenic variants that affect RNA splicing, contributing to more precise genomic medicine and drug development²³.

These advances demonstrate that AI not only accelerates drug discovery but also deepens mechanistic insights that inform safer and more personalized therapeutics.

Figure 5 presents a simplified flowchart of the AI-driven drug discovery process, beginning with compound generation, progressing through target docking, ADMET profiling and ending with candidate selection. Artificial intelligence leverages generative models and molecular simulations to identify novel compounds, predict their binding affinity with biological targets, evaluate pharmacokinetic properties (ADMET) and prioritize drug candidates for further testing. This pipeline illustrates how AI integrates speed, precision and multi-parameter optimization to revolutionize the traditional drug development timeline.

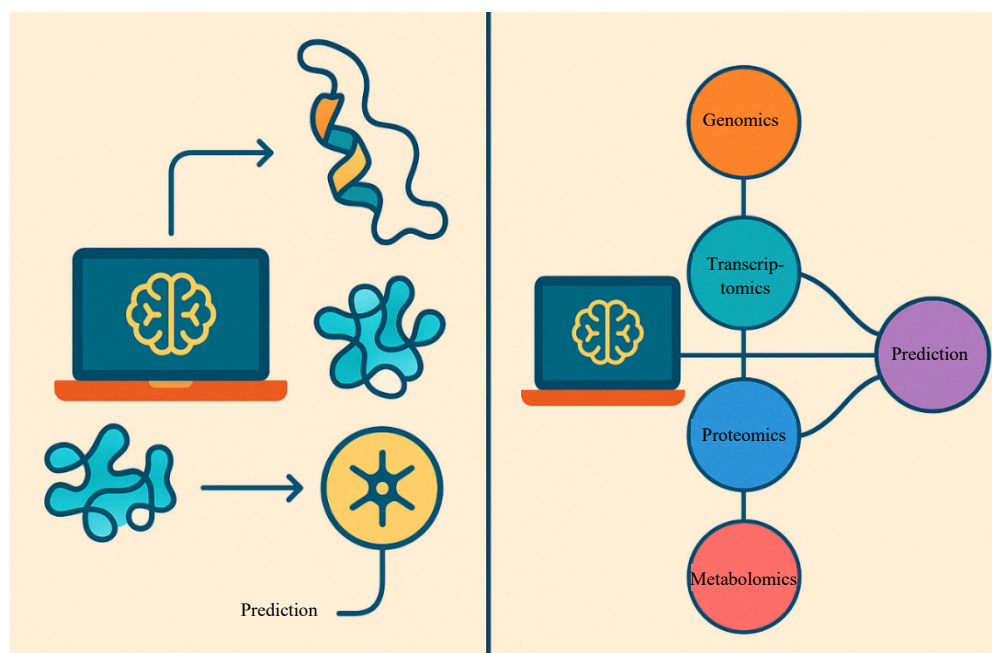


Fig. 6: AI applications in enzyme engineering and omics integration (self-generated)

A flowchart depicting the sequential stages of AI-assisted drug discovery, beginning with compound generation, followed by target docking, ADMET profiling and culminating in candidate selection. This process demonstrates how AI accelerates and optimizes each phase of modern drug development.

AI in enzyme engineering and omics: Artificial intelligence is rapidly transforming enzyme engineering and omics research by enabling predictive modeling, integrative analysis and high-throughput data interpretation. In enzyme engineering, AI models such as deep neural networks and decision trees are used to predict the functional impact of amino acid substitutions, optimize catalytic efficiency and design improved variants with novel activity. Amann *et al.*²⁴ emphasized that incorporating explainability in such models is essential to ensure confidence and traceability in biochemical applications.

Beyond protein-level modifications, AI plays a critical role in multi-omics integration-combining genomics, transcriptomics, proteomics and metabolomics to model complex biological systems.

Figure 6 illustrates the dual role of AI in enzyme engineering and multi-omics data integration. The left panel demonstrates how AI algorithms analyze enzyme sequences and protein structures to predict catalytic activity and

optimize functionality. The right panel depicts AI's capacity to assimilate various omics layers-genomics, transcriptomics, proteomics and metabolomics-into a unified framework for biological prediction. This visualization emphasizes how AI enhances enzyme variant design and interprets complex biological systems through integrative analysis.

Visual representation of how AI supports enzyme structure prediction and integrates multi-omics data (genomics, transcriptomics, proteomics, metabolomics) to generate predictive biological insights.

This holistic view is vital for understanding disease mechanisms and regulatory networks. Vayena *et al.*²⁵ pointed out that while AI facilitates powerful insights in these domains, ethical challenges such as consent, fairness and accountability must guide its application.

To address the evolving risks of AI misuse in biochemical research, the World Health Organization (WHO) published guidelines on ethics and governance. These guidelines advocate for responsible AI development, emphasizing transparency, safety and global equity in access and application²⁶. Adhering to such frameworks is especially crucial in omics studies where patient-derived biological data are highly sensitive.

Together, these efforts are steering enzyme and omics research into a new era where AI-powered innovation is balanced with ethical responsibility and scientific rigor.

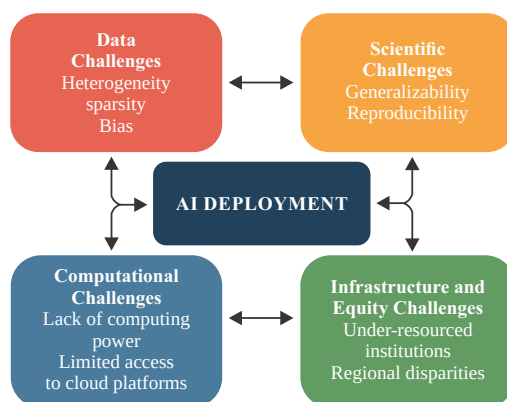


Fig. 7: Barriers to AI deployment in biomedicine: A systems-level framework (self-generated)

Challenges, ethical considerations and future directions in AI-driven biochemistry

Technical and scientific limitations: Although AI has achieved remarkable milestones in biochemistry and biomedical sciences, it faces persistent technical challenges. As outlined by Ching *et al.*²⁷, many AI models struggle with data sparsity, overfitting and poor generalization, especially in heterogeneous biological datasets. Fig. 7 illustrates a systems-level overview of the core barriers limiting the adoption of artificial intelligence in biochemistry and biomedical sciences. These barriers, ranging from poor data standardization and fragmented databases to limited computational access and reproducibility challenges, are interlinked and often exacerbate one another. As Ching *et al.*²⁷ explain, such structural and technical limitations not only impair model reliability but also inhibit broad AI deployment across diverse research settings. The diagram encourages a holistic understanding of the technological and scientific constraints discussed in this section. Training datasets often lack the diversity necessary to support unbiased predictions across populations and biological systems.

Figure 7 outlines the four major categories of challenges—data, scientific, computational and infrastructure-related—that collectively hinder effective AI deployment. It emphasizes the interdependence of these factors in shaping equitable and scalable applications of AI in biochemical research.

Additionally, the integration of multi-modal data from proteomics to metabolomics poses algorithmic and computational difficulties. Without careful normalization and standardization, AI systems risk generating irreproducible or misleading outputs in real-world experiments²⁷.

Foundational applications and structural challenges: AI is already being applied in practical biochemical domains such as drug-target modeling, metabolic pathway mapping and

biomolecular docking. Arowora *et al.*²⁸ have emphasized the utility of AI tools in early-stage drug discovery and the exploration of biochemical mechanisms. These models enhance prediction accuracy for enzyme activity and protein-ligand binding, driving high-throughput experimentation and rational compound screening²⁸.

Nevertheless, many of these applications still suffer from black-box model behavior, which limits interpretability and slows regulatory approval. Arowora *et al.*²⁸ argue for interpretable machine learning approaches tailored to biochemical systems, such as attention-based visualizations or modular networks that reflect domain-specific knowledge.

Infrastructure, access and research equity: Beyond technical capacity, AI research and applications in biochemistry are hindered by resource inequities. Access to computational infrastructure, annotated datasets and cloud services is uneven globally.

Figure 8 visualizes the global disparities in AI infrastructure and resource accessibility that challenge equitable participation in biochemical research. It contrasts regions with high AI capacity, indicated by icons for data servers, internet connectivity and analytics, with underserved areas represented by satellite links and fragmented connectivity. This disparity mirrors the concerns, which emphasize how limited access to computational tools, cloud services and annotated datasets hinders contributions from low-resource laboratories, particularly in the Global South. The image reinforces the need for international collaboration, open-access platforms and inclusive AI development.

Figure 8 highlights disparities in global access to AI resources such as data servers, internet connectivity and computational infrastructure, emphasizing the need for equitable inclusion in biochemical research.



Fig. 8: Global inequities in AI access for biochemical research (self-generated)

Arowora *et al.*²⁸ highlight that these disparities limit meaningful contributions from low-resource laboratories, especially in developing countries, where biological insights are urgently needed.

Solutions such as open-access databases, shared model repositories and international training programs are key to promoting inclusion and accelerating discovery across continents²⁸. Encouraging collaborative platforms between computational and life scientists can also foster responsible and widespread use of AI tools.

Toward explainable and trustworthy AI: The future of AI in biochemistry hinges on building trustworthy and explainable models that can integrate seamlessly into both clinical and laboratory workflows. As emphasized by Jumper and Hassabis²⁹, efforts like AlphaFold have not only advanced structural prediction but also set standards for transparency and open science, offering code, models and data to the global research community.

These standards are essential to mitigate overreliance on black-box systems and to ensure that AI tools remain scientifically accountable and biologically interpretable.

Emerging tools and next-generation applications

Empowering biochemical discovery through precision

AI-driven biomedical image segmentation: The multi-transformer U-Net by Dan *et al.*³⁰ enhances the precision of biomedical image segmentation, which is critical for analyzing complex biochemical data such as histopathology

and proteomic imaging. This advancement supports faster, more accurate interpretation of experimental results. It also paves the way for AI-assisted workflows in biochemistry, enabling real-time analysis and hypothesis generation.

Advancing human health through AI-enhanced microplastic toxicology and biochemical modeling:

In their comprehensive review, Biochemical Effects of Microplastics on Human Health, Anih *et al.*³¹ highlight the urgent need for sophisticated computational models and biomonitoring strategies to evaluate how microplastics impact human biochemistry. Their work points to exciting new directions in AI-driven research, such as tools that can predict organ-specific toxicity, map patterns of exposure and combine omics data to anticipate potential long-term health effects.

Harnessing neurochemical insights for AI-driven innovations in sleep biochemistry:

In their review, Biochemical Mechanisms of Sleep Regulation, Anih *et al.*³² offered a detailed look into the molecular and hormonal systems that govern sleep, providing a critical foundation for the future of AI in biochemistry. By connecting complex pathways involving neurotransmitters and circadian signals to real-world sleep disorders, the authors pave the way for cutting-edge AI applications, such as predictive modeling, personalized diagnostics and data-driven therapy design, to transform sleep medicine and beyond.

Integration of traditional herbal medicine with cutting edge AI technologies in molecular biochemistry:

In their review, Biochemistry of Traditional Herbal Compounds and their Molecular Targets, Anih *et al.*³³ explored how modern techniques like molecular docking and omics technologies are helping decode the complex actions of traditional herbal compounds. By linking chemical structures to specific molecular targets and signaling pathways, their work lays a solid groundwork for the development of AI-powered tools in drug discovery. These insights point to exciting future directions where machine learning can accelerate the design, prediction and refinement of bioactive phytochemicals for precision medicine.

AI-powered exploration of microbiota-derived biochemical networks in host system regulation:

In their review, Biochemically Active Metabolites of Bacteria: Their Influence on Host Metabolism, Neurotransmission and Immunity, Anih *et al.*³⁴ explore how gut microbiota-derived metabolites modulate complex host pathways through receptor signaling, epigenetic control and neuroimmune interactions. By mapping these molecular dialogues, such as SCFA signaling via GPRs and tryptophan-derived modulation of AhR and NMDA receptors, the study lays a compelling foundation for future AI-driven approaches to simulate, predict and therapeutically target host microbiome interactions in systems biochemistry.

CONCLUSION

Artificial Intelligence (AI) is emerging as a transformative force in biochemistry and biomedical sciences, redefining the pace and depth of molecular research and clinical innovation. By enhancing diagnostic precision, enabling accurate protein modeling, accelerating drug discovery and facilitating integrative multiomics analysis, AI is reshaping scientific workflows and expanding the possibilities of personalized medicine. This review highlights AI's pivotal role in deepening our understanding of complex biological systems and promoting interdisciplinary collaboration. However, for this potential to be fully realized, challenges such as data bias, limited interpretability, ethical concerns and global disparities must be addressed. The development of explainable and equitable AI systems will be essential for sustainable and inclusive progress. Ultimately, AI stands as a central pillar in advancing modern biochemistry and improving health outcomes worldwide.

SIGNIFICANCE STATEMENT

This study discovered the transformative potential of Artificial Intelligence (AI) as both a computational engine and a scientific collaborator in biochemistry and biomedical sciences. It can be beneficial for enhancing diagnostic accuracy, accelerating drug discovery, improving protein structure prediction and integrating multiomics data for better disease understanding. The study also emphasizes the importance of ethical governance, equitable access and explainable AI to ensure responsible deployment across diverse settings. By providing practical examples in areas such as neurodegeneration, toxicology and systems biology, this study will help researchers to uncover the critical areas of molecular research and data integration that many were not able to explore. Thus, a new theory on AI-driven biochemical innovation may be arrived at.

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