

Transforming Biochemistry with Artificial Intelligence: Applications in Protein Structure Prediction, Drug Discovery, Clinical Diagnostics and Laboratory Automation

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ABSTRACT

Artificial Intelligence is rapidly transforming the landscape of biochemistry and enabling the smart interpretation of biological complexity in clinical, laboratory, and research settings. The review provides an overview of various applications of AI in molecular modelling, drug discovery, clinical diagnostics, lab automation, and emerging technologies, along with associated challenges, ethical implications, and future research avenues. The literature was searched in the Scopus, Google Scholar, PubMed, and Web of Science databases (2015–2025) using MeSH Terms and keyword combinations. A narrative-systematic synthesis of 312 articles was completed for a total of 95 full-text publications that met the inclusion criteria. From protein structure prediction to biomarker discovery, metabolic pathway analysis, drug design, enzyme engineering, clinical decision support, and many new applications such as synthetic biology and federated learning, AI has made a difference. Moreover, machine learning models achieve high performance in disease risk stratification for most diseases. Although challenges exist in data quality, interpretation, regulation and ethics, AI can offer unprecedented advances in biochemical research, diagnostics and create the capacity to tailor and customise patient care.

1. INTRODUCTION

Biochemistry is a branch of chemistry that integrates biology, medicine, and molecular science to study the chemical processes in living organisms. Biochemical research and clinical practice have used manual analytical methods, hypothesis testing, and statistical models for decades; these are powerful tools but have limited capacity to address the increasing

complexity and volume of biological information. AI (artificial intelligence) has revolutionised this landscape (Jumper et. al., 2021; Rajpurkar et. al., 2022; Topol, 2019).

AI involves a wide-ranging variety of computational methods comprising machine learning (ML), deep learning (DL), natural language processing (NLP), and generative AI that enable

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computers to learn from facts, recognise patterns, make estimates, and accomplish tasks that are usually for vital human aptitudes (Topol, 2019). The past decade has seen unprecedented advances in the availability of high-throughput biochemical data, such as genomics, proteomics, metabolomics, eHRs, and imaging data, and in computational power, which together have sparked an AI revolution in the field of biochemistry and other biomedical sciences (LeCun et al., 2015).

The implications are far-reaching. AI systems are now used in clinical biochemistry to interpret complex laboratory reports, predict disease progression, automate quality control, and provide real-time decision support. AI tools like AlphaFold2 have solved the longstanding 50-year-old problem of precisely predicting the 3D protein structure from its amino acid sequence (Alhamzi, 2024; Gupta et al., 2025; Rajpurkar et al., 2022). Generative AI models are creating new molecules in silico with desirable pharmacological properties in drug discovery, significantly accelerating the discovery process. The use of intelligent automation—comprising of robotics, computer vision, and AI-enabled laboratory information systems (Anih et al., 2025; Baum et al., 2021; Huang et al., 2025; Jumper et al., 2021; Senior et al., 2020; Singhal et al., 2025; Yang et al., 2019)—has reshaped laboratory operations.

Yet all this amazing development has not yet been fully realised in the field of biochemistry. A range of issues of data divergency, explainability, transparency, comprehensibility, regulatory uncertainty, ethical considerations regarding bias and privacy and the requirement for validated prospective studies remain to limit the broad clinical use of challenges. In addition, a major gap exists in the literature regarding the comprehensive reviews of the growing role of AI in biochemistry, which incorporate all facets of the field, both clinical and academic, and laboratory and ethical (Anih et al., 2025; Balti et al., 2025; Huang et al., 2025; Junaid, 2025; Rajpurkar et al., 2022).

This review deals with that. We provide a systematic and integrated overview of the range of applications of AI in biochemistry, from clinical diagnostics and laboratory processes to research discovery and cutting-edge research. Current challenges are also critically discussed and a research agenda is outlined for future research to create a roadmap that informs researchers, clinicians, lab professionals and policy makers about the transformational yet complex role of AI in modern biochemistry.

2. METHODOLOGY

The methodology adopted for this study is a narrative-systematic synthesis, combining the rigour of systematic literature identification with the depth of narrative synthesis, as the applications of AI in biochemistry are very broad and multidisciplinary. A protocol was used to plan the review and followed the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2020) guidelines as applicable (Junaid, 2025).

The electronic literature search was carried out on four main bibliographic files, including PubMed/MEDLINE, Scopus, Web of Science, and Google Scholar. A search was conducted in journals from January 2015 to May 2025 to reflect the current direction of AI in biochemistry. The following MeSH terms and combinations of keywords were used for the searches:

- "Artificial intelligence" AND "biochemistry" OR "clinical biochemistry"
- "Machine learning" AND ("biomarker" OR "laboratory diagnostics" OR "metabolomics")
- "Deep learning" AND ("protein structure" OR "drug discovery" OR "enzyme engineering")
- "Natural language processing" AND ("laboratory information system" OR "clinical report")
- "AI" AND ("laboratory automation" OR "quality control" OR "point-of-care testing")
- "Generative AI" OR "large language models" AND "biochemistry" OR "drug design"
- "Federated learning" OR "explainable AI" AND "clinical biochemistry"
- "AlphaFold" OR "MolGPT" OR "ChemBERTa" AND "biochemistry"

Inclusion Criteria:

- Peer-reviewed original research articles, systematic reviews, and meta-analyses
- Studies informing AI/ML application specifically in biochemical domains (clinical, laboratory, or molecular)
- Publications in English with available full text
- Studies involving human, animal, or in silico biochemical data
- Publications in indexed journals with clear methodology

Exclusion Criteria:

- Abstracts from conference, editorials, and letters without primary data

- Searches principally directed on radiology, pathology imaging, or genomic sequencing outside biochemical context
- Duplicate publications or studies without reproducible AI methodology
- Non-peer-reviewed preprints without subsequent journal publication

For each author, web scraping was done independently and a pre-structured extraction form was used to capture: study design, database/dataset used, AI technique used, biochemical domain, key findings, performance metrics (sensitivity, specificity, AUC-ROC), and limitations. Studies included were quality analysed using QUADAS-2 for diagnostic accuracy studies (Stokes et al., 2020) and CASP (Critical Appraisal Skills Programme) for systematic reviews and cohort studies (Topol, 2019; Zhavoronkov, 2018).

Given the variety of study designs and AI techniques in the literature, a quantitative meta-analysis was not performed. Instead, a themed narrative fusion approach was used, breaking outcomes into six broad areas: (Aliper et al., 2016;

Dobson, 2001; Miotto et al., 2018; Rives et al., 2021; Wainberg et al., 2018):

- (1) AI techniques overview,
- (2) clinical biochemistry applications,
- (3) academic and research applications,
- (4) laboratory automation,
- (5) challenges and ethical considerations, and
- (6) Research prospects.

3. RESULTS AND DISCUSSION

3.1 Overview of AI Techniques Applied in Biochemistry

After full-text screening, 95 scientific papers were considered eligible. Research covered multiple AI paradigms across the range of biochemical fields. The top five techniques reported were supervised machine learning (n=38, 40%), deep learning (n=29, 30.5%), NLP/LLMs (n=12, 12.6%), generative AI (n=9, 9.5%) and other techniques such as robotic automation, federated learning, and XAI (n=7, 7.4%). The main identified techniques of artificial intelligence, the main underlying mechanism, and the biochemistry-specific applications and representative clinical examples are summarised in Table 1.

Table 1. AI Techniques and Their Applications in Biochemistry

AI Technique	Core Mechanism	Biochemistry Application	Clinical Example
Machine Learning (ML)	Pattern recognition in large datasets	Biomarker identification, disease risk prediction, lab QC	Disease risk scores; lipid panel anomaly flags
Deep Learning (DL)	Deep neural network models for learning complex data representations.	Protein structure prediction (AlphaFold2), image-based diagnostics	Retinal OCT analysis; urine sediment classification
Natural Language Processing (NLP)	Text scooping from biomedical literature and EHRs	Literature mining, clinical report generation, ICD coding	Automated lab report interpretation; drug interaction alerts
Generative AI / LLMs	Novel molecular design; content generation	De novo drug design (MolGPT), synthetic biology, education	Scaffold generation for novel enzyme inhibitors
Robotic Process Automation (RPA)	Rule-based workflow automation	Sample handling, barcode tracking, LIS integration	Automated specimen routing in hospital labs
Federated Learning	Distributed model training without sharing raw data	Multi-institutional biochemical research, privacy-preserving diagnostics	CKD prediction models across hospital networks
Explainable AI (XAI)	Interpretable model outputs	Clinical decision support, regulatory compliance	SHAP values for HbA1c risk model outputs

Abbreviations: CNN – Convolutional Neural Network; LIS – Laboratory Information System; ADMET – Absorption, Distribution, Metabolism, Excretion, Toxicity; SHAP – SHapley Additive exPlanations

Table 2. AI Applications in Clinical Biochemistry by Disease Domain

Disease Domain	Biochemical Parameters	AI Approach	Clinical Impact
Diabetes & Metabolic Syndrome	HbA1c trend prediction, insulin resistance scoring	ML models integrating HbA1c, fasting glucose, lipid profiles	Early T2DM risk up to 5 years before diagnosis
Cardiovascular Disease	Troponin, BNP, lipid panel AI interpretation	Deep learning on lipid subfractions and apolipoprotein patterns	Reduced false-positive ACS admissions by ~18%
Chronic Kidney Disease (CKD)	eGFR trajectory modeling, cystatin C analysis	Federated ML across hospital networks	CKD staging accuracy improved by 12%
Liver Disorders	LFT pattern recognition (AST/ALT/GGT/ALP)	Time-series DL on serial liver enzyme trends	NASH vs. ALD differentiation without biopsy
Thyroid Disorders	TSH/FT4/FT3 multi-marker AI models	Ensemble classifiers on TFT panels	Subclinical hypothyroidism detection in early stages
Cancer Biomarkers	Tumor marker panel interpretation (AFP, CEA, CA-125, PSA)	LLM-assisted liquid biopsy result synthesis	Improved sensitivity for early-stage malignancy
Inborn Errors of Metabolism (IEM)	Urine metabolite profiling, tandem MS data	Pattern recognition on organic acid chromatography profiles	Automated newborn screening flagging
Infectious Diseases	Procalcitonin, CRP, ferritin sepsis models	Real-time ML on serial inflammatory markers	Sepsis prediction 6 hours before clinical deterioration

Abbreviations: ACS - Acute Coronary Syndrome; CKD - Chronic Kidney Disease; NASH - Non-Alcoholic Steatohepatitis; IEM - Inborn Errors of Metabolism; T2DM - Type 2 Diabetes Mellitus

3.2 AI in Clinical Biochemistry

Clinical biochemistry applications were the largest group of included studies (n=41, 43.2%). AI has been shown to make meaningful contributions in several areas of disease, including interpreting biochemical laboratory parameters, stratifying disease risk, and detecting disease early.

Diabetes and Metabolic Disorders: The machine learning models using HbA1c, FPG, lipid profile, insulin resistance indices, and anthropometric data had AUCs ranging from 0.85 to 0.92 for predicting T2DM over 5 years prior to the clinical diagnosis of T2DM. With the help of artificial intelligence, interpreting serial HbA1c trends enabled personalised glycemic trajectory mapping, providing a more accurate representation of monitoring than alerts based solely on thresholds. Models of microalbuminuria (MA) prediction with UACR added with renal function biomarkers shown better early nephropathy detection than using only single markers (Gupta et al., 2025; Obermeyer & Emanuel, 2016).

Cardiovascular Disease: Emergency department validation studies of AI systems

analysing cardiac biomarker panels (high-sensitivity troponin, BNP/NT-proBNP, CK-MB) demonstrated that they improved the ability to discriminate acute coronary syndrome from non-cardiac chest pain, with an about 18% reduction in false-positive emergency admissions. When applied to the data of lipid subfractions (LDL particle size, HDL functionality, apolipoprotein B/A1 ratios), deep learning models outperformed traditional Framingham-based scoring (Chen & Asch, 2017; Deo, 2015; Esteva et al., 2017; Manzur et al., 1990; Obermeyer & Emanuel, 2016; Rajpurkar et al., 2022; Topol, 2019).

Kidney and Liver Disorders: The federated machine learning models achieved a 12% increase in accuracy for CKD staging and an 87% sensitivity for predicting the development of end-stage renal disease when using multiple hospital networks that included information on serum creatinine, cystatin C, phosphate, and parathyroid hormone. In the field of hepatic disorders, time-series deep learning was used to visualise serial liver enzyme patterns (AST, ALT, GGT, ALP, albumin, bilirubin) and achieved non-invasive differentiation of non-alcoholic steatohepatitis (NASH) from alcoholic liver disease

with 81% accuracy (Baldi, 2012; Buczak & Guven, 2016; Gupta et al., 2025; Litjens et al., 2017; Obermeyer & Emanuel, 2016).

Cancer Biomarkers and Thyroid Disorders:

AFP, CEA, CA-125, PSA, and CA 19-9 cancer markers were synthesised using LLM, and the performance of the multi-marker cancer panel was compared with single-marker interpretation. AFP, CEA, CA-125, PSA, and CA 19-9 cancer markers were synthesised with the help of LLM, and the performance of the multi-marker cancer panel was compared with that of single-marker interpretation. In populations diagnosed as "euthyroid," the use of ensemble classifiers on thyroid function test (TFT) panels, which included TSH, FT3, FT4, anti-TPO antibodies, and thyroglobulin, allowed for the accurate detection of subclinical hypothyroidism for thyroid disorders (Gupta et al., 2025; Junaid, 2025; Obermeyer & Emanuel, 2016; Vaswani et al., 2017).

3.3 AI in Academic and Research Biochemistry

A large body of evidence (n=31, 32.6%) showed the transformative role of AI in molecular and translational biochemistry research, revolutionising the scope of what can be computed in structural molecular biology, pharmaceutical research, and multi-omics integration and drug prospecting (Baum et al, 2021; Goodfellow et al, 2014; Jumper et al, 2021; Junaid, 2025).

Protein Organisation Prediction: Created with DeepMind, AlphaFold2 made predictions of 3D protein structures from critical amino acid sequences with near-atomically precise accuracy, a feat that has been impossible for more than 50 years. AlphaFold now has structural predictions for more than 200 million proteins from essentially all known organisms, allowing structural biochemists to begin unearthing the structures of unknown enzymes, receptors, and transport proteins. The successor models, ESMFold and RoseTTAFold, extended these features to multimeric protein complexes and intrinsically disordered regions (Jumper et al., 2021; Rives et al., 2021; Senior et al., 2020).

Drug Discovery and Molecular Design:

Industry and academia are turning to generative AI models like MolGPT and ChemBERTa, which were trained on millions of known molecular structures and that design novel drug scaffolds with desired pharmacological properties in silico. The binding affinity, ADMET, and off-target predictions of graph neural networks (GNNs) are in close agreement with experimental validation. The potential savings from the incorporation of AI into preclinical drug discovery pipelines have been estimated as up to 40–60% of the lead optimisation phase, which works out to billions of dollars saved per approved drug (Aliper et al., 2016; Baum et al., 2021; Yang et al., 2019).

Enzyme Engineering and Synthetic Biology:

Enzymes with enhanced thermostability, substrate specificity, turnover rate (kcat), and resistance to inhibition can be rationally engineered using AI models such as ProteinMPNN and ESM-2. AI-powered Design-Build-Test-Learn cycles have been used to automate iterative optimisation of biosynthetic pathways that enable the production of microbes for the invention of new drugs, biofuels, bioremediation, etc. (Baum et al., 2021; Rives et al., 2021; Zhavoronkov, 2018).

Multi-Omics and Metabolomics Integration:

The computational approaches, such as MOFA+ Multi-Omics Factor Analysis and DIABLO, combine genomic, proteomic, and metabolomic data to discover cross-platform biochemical signatures of disease. The AI-powered metabolomics platforms, MetaboAnalyst AI and XCMS-ML, allow for high-throughput untargeted metabolite profiling, pathway enrichment analysis, and biomarker panel construction, utilising mass spectrometry data. These novel multi-omics AI technologies have revolutionised the field of precision oncology, rare disease identification, and personalised nutrition (Baum et al., 2021; Junaid, 2025).

3.4 AI in Laboratory Biochemistry and Automation

Laboratory automation (pre, during and post analytical processes) was a fast-growing application of AI (n=23, 24.2%). The use of AI in the laboratory has shown promising results in reducing errors, streamlining turnaround times, and enhancing diagnostic accuracy (Alhamzi, 2024; Anih et al., 2025).

Automated Urinalysis and Haematology: The image recognition system, based on a convolutional neural network (CNN), for urinalysis sediment classification achieved a high recognition sensitivity of 92-96%, significantly reducing the workload of manual microscopy and ensuring that the recognition results are comparable to those of laboratory scientists with more than 10 years of experience. Similarly, peripheral blood smear images were used with deep learning models, resulting in per-haematologist accuracy for WBC differential counting and red cell morphology classification (Alhamzi, 2024; Anih et al., 2025).

Quality Control and Laboratory Information Systems: Reagent lot failure, instrument drift, and impending QC rule violation can be predicted up to 24 hours in advance of manual detection by ML-based QC systems trained on historical QC data, allowing for preemptive corrective action and minimising reagent wastage. NLP-equipped Laboratory Information Systems (LIS) that also include AI engines automate critical value notifications, delta-check verification, reflex testing order and turnaround time monitoring, resulting in virtually 0 missed critical

value communications (Alhamzi, 2024; Anih et al., 2025).

Point-of-Care Testing and Microfluidics: Edge AI for biosensor chips facilitates real-time interpretation of point-of-care test results for glucose, troponin, CRP and creatinine, seamlessly integrated into clinical decision pathways. Sepsis biochemical

panels (procalcitonin, IL-6, lactate, and CRP) can be performed within 30 minutes with a single blood draw on an AI-integrated lab-on-chip microfluidic platform, with great potential in emergency and resource-limited environments (Deo, 2015; Huang et al., 2025).

Table 3. AI Applications in Academic and Research Biochemistry

Research Domain	Key AI Tools/Models	Key Achievement	Application Area
Protein Structure Prediction	AlphaFold2, RoseTTAFold	Near-atomic accuracy for >200 million proteins in UniProt	Enzyme engineering, drug target identification
Drug Discovery	ChemBERTa, MolGPT, Graph Neural Nets	ADMET prediction, scaffold hopping, lead optimization	Accelerated preclinical pipeline by 40–60%
Enzyme Engineering	ProteinMPNN, ESM-2, directed evolution ML	Thermostability, substrate specificity, kcat optimization	Industrial biocatalysis, biosensor design
Metabolic Pathway Analysis	Flux Balance Analysis + ML, MetaboAnalyst AI	Multi-omics pathway enrichment, metabolic network mapping	Identifying novel therapeutic targets
Genomics-Proteomics Integration	Multi-omics fusion models (MOFA+, DIABLO)	Cross-platform data integration for systems biochemistry	Precision oncology, rare disease research
Synthetic Biology	Automated Design-Build-Test-Learn (DBTL) cycles	AI-designed genetic circuits and biosynthetic pathways	Biofuel production, recombinant protein manufacturing
Nutritional Biochemistry	Microbiome + metabolomics ML models	Personalized dietary recommendations, nutrigenomics	Gut-brain axis research, obesity interventions
Toxicological Biochemistry	QSAR/QSPR models, DeepTox	Hepatotoxicity and nephrotoxicity prediction from structure	Reducing late-stage drug attrition in clinical trials

Abbreviations: ADMET – Absorption, Distribution, Metabolism, Excretion, Toxicity; DBTL – Design-Build-Test-Learn; MOFA – Multi-Omics Factor Analysis; QSAR – Quantitative Structure-Activity Relationship

Table 4. AI in Laboratory Biochemistry – Automation and Workflow Applications

Laboratory Domain	AI Technology	Function	Outcome
Automated Urinalysis	CNN-based image recognition	Urine sediment classification (RBC, WBC, casts)	Reduced manual microscopy workload by >70%
Haematological Analysis	DL on peripheral smear images	WBC differential, reticulocyte maturation index	Accuracy comparable to trained haematologist
Point-of-Care Testing (POCT)	Edge AI on biosensor chips	Real-time glucose, troponin, CRP interpretation	ICU bedside monitoring, rural diagnostics
Quality Control (QC)	ML-based Westgard rules, Levey-Jennings AI	Predictive QC failure detection, drift correction	Reduced reagent wastage; 24/7 automated QC
Laboratory Information Systems (LIS)	NLP + rule-based engines	Critical value alerts, delta-check automation, reflex testing	Faster clinical notification; zero-missed criticals
Spectroscopy / Chromatography	Peak deconvolution ML, NIRS + AI	Automated HPLC peak identification, mass spec data analysis	Hemoglobin variant identification (HPLC-AI)
Microfluidics + AI	Lab-on-chip with integrated ML inference	Rapid multi-analyte biochemical profiling	Sepsis panels in <30 minutes from blood draw
Robotics / RPA	Computer vision + robotic arms	Sample sorting, aliquoting, barcode verification	Reduced pre-analytical errors by up to 85%

Abbreviations: CNN – Convolutional Neural Network; LIS – Laboratory Information System; POCT – Point-of-Care Testing; RPA – Robotic Process Automation; QC – Quality Control; HPLC – High-Performance Liquid Chromatography

4. DISCUSSION

The results of this thorough review have demonstrated that AI has become an integral part of virtually all significant areas of biochemistry and is not merely a convenience but a paradigm shift reshaping the landscape of scientific and clinical possibilities. AI's applications in biochemistry can be broken down into three converging approaches: speeding up discovery (research), improving precision (clinical), and optimising operations (laboratory) (Junaid, 2025; Rajpurkar et al., 2022; Topol, 2019).

Perhaps the most significant advancement in AI in biochemistry is the resolution of the protein folding problem. What had been impossible for decades - experimental crystallography and NMR spectroscopy - was done by AlphaFold2 in a single go: the rapid, accurate and scalable prediction of three-dimensional protein structures. Rational drug design of new protein conformations, as well as redesign of industrial enzymes for biocatalysis, have a cascading significance. Access to the predicted structures of more than 200 million proteins in an open-access database makes structural biochemistry accessible to all investigators, even those in geographically remote regions, who want to carry out prime-excellence in silico biochemical investigations (Dobson, 2001; Jumper et al., 2021; Senior et al., 2020).

De novo molecular design using generative AI is another transformative trend in drug discovery. Models like MolGPT and ChemBERTa can predict chemically valid, synthetically accessible molecules with the desired binding affinity and ADMET profiles, reducing years of lead generation to only weeks. Yet, the gap between in silico prediction and experimental validation remains significant, and prospective studies for clinical validation remain limited (Aliper et al., 2016; Baum et al., 2021; Yang et al., 2019).

The depth of AI's reach into clinical biochemistry aligns with its ability to combine multiple parameters into clinical intelligence. Laboratory results are typically interpreted using binary reference ranges, a system that is reductive for complex, multifactorial diseases such as diabetes, CKD, or metabolic syndrome. These AI models enable the detection of dynamic patterns in biochemical data trajectories that are not apparent from single-timepoint analysis, thereby offering insights into disease progression. These AI models can identify patterns in biochemical data trajectories that are dynamic and not detectable from single-timepoint analysis, providing insights into disease progression.

The validated power of ML models to predict T2DM risk long before the clinical threshold is reached, to detect CKD in its early stages, and to non-invasively differentiate NASH from ALD represents a paradigm shift from reactive to proactive biochemical medicine. Importantly, these models are designed to be most useful not in lieu of lab tests, but by intelligently using the context of the patient's available data—the sum of all the conditions a patient has (comorbidities), the medications prescribed (or not prescribed), the patient's demographic characteristics, and the patient's history over time (longitudinal trends) (Gupta et al., 2025; Junaid, 2025; Obermeyer & Emanuel, 2016).

One important, clinically relevant application is predicting sepsis using AI, based on repeated inflammatory biomarker panels. The ability of AI to forecast septic shock six hours prior to clinical deterioration, based on trajectories of procalcitonin, CRP, ferritin, and IL-6, carries significant implications for critical care medicine, particularly in the field of intensive care unit (ICU) biochemistry (Alhamzi, 2024; Gupta et al., 2025).

The idea of the 'Intelligent Automated Laboratory' (IAL), where AI systems monitor the entire testing process, detect pre-analytical errors, and automatically validate results, is no longer a theory. In high-throughput hospital laboratories, pre-analytical errors such as improper sample handling, labelling, and haemolysis detection can be reduced by up to 85% using AI-based robotic specimen-processing systems. Unlike traditional Westgard multi-rule systems, which only detect analytical imprecision when patient results are impacted, ML-based QC engines can provide predictive maintenance and early warning of QC failure (Alhamzi, 2024; Anih et al., 2025; Goodfellow et al., 2014; Huang et al., 2025; McKinney et al., 2020).

By incorporating NLP into LIS platforms, the laboratory report is no longer a mere data output but a dynamic, intelligent document that automatically identifies critical values, offers reflexive test recommendations, and provides clinically relevant interpretive remarks. This expertise not just enhances clinical safety but also significantly decreases the cognitive burden on clinical biochemists and pathologists (Alhamzi, 2024; Anih et al., 2025).

While there is strong evidence of its effectiveness, AI currently faces significant structural, technical, and ethical challenges to its integration into everyday medical and laboratory procedures. Data

quality and heterogeneity are the most common problems. This can create systematic bias in laboratory reference ranges, analytical platforms, and even reporting practices, which may hinder the generalizability of AI training datasets (Char et al., 2018; Junaid, 2025; Obermeyer & Emanuel, 2016; Rajpurkar et al., 2022).

The interpretability of models remains a significant unanswered question in clinical biochemistry. If the clinician does not know what the AI system is based on, he or she cannot trust the recommendation to make to the patient or defend in front of the patient. Explainable AI approaches, like SHapley Additive exPlanations (SHAP) and Local Interpretable Model-agnostic Explanations (LIME) (Char et al., 2018; Rudin, 2019), yield post hoc feature importance attributions but are not yet as causal intuitive as clinical practice would require.

The global regulation of AI-based In Vitro Diagnostic (IVD) devices is still in its infancy. The FDA's Software as a Medical Device (SaMD) guidelines and the EU AI Act offer some initial structure, but prospective validation requirements, post-market surveillance duties and performance drift monitoring requirements for AI diagnostic products are not yet sufficiently specified. Commercial uptake is likely to be slow if there are no clear regulatory avenues (Char et al., 2018; Price & Cohen, 2019).

Perhaps the most ethically problematic issue is algorithmic bias due to non-representative training sets. There are several studies that have been published in multiple journals that noted that AI replicas that are trained using mainly Western, Caucasian clinical data perform poorly with populations of South Asian, African or indigenous populations, which have different biochemical phenotypes, disease prevalence and genetic makeup. There is a potential for biochemical AI systems to cause inequities in health outcomes (Bibault et al., 2016; Murdoch & Detsky, 2013; Obermeyer et al., 2019; Parikh et al., 2019; Somashekhar et al., 2018).

5. CONCLUSIONS

This extensive review has confirmed that AI is not just a bolt-on to biochemistry but a transformative technology that is changing the scope and practice of the field at all stages, from molecular discovery to clinical diagnosis to laboratory management. The evidence collected and summarised here supports the measurable and validated impact of AI in the following areas: protein structure prediction, drug design, biomarker discovery, metabolic pathway analysis, enzyme engineering, clinical decision support, laboratory automation, and quality

management. The protein-folding advances represented by AlphaFold2, the de novo molecular design capabilities of generative AI, and the clinical risk-stratification capabilities of ML models all point to a paradigm shift akin to the new standards of practice in biochemistry ushered in by the spectrophotometer or the polymerase chain reaction. There is a need for concerted effort by diverse stakeholder communities to recognise the potential of AI in biochemistry. To benefit from AI tools, biochemists and clinicians also need to be proactive, providing their domain expertise to design and validate models. Biological and clinical plausibility should be prioritised over statistical performance metrics. It will be important for regulatory agencies to create flexible, evidence-based policies that allow for the safe development and utilisation of AI without stifling innovation. Laboratory and clinical staff need to be made AI literate. Researchers need to be prepared to engage in future multi-institutional, prospective, real-world validation studies with diverse populations to validate AI models. The future of biochemistry is one in which AI complements rather than supplants the biochemist or clinician, providing computational intelligence integrated into the analytical and interpretive process. Making this future will require not only technological progress but also scientific integrity, ethical engagement, and institutional courage to think and act intelligently while remaining faithful to the first principles of evidence-based medicine and laboratory science.

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