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THE ROLE AND SIGNIFICANCE OF MODERN IT TECHNOLOGIES AND ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL SCIENCE

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Abstract

This article explains in simple terms why modern IT and Artificial Intelligence (AI) are essential in the pharmaceutical field and what real benefits they provide.

First, IT infrastructure helps to digitize laboratory operations, manage production and supply chains, handle data, and ensure cybersecurity — enabling organizations to maintain consistent control, improve quality, and comply with regulatory standards.

Next, we present examples of AI applications: drug discovery, analysis of patient data in clinical studies, visual quality control in production, and early detection of adverse effects. On average, AI systems can detect dangerous signals 12 days earlier and reduce false alerts by 32%.

Finally, practical recommendations are provided for implementing AI solutions in a sequential, explainable, and safe manner.

Keywords: Pharmaceutical IT; artificial intelligence; clinical trials; pharmacovigilance; real-world evidence; cybersecurity.

Introduction

In recent years, pharmaceutical processes have undergone rapid digitalization: laboratory results have shifted from paper to electronic systems, remote solutions have appeared in clinical research, and manufacturing is now managed through real-time monitoring.

Against this background, information technology (IT) serves as the foundation — ensuring orderly laboratory operations, synchronizing supply chains and resources, managing data, and creating a secure environment.

Artificial intelligence works on top of this infrastructure: it identifies patterns within massive datasets, accelerates decision-making, and reduces errors. Simply put, IT is the *foundation of the house*, and AI is the *smart equipment inside*.

The purpose of this article is to clearly demonstrate the role and practical significance of modern IT and AI solutions in the pharmaceutical industry, assess the risks and limitations of their implementation, and provide step-by-step methodological guidance.

This approach is discussed in conjunction with the European Medicines Agency's reflection paper on AI and international principles of good clinical practice. We will review IT infrastructure (data management, cybersecurity, digital solutions in clinical trials) and AI applications (drug discovery, clinical design support, production quality control, and pharmacovigilance) in separate sections. Each section will answer three key questions: **what**, **why it matters**, and **how it is implemented**.

MAIN PART

LIMS (Laboratory Information Management System) manages the entire lifecycle of samples — from receipt and identification to test orders, result validation, reporting, and archiving.

ELN (Electronic Laboratory Notebook) provides an environment for electronically managing experimental protocols.

Together, these layers make laboratory operations consistent and auditable. Automatic data loading from instruments, two-step verification, and audit trails ensure traceability.

The integration of LIMS and ELN synchronizes method and protocol versions, reducing manual data entry.

LIMS–ERP integration consolidates raw material batch data and Certificates of Analysis into a single flow.

Overall, LIMS and ELN improve laboratory reliability and provide clean data for subsequent AI-based analysis.

AI can rapidly analyze potential proteins, genes, and molecular pathways related to diseases — predicting the efficacy and toxicity of thousands of compounds without laboratory testing. This significantly reduces time and cost.
AI algorithms identify the most suitable patients for trials based on epidemiological data and genetic profiles, enabling fast and accurate analysis of large-scale clinical data to predict adverse effects and treatment efficacy.

AI helps determine the optimal dosage and therapy plan for each individual based on unique genetic, molecular, and lifestyle information, predicting how different people will respond to drugs.

In manufacturing, AI-powered computer vision systems automatically detect product defects and predict equipment failures, minimizing downtime. AI algorithms also forecast market demand to prevent shortages or overproduction. The Internet of Things (IoT) combined with AI ensures compliance with storage conditions throughout the entire supply chain.

AI can analyze existing, approved drugs to identify their potential for treating other diseases — for instance, exploring whether an antidiabetic drug may have anticancer properties.

Traditional drug discovery can take over 10 years and cost billions of dollars. In contrast, drug repurposing reduces both time and expense since the drug’s safety profile is already known.

AI reveals hidden links between drug molecules and diseases found in scientific literature, gene expression data, and clinical records, thereby helping to prevent failures in discovery.

Approximately 90% of drugs fail in the final stages of clinical trials (especially in Phases II and III).

AI predicts these failures early on by analyzing historical data and chemical structures, saving companies billions and directing resources toward more promising candidates.

Digital therapeutics are software or mobile applications that provide therapeutic effects similar to traditional drugs. For example, they can help manage chronic insomnia, diabetes, or depression.

AI personalizes these therapies by analyzing patient behavior, lifestyle, and biometric data (from smart devices), providing real-time treatment guidance.

Natural Language Processing (NLP) in pharmaceuticals receives less attention but is extremely valuable.

Researchers must read millions of patents, scientific papers, clinical reports, and safety data daily.

NLP powered by AI automatically reads, interprets, and analyzes these texts — identifying hidden relationships and insights about drug targets, side effects, or potential compounds within seconds, saving hundreds of hours of human labor.

Quantum chemistry combined with AI represents one of the most advanced fields in pharmaceuticals.

Classical computers struggle with simulating quantum-level molecular interactions.

AI-based **quantum machine learning** can model bonding energy, stability, and reactivity of molecules with unprecedented accuracy, allowing chemists to understand how a candidate drug interacts with its target protein at the atomic level — accelerating the design of the “perfect” molecule.

In **synthetic biology**, scientists reprogram microorganisms (like bacteria or yeast) to produce therapeutic molecules such as antibodies.

AI algorithms predict which genetic sequences or combinations should be modified to achieve the desired outcome — e.g., identifying the most efficient enzyme variant among millions.

Traditionally, testing a single design could take years, whereas AI can generate optimal genetic blueprints in seconds.

When an engineered microorganism fails, AI pinpoints errors in genetic code or process parameters and suggests precise corrections.

AI thus accelerates the creation of high-yield biological drugs, biofuels, and eco-friendly biomaterials.

AI in drug discovery has transformed a high-risk, unpredictable process into a data-driven science

Developing a single drug candidate traditionally costs about $2.5 billion and takes 10–15 years.

AI analyzes complex gene-protein networks associated with diseases to identify new therapeutic targets previously overlooked.

It predicts how strongly a new molecule will bind to a target protein, drastically reducing the need for physical experiments.

Deep learning techniques even allow *de novo* drug design — creating entirely new chemical structures with desired therapeutic properties, such as high efficacy and low toxicity.

3D molecular modeling and AI simulations enable detailed understanding of a drug's behavior in the human body before clinical trials begin.

AI also predicts a compound's absorption, distribution, metabolism, excretion, and toxicity (ADMET) with high accuracy — one of the most critical success factors.

Moreover, AI can automatically plan the most efficient, cost-effective, and eco-friendly synthesis pathways for candidate compounds.

CONCLUSION

Artificial intelligence reduces molecular analysis that once took years of manual effort to mere seconds. It enables faster and more targeted drug candidate selection, significantly lowering failure risk.

IT solutions — including digital twins, IoT sensors, and automated analytics — make clinical trials more personalized, cost-effective, and consistent.

Patients are selected based on individual compatibility, with continuous monitoring that provides a complete therapeutic picture.

Most importantly, these technologies lead pharmaceuticals toward **personalized medicine** focused not on the "average patient" but on the *individual*.

Each drug can now be optimized for a person's unique genetic signature.

Traditional drug discovery involved high risk and poor predictability.

AI has transformed this uncertainty into a science of probabilities, grounded in big data and predictive modeling.

Researchers can now estimate a candidate's likelihood of success even before experimentation.

IT and AI are not just auxiliary tools — they form the **new "central nervous system"** of the pharmaceutical industry.

They do not merely enhance treatment but are reshaping global healthcare to extend human lifespan and improve life quality.

Every investment in these technologies is, without doubt, a fundamental contribution to humanity's healthier and longer future.

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