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# ROLE OF ARTIFICIAL INTELLIGENCE IN THE PHARMACEUTICAL INDUSTRY FOR PRODUCT DEVELOPMENT

**Mr. Aniket Sudhakar Sutar[1]*, Dr. Abid Shaikh[2], Dr. Sunil S. Jaybhaye[3]**

Institue of Pharmacy, Badnapur, Jalna 431202.

Dr. Babasaheb Ambedkar Technological University, Loner, Raigad.

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**Corresponding Author: Mr. Aniket Sudhakar Sutar**

**Address:** Institue of Pharmacy, Badnapur, Jalna 431202.

## ➢ ABSTRACT

Artificial intelligence (AI) has become a powerful tool that combines human intelligence and knowledge with machine capabilities and provides solutions to complex challenges. AI technology has brought about a transformation in drug discovery, formulation and testing of pharmaceutical dosage forms. Using AI algorithms, it is possible to analyze a lot of data, including searches. This allows for a more efficient and targeted approach to drug discovery, increasing the success of drug approvals. AI helps reduce costs by optimizing research and development processes. The personalized medicine approach can be facilitated with AI that analyses patient data, leading to more effective treatment outcomes and better patient treatment compliance. This review article explores the wide range of AI applications in drug discovery, drug delivery dosage form design, process optimization, pharmacokinetic testing and pharmacodynamic studies. This article provides an overview of the different AI-based approaches used in pharmaceutical technology, highlighting their advantages and disadvantages. However, continued investment and exploration of AI in the pharmaceutical industry offers exciting prospects.

## ➢ KEYWORDS

Artificial Intelligence (AI), Machine learning, Drug discovery, Formulation, Dosage form testing, Pharmacokinetics, Pharmacodynamics, PBPK; QSAR, Target identification, Lead optimization, Personalized medicine.

## ➢ INTRODUCTION

- The adoption of AI in the pharmaceutical industry has evolved significantly over the past few decades. Initially, in the 1980s and 1990s, AI applications in drug discovery were limited to basic computer models, used mainly for molecular modeling and chemical structure prediction. These initial efforts laid the foundations for more sophisticated approaches as computing power and algorithms improved. In the early 2000s, AI began to gain traction with the introduction of machine learning algorithms capable of analysing complex data sets, which helped improve the drug discovery process by predicting molecular interactions and optimizing drug formulations. However, the widespread adoption of AI in pharma took off in the 2010s, driven by advances in big data, deep learning, and access to large biological and chemical datasets, such as genomics, proteomics, and high-throughput screening. Pharmaceutical companies are beginning to integrate AI into various stages of drug development, from target identification to clinical trial design. In recent years, AI has become an indispensable tool for accelerating drug discovery, optimizing clinical trials and personalizing treatments, marking a shift towards more efficient and data-driven pharmaceutical research and development.

- The convergence of artificial intelligence (AI) with new drug development has ushered in a new era of innovation that has significantly transformed many aspects of drug discovery and delivery. AI encompasses a wide range of techniques applied by pharmaceutical companies in recent decades, including machine learning, deep learning and other advanced computing techniques. This has created unprecedented opportunities to accelerate drug discovery and delivery processes, leading in turn to optimizing treatment regimens and improving patient outcomes.

- Traditionally, the drug discovery process has been characterized by high costs attributed to long lead times and high failure rates. By integrating AI-based approaches, pharmaceutical companies can navigate this complex landscape more effectively. For example, machine learning algorithms can analyze large databases to identify complex patterns. This enables the discovery of new therapeutic targets and the prediction of potential drug candidates with greater accuracy and at a faster rate than traditional trial-and-error methods. This has accelerated the drug development process for many diseases.

- Similarly, AI algorithms can analyze large-scale biomedical data and discover hidden relationships between drugs and diseases. This has enabled AI to enhance drug repurposing, facilitating the identification of new therapeutic uses for existing drugs and accelerating their clinical translation from bench to bedside. This is particularly important for some diseases, such as parasitic diseases that affect developing countries and even orphan diseases. In the era of personalized medicine, AI algorithms can analyze different patient data sets, such as genomics, proteomics, and clinical data, and provide personalized treatments for each patient based on their genetic makeup, lifestyle factors, and disease characteristics.

- This can minimize adverse effects and improve patient outcomes. Although the tremendous progress made so far is evident, integrating AI into drug discovery and delivery is not without challenges. Ethical considerations, regulatory hurdles and data privacy concerns continue to pose significant barriers to widespread adoption. Continued collaboration between researchers, clinicians, industry stakeholders and regulators is essential to drive AI innovation in pharma.

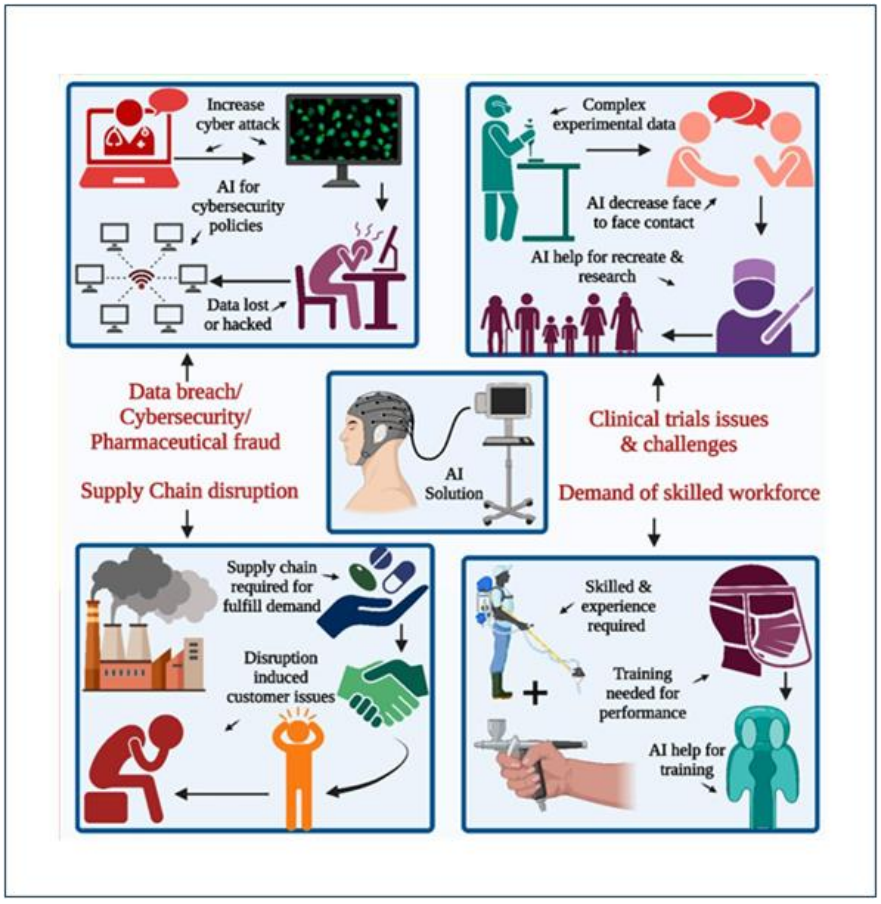


**Fig 1: Depicts a possible artificial intelligence (AI)**

## ➢ EMPLOYING AI IN PRODUCT DEVELOPMENT

Developing a high-quality product and a manufacturing process that guarantees reliable production of the necessary high-quality product are the two main objectives of pharmaceutical development. The design of new drugs, formulation development, drug repurposing, increasing R&D efficiency, aggregating and analysing biomedicine data, and streamlining the decision-making process to recruit study participants in clinical trials are just a few of the stages of product development where AI-enabled technologies have developed into flexible tools . These possible AI uses present a chance to reduce bias and human involvement while mitigating the inefficiencies and uncertainties that come with conventional product development techniques.43 Different kinds of AI algorithms are employed in the creation of new products.

- AI algorithms employed in product development and their applications

1. One tool for estimating drug behaviour in vivo and compensating for variations in drug release kinetics under different circumstances is the general regression neural network44,45 (GRNN). In their study, Stanojevi’c et al. employed two different kinds of artificial neural networks (ANN) to forecast the dissolution curve of 3D printed atomoxetine tablets. A self-organising map was used to visualise the impact of the inputs on the release of atomoxetine, and a GRNN was used to predict the release of atomoxetine.
2. It was discovered that the two testing formulations' predicted dissolution profiles matched the experimental data. The GRNN created in this study was therefore reasonably capable of forecasting the drug's dissolution behaviour. GRNN also conducts research in many other areas of pharmaceutical science.
3. Drug release from modified-release formulations is modelled or characterised using recurrent neural networks (RNNs). An extended-release aspirin neural network with four inputs and a single tablet output was designed by Ibric et al. using the multi-layered perceptron (MLP).
4. The NEURAL programme was used to create ten aspirin matrix tablets. Portions of MCC and GMS in the formulations, in vitro dissolution–time profiles at four different sampling time points, and the difference between the sampling time points, as well as coefficients n release (release order) and log k (release constant) from the one similarity factor, f as release parameters, Peppas equation was estimated.
5. Genetic algorithms and artificial neural networks (ANN&GA) - It is used for nanoparticle formulation of verapamil hydrochloride. Using the spherical central composite design and

the ANN methodology, they successfully optimized the formulation.

6. The resulting formulation had a high drug loading efficiency (92%) and a small mean particle size (100 nm), which is ideal for lymphatic transport via oral administration. It is found that ANN fit the experimental data better than (Response Surface Methodology) RSM, owing to ANN's ability to accommodate more complex and non-linear functional relationships.

➢ **Types of Artificial intelligence (AI)**

**1. Based On Capabilities**

- Narrow AI
- General AI
- Super intelligent AI

**2. Based On Functionalities**

- Reactive AI
- Limited AI
- Theory of mind
- Self-aware AI

**3. Based On Technologies**

- Machine language
- Deep learning
- Natural learning processing
- Robotics
- Computer vision
- Expert System

➢ **Application of AI In Pharm**

1. Quality Control & Quality Assurance (QA&QC)
2. Pharmaceutical Product Management
3. Pharmaceutical Product Development
4. Clinical Trial Design And Monitoring
5. Drug Design
6. Pharmaceutical Manufacturing

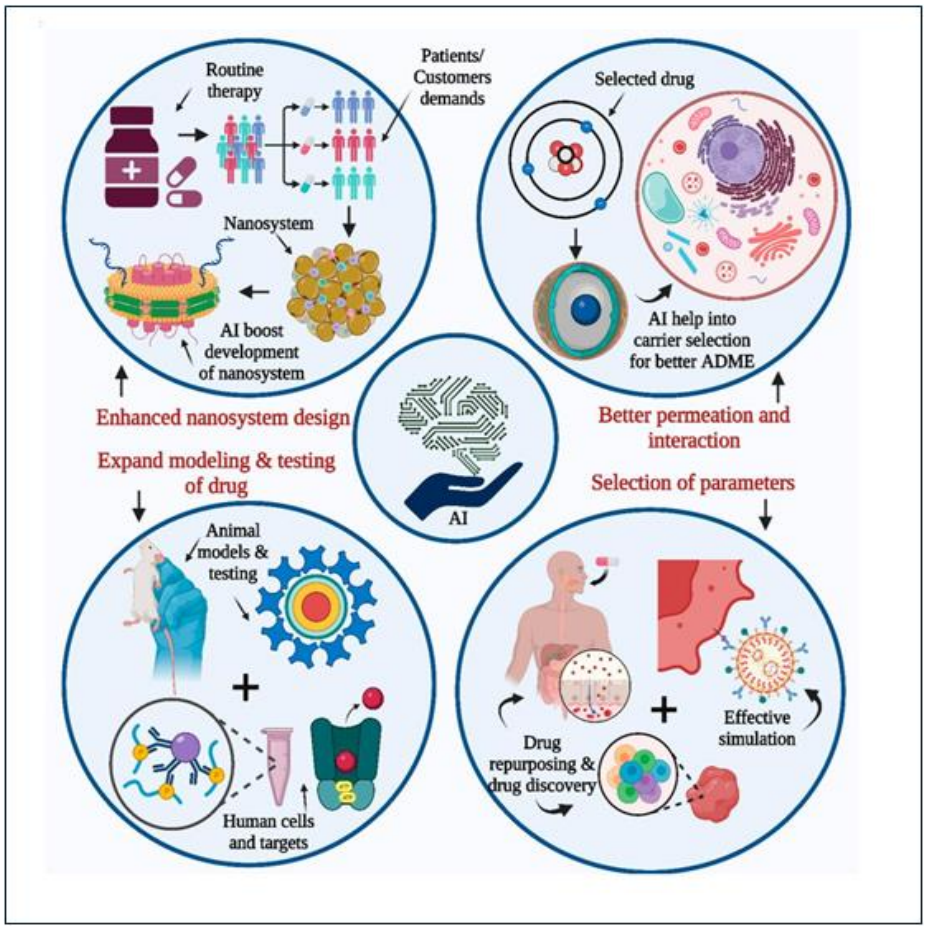


**Fig. 2: AI Tool Application in Dosage Form Designs.**

## ➢ Research Objectives

1. Examine how AI is used at different phases of drug development, design, and discovery.
2. Examine how AI might shorten the time and expense involved in introducing new medications to the market.
3. Evaluate how AI-powered prediction models can enhance medication safety, effectiveness, and clinical trial results.
4. Determine the obstacles and constraints to incorporating AI into pharmaceutical R&D processes.
5. Examine upcoming prospects and moral issues surrounding the application of AI in the pharmaceutical sector.

## ➢ Literature Review

- 2.1 Target Identification and Validation

AI helps exploit large biological/omic/pathway datasets to identify potential drug targets (proteins, genes) more quickly. Example: Using deep learning/neural networks to predict

protein binding, interactions and structural features with the target disease. A recent review says: "Identifying and validating the most effective drug targets with the help of AI."

- **2.2 Hit generation / Compound screening / Lead optimization**

Virtual screening: AI / ML models predict activity, ADMET properties (absorption / distribution / metabolism / excretion / toxicity), binding affinity. New drug design: Generative AI can propose entirely new molecules or design antibodies in silicon. For example, a 2023 article noted that a generative AI model created de novo (zero-shot) therapeutic antibodies, reducing lead identification time. Lead optimization: ML models help refine molecular structures to improve efficacy, reduce toxicity, and improve pharmacokinetics. Screening of large chemical areas becomes feasible.

- **2.3 Preclinical / in vitro / in vivo studies**

AI models can predict toxicology, off-target effects, drug interactions, thus reducing risks before expensive animal studies or first human trials. Simulation / Modeling: Molecular Dynamics, ML augmented constraint free energy predictions.

- **2.4 Clinical trials and development**

Patient recruitment and matching: AI helps identify appropriate patient populations, predict dropout and stratify subgroups. Adaptive trial design: Predictive analytics help optimize dose, arms and recruitment, speeding up time to trial results. Several reviews highlight the role of AI in clinical outcomes: for example, a study found in a sample that 40.9% of AI methods used were ML, 20.7% molecular modeling, 10.3% deep learning; oncology predominated (72.8% of studies) in one review. Real-time monitoring and analysis of test data with AI.

- **2.5 Formulation, manufacturing and quality control**

Once a drug candidate is approved, AI is used in pharmaceutical manufacturing: process analysis technology (PAT), predictive maintenance, supply chain optimization, quality assurance. For example: A study shows AI in manufacturing, quality control and post-market surveillance. AI enables pharmaceutical industry digitized/connected manufacturing and use of lifecycle data.

- **2.6 post-market surveillance/pharmacovigilance**

After market launch, AI can analyze real-world data (electronic health records, adverse event reports) to detect safety signals, optimize use and support life cycle management.

## ➢ Research Methodology

### 1. Research design

This project follows a descriptive and analytical research design, focusing on secondary data to explain how artificial intelligence (AI) is applied in different stages of pharmaceutical product development, from drug discovery to post-market surveillance.

### 2. Data collection

#### ❖ Primary data (if applicable)

Interviews or short questionnaires can be conducted with pharmacy professionals, researchers or industry experts to understand their views on AI integration.

#### ❖ Secondary Data

- Information collected from:
- Research journals (PubMed, ScienceDirect, SpringerLink, etc.)
- Journal articles, white papers, and case studies on AI in the pharmaceutical industry
- Company reports on major pharmaceutical companies using AI (Pfizer, Novartis, etc.)
- Government and regulatory databases (FDA, EMA, CDSCO.)

### 3. Data analysis

- The data will be analyzed qualitatively to identify key patterns, advances and challenges in AI-based product development.
- A comparative analysis between traditional and AI-assisted approaches will be conducted based on
- Time efficiency
- Cost reduction
- Predictive accuracy

## ➢ Statement of Problem

The pharmaceutical sector still faces major obstacles in drug discovery, development, and production despite quick technology developments, such as high costs, lengthy lead times, and poor success rates. Conventional approaches to product development sometimes rely on time-consuming and ineffective trial-and-error techniques. With its ability to analyze massive datasets, forecast molecular behavior, optimize formulations, and improve decision-making, artificial intelligence (AI) has become a game-changing tool. However, little is known about the obstacles to AI's general acceptance and how well it may be incorporated into the

pharmaceutical product development process. Investigating the effects, possibilities, and constraints of AI in enhancing and expediting the development of pharmaceutical products is crucial.

- **Hypothesis**

**1. $H_1$ (Alternative Hypothesis)**

When compared to conventional approaches, the use of artificial intelligence in pharmaceutical product development greatly increases productivity, lowers expenses, and expedites the drug discovery and formulation process.

**2. H0 (Null Hypothesis)**

When compared to conventional approaches, the use of artificial intelligence in pharmaceutical product development has no appreciable effect on productivity, cost savings, or timeliness.

- **Aim & Objective**

To assess how artificial intelligence (AI) might improve productivity, accuracy, and creativity in the pharmaceutical product development process, from medication discovery to formulation and production.

- **Objective Of Study**

1. To comprehend the fundamental ideas and methods of artificial intelligence applied to the pharmaceutical sector.
2. To investigate how AI is used in several phases of the creation of pharmaceutical products, including drug discovery, formulation design, and clinical trials.
3. To determine how AI might shorten development times, lower costs, and increase productivity.
4. To examine case studies or real-world instances of AI's effective application in pharmaceutical research and development.
5. To investigate the difficulties, moral dilemmas, and restrictions related to the application of AI in the creation of pharmaceutical products.
6. To make recommendations on how to successfully use AI technologies into the pharmaceutical sector for upcoming developments.

## ➢ Findings and Discussion

Our findings from the study are presented in this section of the article. The effect of AI on business process changes unique to the pharmaceutical sector. We will go into greater detail about how AI is affecting the main business processes that are unique to the industry we are focusing on, as well as some important quotes that frequently came up in conversations.

### • 4.1. Research and development

Whereas conventional techniques would take months or even years, algorithms enable researchers to search databases containing millions of molecules in a matter of hours. However, the fact that AI is unable to create a drug may suggest that a specific molecular combination has a higher likelihood of producing a medication for a given illness. "Using machine learning methods for R&D is the backbone of our business [target identification]."

Following that, businesses might cut back on the number of combinations and keep creating drugs the old-fashioned way.

AI is used by small businesses to complete a variety of extremely specific tasks by providing medium-sized and large businesses with services and outputs, such as target identification, scoring, and the creation of innovative small molecules. The foundation of small businesses' operations is how they achieve outcomes and raise the probability of success in drug discovery and development; this information is not required to be disclosed. As evidenced by the following statement from Medium Company 1's founder, medium-sized businesses aim to establish an R&D conveyor:

### • 4.2. Organizing Large and medium-sized businesses' planning

Procedures have undergone substantial change, mostly during the clinical trial phase. Before putting new medications on the market, pharmaceutical companies must test them for safety and effectiveness in controlled samples in accordance with FDA standards. The founder of Medium Company 5 pointed out that AI-based applications have the potential to significantly alter conventional clinical trials and raise the required parameters.

"There are machine learning-based trial planning solutions available on the market, but it is worthwhile to give them more consideration." The respondents stated that an early evaluation of the probability of success could result in a 70% reduction in the number of required experiments. Since their business models are built on services to boost drug development efficiency, small businesses have more optimistic outlooks. Existing databases that were

gathered prior to the widespread adoption of new technologies can be digitized by large corporations. Businesses can plan and forecast outcomes at various phases of drug development, particularly during clinical trials, using data that has been gathered and AI-analyzed. Big businesses are capable of organizing their marketing and sales campaigns.

- **4.3. Purchasing**

Few AI-based procurement systems have been effectively incorporated into the pharmaceutical and other sectors. Nonetheless, a number of software integrators that have the potential to work with pharmaceutical companies provide supply chain management, AI-based procurement decision-making, and smart contract management. As stated by a representative of Large Company "I believe we are the first in this market," the respondents suggested that AI-based procurement solutions might have an edge over industry experts. The suggested solutions can help with supplier selection (optimization of data collection and processing), procurement policy decisions (reduction of manual labor and supply chain flaws), and scaling. Numerous repetitive tasks can be replaced by AI applications, which can also provide decision support.

- **4.4. Manufacturing**

There aren't many instances of small and medium-sized businesses successfully employing AI capabilities in drug production. We anticipated that contract and generic manufacturing would serve as representatives of this sample during the study's preparatory phase. Our interviewees, however, questioned whether AI solutions were necessary in these situations; for instance, the founder of Small Company stated: "Manufacturing is not typical for small companies operating in the pharmaceutical industry." Large corporations house the great majority of pharmaceutical manufacturing facilities. Based on incoming and available internal and external data, these businesses may create production plans using AI-based applications.

- **4.5. Control of quality**

When it comes to quality and compliance, there is some misunderstanding. In the field of drug development, both are significant, but they differ in some ways. Quality is the sum of the factors that customers consider and that influence how satisfied they are with a product or service. The guidelines and standards that must be adhered to in order to finish the FDA registration process are known as compliance. Large businesses are more likely than medium-sized businesses to use quality control software, while small businesses are less likely to do so. Additionally, a representative from Large Company 2 stated:

➢ **Advantages & Disadvantages of AI Integration**

- **Advantages**

**1.** Faster Drug Discovery

AI systems can look at huge collections of chemical and biological data to find possible drug candidates faster than traditional approaches. This cuts down on the time it takes to produce drugs by a lot.

**2. Cost Reduction**

AI helps minimise the overall cost of R&D and resource use by making tests more efficient and cutting down on failed attempts.

**3. Better Predictive Accuracy**

Machine learning models make predictions about drug-target interactions, toxicity, and efficacy more accurate, which makes clinical trials safer and more successful.

**4. Personalised Medicine**

AI helps create medicines that are tailored to each patient by looking at their genetic, clinical, and lifestyle data to make predictions about how well they will work.

**5. Automation and Efficiency**

AI takes care of boring processes like data filtering and compound testing, which boosts productivity and lets scientists focus on coming up with new ideas.

- **Disadvantages**

**1. Problems with Data Quality and Availability**

Large, high-quality datasets are essential to AI systems, and biased or inadequate data might result in erroneous predictions.

**2. High Implementation Cost**

The development and upkeep of AI systems necessitate large investments in technology, infrastructure, and qualified staff.

**3. Lack of Transparency (also known as the "Black Box" Problem)**

Many AI models, particularly deep learning systems, have poor interpretability, which makes it challenging to comprehend or defend choices in regulatory settings.

**4. Ethical and Regulatory Issues**

Adoption of AI is hampered by issues with patient permission, data privacy, and adherence to health legislation

**5. Limited Human Expertise in AI**

Effective integration and utilisation may be hampered by the lack of experts in both pharmaceutical sciences and AI.

- **Suggestion**

**1. Improve Data Quality and Accessibility**

To increase the precision and dependability of AI models, pharmaceutical businesses should make investments in developing standardised, high-quality, and interoperable datasets.

**2. Encourage cooperation between pharmaceutical scientists and AI specialists**

Multidisciplinary cooperation can guarantee that AI systems are created with a thorough comprehension of chemical and biological processes, resulting in more useful applications.

**3. Use Explainable and Transparent AI Models**

The industry should concentrate on explainable AI (XAI) techniques that enable transparent interpretation of model predictions and decisions in order to solve ethical and regulatory issues.

**4. Invest in Workforce Training**

Businesses and academic organisations should put in place training initiatives to produce experts in pharmaceutical sciences and AI technology.

**5. Boost Ethical and Regulatory Frameworks**

To guarantee the safe, moral, and responsible application of AI in drug discovery and product development, governments and regulatory organisations should revise their rules.

**6. Promote Public-Private Partnerships**

Working together, academic institutions, pharmaceutical businesses, and IT companies may effectively exchange AI-driven findings and promote innovation.

**7. Continuous Assessment and Validation of AI Models:**

To preserve dependability and adjust to new scientific facts, AI models must be regularly tested, validated, and improved.

## ➢ CONCLUSION

New technology have advanced many facets of living in recent decades. Business and society are paying more attention to AI. One sector where the pursuit of novel solutions is linked to large and extremely hazardous investments is the pharmaceutical business. AI's impact on pharmaceutical business procedures is significant, but it hasn't been thoroughly examined in the past.

We were able to examine which business activities are impacted by AI and how by doing research on fifteen pharmaceutical companies. We discovered that businesses convert essential and support business operations in different ways based on their size. Small businesses are more concerned with utilising AI to alter their R&D strategy and commercial procedures.

Big businesses are altering their manufacturing, sales, and marketing procedures. Consequently, medium-sized businesses are compelled to modify their business procedures based on their area of expertise.

However, there aren't many effective AI integrations in the pharmaceutical sector. Furthermore, some of the initiatives that have been effectively completed are carried out in particular regions and are not widely recognised in the marketplace.

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