



It can perform automated tasks based on the data provided to it. Idea organization and optimization streamlines the complexities and facilitate favourable outcome. Involvement of AI is increasing in numerous areas such as robotics, medical image analysis, calibrate standards, toxicity analysis as well as increase productivity. Various novel technologies are coming up few of which are beneficial in fields such as chemistry, biology, pharmaceutical sciences and one of the major sectors which is boosted by the use of AI is the healthcare sector[2]. The use of AI in fields such as healthcare and pharmaceutical research has led to many innovations and advancements which ensures patients well-being by coming up with faster solutions. Artificial Intelligence has played a significant role in disease diagnosis, medication management, research and clinical trials. The pharmaceutical industry has evolved prominently and AI is revolutionizing processes such as drug discovery, drug development, drug effectiveness and drug dispensing. These are not yet routinely practiced in Computer Aided Drug Design but can be used to unfold complex drug related problems. Utilization of such technology leads to the automation of the various manually driven operations

which provides time-saving and efficient ways of medicine development, dispensing and management for better patient care. Machine learning which is a branch of AI helps in determining drug stability, forced degradation studies, drug-drug interactions and side-effects which thereby assists in formulation development and also provides an overview of drug safety. AI and machine learning may improve the quality of formulation and it may enhance drug stability.

It can outperform humans in cognitive tasks and save time as well as reduce stress. Drug development techniques and procedures have significantly changed due to AI as it may predict hypothetical formulations as well as new combinations which may also avoid unfavorable results. Drug dispensing methods used earlier are slowly being morphed by AI which replaces manpower and eases the management of medications such as segregation, manufacturing, and expiry date as well as analyzing the drug contents, accurate dosage and administration. If we provide these skills to humans, it would be more beneficial for society, and being updated with AI won't affect jobs and employment.

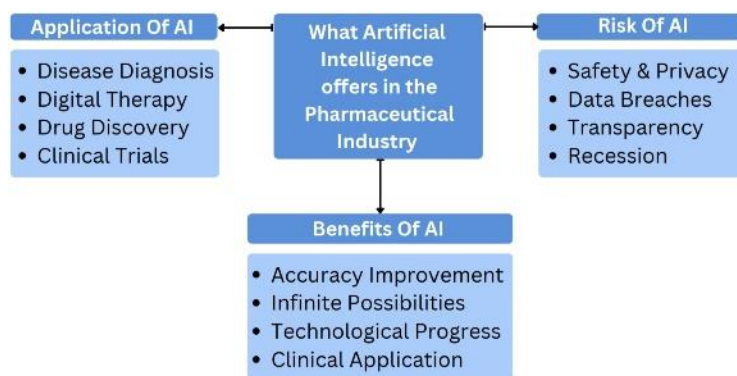


Diagram 2- Role of AI in Pharma Industry

Impact Of AI:

AI has a tremendous impact on the operations taking place in the lab as the development of drug molecules earlier was laborious and lengthy. Carrying out such processes in a restricted area and the lack of technologies led to increasing expenses and wastage of resources. Drug discovery is a process through which new therapeutic entities are identified. A lot of data and information needs to be provided to AI and it needs to be

trained in advance to acquire expected results. AI-aided organisations find it easy to discover various parameters such as structure-activity relationship, toxic concentrations, shelf life, contraindications, incompatibility and many more of various hypothetical drugs that are yet to be used in formulations. The specific proteins or genes which is the major cause of the succession of a disease can be analyzed using machine learning and thus drug action, effect and relevance on the



target sites could be studied. It helps in selecting the accurate and appropriate compounds which can effectively act on the causing agents and on the specific sites. The biochemical and physiologic properties of drugs can be studied and the chemical structures which are convenient for the same could be predicted. Thus the pharmacodynamic studies of the drugs can be known.

Thus the pharma companies are nowadays advancing various processes by working in coordination with software companies and adapting new technologies.

The Drug Discovery and Development Lifecycle includes the further steps –

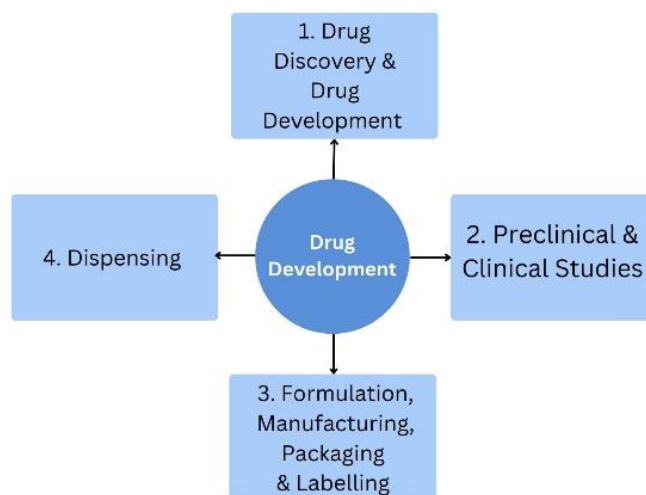


Diagram 3- Life cycle of drug discovery & drug development

1. Drug Discovery and Development:

Discovery of Drugs starts with the identification of the target as in the disease or condition to be treated and development of a new molecule which could potentially act on the target. The only loophole present is the tremendous consumption of time and energy. Artificial Intelligence overturned this by aiding in analysing biological data, identification of receptor and target, prediction of target-receptor interactions, compound screening, lead Identification and modification. It includes inductive-deductive cycle leading to optimised lead compounds[3]. Machine learning algorithms are used to determine which drug molecule would be efficient for further research and which wouldn't [4]. Molecular simulations imitate the operations of a system using computers which further reduces the need for physical testing of the drug compound [5]. AI/ML has the wide potential to select drug molecule for a particular disease according to its seasonability, local health trends based on external factors like weather patterns and demands for medications [6]. Pathogenesis of the disease

as well as Mechanism of Action of the drug is predicted using AI and it further assists to reduce occurrence of error during clinical trials and saves time [7]. Based on previous statistics, companies create their own database and train its models which can efficiently identify the target and response of drug that has not yet been tested. Even development of their own dataset and acquiring it from third parties is done by the companies to improve precision[8]. Medication errors in formulations and adverse drug reaction's patterns are identified which upgrades the drug molecule design [6]. The structure activity relationship of the drug affects various factors which greatly change the characteristics of the drug justifying the biological safety, efficacy and adverse effects of the drug [9]. Once a lead compound has been identified it brings about the establishment of drug development step and it begins long before the clinical testing. Various chemical databases are available based on which the Artificial Intelligence algorithms function to determine the characteristics of the lead compound and data preprocessing, standardization is done. Further,



Machine learning is used to create models based on acquired data which are then evaluated and the best model is selected for the further screening of drug [10]. Besides manual development of drug, more detailed and accurate decisions can be made for development of new drug using artificial intelligence[11].

While development is done manually, there are certain drawbacks which are needed to be considered-

1) Prediction of relationship amongst the formulation factors is difficult.

2) Response of drug molecule after development is in contrast with the one expected before development.

Thus it is rational to assume that Artificial Intelligence plays a major role in development of pharmaceutical compounds from bench to bedside.

2. Preclinical and Clinical Studies:

i) Preclinical Trials:

In preclinical studies, effectiveness and potency of novel medicinal substances are evaluated using tests which are conducted in vivo, in vitro and is mandatory before human trials initiate [12]. Preclinical studies is the research using animals to find out the approach of a drug which can be possibly utilize in various formulations to treat diseases. Animal models are used as they can replicate the aspects of human physiology and pathophysiology of disease[8]. Using AI in preclinical research can improve and optimize processes, but it's shouldn't completely replace traditional methods. Instead, AI can work alongside existing approaches to enhance efficiency and outcomes[13]. In-vitro involves studies outside the biological surrounding that includes tissues, organs, cells, etc. The AI supports in-vitro studies in completing the deadlines of experiment and particularly distinguish the results of each drug molecules[9]. Artificial Intelligence within in-vivo involves studies inside the biological surroundings and contribute to address unmet medical needs based on toxicology, efficacy, pharmacokinetic and pharmacodynamic parameters[14]. It is based on assumptions but does not fail to provide accurate, relevant and reliable results which are comparable to the existing human population.

ii) Clinical Trials:

It is an ethically designed investigation which involves testing and experiments on human candidates once it is proven to be effective and safe in preclinical trials. Thus evaluation of safety and efficacy as well as optimal use of drugs and its administration becomes easier.

Clinical Trials involve following phases[15]

Phase I: First in human studies

Phase II: Therapeutic Exploratory Studies

Phase III: Therapeutic Confirmation Trials

Phase IV: Post-marketing Surveillance

AI based technologies applied in clinical trials minimize the burden on humans, drug sponsors and regulatory bodies. It is performed virtually and involves the use of electronic hardware and software that can identify clinical end points and biological markers[13]. It mimics the human body and provides hypothetical insights of the disease progression and treatment as well as characteristics of the administered drug under surveillance. Patient condition, side effects and toxicity, pharmacokinetics and pharmacodynamic parameters become easy to understand and without any tedious and time consuming procedures. Drugs which can possibly be labelled with radioactive tracers can be much helpful by injecting it or providing it to the subject and tracing is overall path inside the human body i.e pharmacokinetics. Generally, clinical trials is a very tedious and laborious process and which requires 7-8 years of consistent efforts and a huge sum of money to be invested with a little success rate. Thus implementing right strategy and executing it becomes better with AI. The process could be appreciably sped up with investment of less time and lower economic burden [12]. AI can assist real world trials with design, conduct and analysis. Selection of the site of administration, dose to be administered and the resulting analysis is no more complicated with the aid of artificial intelligence. Overall accuracy is improved and precise outcomes are acquired [8]. Bayesian nonparametric models (BNMs) has come out as an efficient tool in clinical trials with numerous advantages having non parametric approach and being flexible. It is employed in applications such as dose selection which is strenuous due to heterogeneity in human patients and cell therapy trials in immuno-oncology and cancer patients.



Markov Chain Monte Carlo (MCMC) and Dirichlet Process Mixture Models are a few examples of BNMs [9]. Eligibility of patients is a major factor in selecting patients based on trial eligibility criteria. AI helps in matching suitable patients for suitable clinical trials and eliminates or reduces the chance of errors[16]. Phase III clinical trials include testing on nearly 300 to 3000 individuals at once and it manually troublesome to collect, compile and manage all the data at once. Thereby, AI makes it simple to combine patient data with Electronic Medical Record and thus helps in characterization, identification and selection of patients. It can examine patient data, their history and past treatments, statistical characteristics and to determine which patient would effectively respond to a new treatment [11]. Using the available data, adverse

reactions and certain risks can be found out before employing the subject in testing of drugs and the safety of new treatment.

3. Manufacturing and Formulation Development:

Once the drug is proved to be effective and passes the clinical trials process, it is sent to the FDA for evaluation. Thus, the safety of the drug, its efficacy and quality can be determined and a review is made accordingly. The different members or different professions review the respective data such as medical officer who reviews the clinical data and pharmacologist reviews the animal studies[17]. Inspection of the premises used for clinical trials is also carried out and evidence of adulteration, manipulation or any other errors are taken into consideration[17].



Diagram 4- FDA Approval steps

Thus approval of the drugs provides a green signal for its use into manufacturing. Top pharmaceutical companies are collaborating with AI vendors to employ it in manufacturing and get better outcomes based on more

efficient and precise operations[1]. Robotic Technologies are used to bring in innovation and get the work done faster in the manufacturing processes[18].



Diagram 5-AI in Manufacturing & Formulation

The major advantage of employing AI is predicting failure and reducing financial costs and shorten design time[19]. It reduces operational expenses by regulating quality control within the given standards, reducing

human interactions and automation in robotics and machinery[20]. While high level of accuracy and precision is achieved in weighing and compounding, the machinery used ensures the appropriate and uniform



mixing of the drug and excipients leading to reduction in deviation and improving quality[20].

Robots can perform tasks in snap of fingers which humans would require a large amount of time to get done. Eg. Rotary Tablet Press machine for tablets, Automatic Encapsulation machine for capsules, Different Ampoule Filling machines for parenterals etc. They reduce the defects and deviation and provide a stable, uniform and reliable product. Any defects or deviation can be removed using robots and the formulations are sidelined and discarded, thereby it can work in coordination with humans and lead to automation of this time consuming process. Productivity increase and labour cost as well as time consumption is reduced in labelling, packing, stacking as well as dispatching following GMP (Good Manufacturing Practices). Continuous production is an important method in manufacturing which eliminates the manual and batch processes and increases efficiency. Thus it limits the dissimilarity in the final products and minimize variations in patient outcome[20]. Using Artificial Intelligence and Machine Learning in these processes makes it well-regulated, cost-effective, labour-saving as well as energy efficient. Various dosage calculations as well as numerical entities play a major role in drug formulations and error in these procedures may be caused by humans. To manage this, Computer Numerical Control (CNC) powered by machine learning algorithms is proved to be advantageous[21]. Artificial Intelligence also gives rise to new and innovative strategies, inestimable outcomes in the favour of patient compliance by redefine the future of pharmaceutical manufacturing processes.

Once the manufacturing is completed it is mandatory for the formulations to go under various quality control tests for it to be proven of appropriate quality standards. Thus quality is an important requirement for a formulation to be marketed and sold which also determines the profit scale of the respected product. So it is vital that the pharmaceutical products must be manufactured to meet stringent regulatory standards. The quality control tests were carried out manually on a large scale which is taken over by artificial intelligence and machine learning processes. But manual tests involve a number of limitations as it being time-consuming, cost-intensive, repetitive-tasks, limited scalability and inadequate test coverage. Also human errors lead to decrease in accuracy and precision which compromises the quality of product

and human life. The machine learning tools dominate manual testing in various aspects such as reducing human error, saving time, reducing cost by using more efficient techniques, eliminating repetitive tasks and increasing scalability[22]. The formulations which pass the tests as per provided standards are then eligible for packaging. Using Artificial Intelligence in packaging science offers significant benefits like waste reduction, elimination of extra and unused products, overproduction and selection of appropriate packaging for certain drugs according to it's properties leading to reduction in testing procedures. It also suggests an alternative packaging for harmful materials such as plastic such as traditional materials and green packaging.

Considering the predominant part that AI plays in pharmaceutical industry, it is a transformative technology and has proven to be a revolution of it's own more than an evolution.

Risk Factors of Artificial Intelligence :

AI has shown appreciable development in the pharmaceutical industry and is constantly growing. Although it has impressively helped in the evolution of the drug discovery and dispensing processes, it possesses few drawbacks which could be unfair or maybe harmful for humans. As AI automates a wide range of tasks and functions more efficiently than humans, it leads to utilisation of technology in most of the tasks and creates unemployment minimising the need for human personnel. AI/ML being Information Technology based, it is difficult for workers to learn and adapt it as it is a difficult field of interest[12]. The biggest risk of using AI is data breaches and data piracy which is not safe and could cause harm to the common people as it becomes vulnerable to cyber-attacks[11]. The use of AI in drug development and dispensing may turn dangerous if there are ambiguities in it's functioning. Errors while monitoring a drug development process and its formulation may cost several lives. The models developed using Artificial Intelligence are purely based on data quality and availability of datasets. AI needs to be filled with appropriate data to provide relevant solutions and if it is inserted with poor quality data, it may affect the model's output. They should be validated before taking into consideration and using them in prediction of medications for rare diseases[25]. Hence proper measures must be taken to mitigate such risks and



ensure the privacy and security of data as well as the patient. Lack of transparency can be harmful for patients as it is difficult for the patients as well as doctors to understand from where data is used and decisions are made[22].

Conclusions:

AI are transforming landscape of drug discovery, drug development, preclinical & clinical trials, manufacturing, dispensing and offering significant improvement in pharmaceutical industry. The demands of digital transformation & new technologies are need of industry as to keep huge amount of health data efficiently. While challenges remains, the growing interest and attention of artificial intelligence from pharmaceutical industries and regulatory agencies combined with the potential benefits of AI, make it an exciting and promising area of research & development. Comparing machinery with manpower, the machines work with greater efficiency without limitations and are devoid of any emotions which bring about better precision. AI technology should be tested alongside with the existing technology it aims to complement or replace, and its value needs to be investigated precisely. Considering the increased utilization of artificial intelligence, unemployment could become an issue but can be tackled by assisting the humans and making them familiar with upcoming technologies. Thus looking forward towards the benefits AI does to the pharmaceutical industry, it has enhanced technological progress rate.

References

1. Raza A, Aziz S, Noreen M, Saeed A, Anjum I, Ahmed M, Raza S; Artificial Intelligence (AI) in Pharmacy: An Overview of Innovations; National Library of Medicine; 2022,10.24926/iip.v13i2.4839; 12,13(2).
2. Sharma V and Bharatam P; Artificial Intelligence in Drug Discovery (AIDD); Current Research & Information on Pharmaceutical Sciences (CRIPS); 2022, Volume 16, No. 1; 3 - 7.
3. Mak K and Pichika M; Artificial intelligence in drug development: present status and future prospects; Science Direct; 2019, Volume 24, Issue 3; 773 - 780.
4. Mali A, Nambiar A, Agrawal A, Kumar D; Trends and Scope of Artificial Intelligence and Machine Learning in Pharmaceutical Industry; Current Research & Information on Pharmaceutical Sciences (CRIPS); 2022, Volume 16, No.3; 42 - 49.
5. Chun M; How Artificial Intelligence is Revolutionizing Drug Discovery; Bill of Health; 2023.
6. Meslamani A; Applications of AI in pharmacy practice: a look at hospital and community settings; Journal of Medical Economics; 2023, Volume 26, Issue 1; 1081 - 1084.
7. Singh N, Kumar S, Prabhu K, Shukla A, Yadav A; A Review on Artificial Intelligence in Pharma; International Journal of Pharmaceutics; 2023; 10.47583/ijpsrr.2024.v84i01.006; 33 - 39.
8. <https://www.who.int/publications/i/item/9789240088108>
9. Bhattamisra S, Banerjee P, Gupta P, Mayuren J, Patra S, Candasamy M; Artificial Intelligence in Pharmaceutical and Healthcare Research; Big Data and Cognitive Computing; volume 7; Issue 1; 2023.
10. Tripathi M, Nath A, Singh T, A. S. Ethayathulla, Kaur P; Evolving scenario of big data and Artificial Intelligence (AI) in drug discovery; Molecular Diversity; Volume 25; pages 1439–1460; 2021
11. Patil P, Nrip N, Hajare A, Hajare D, Patil M, Kanthe R, Gaiwad A, Vidyapeeth B; Artificial Intelligence and Tools in Pharmaceuticals: An Overview; Research Journal of Pharmacy and Technology; 2023
12. Choudhary H, Sharma A, Dr. Ahuja D; Applications of Artificial Intelligence in Pharmaceutical Industries; International Journal of Pharmaceutical Sciences Review and Research; Article No.27; pages: 159-164; 2023
13. Hons L, Flepisi B PhD, Brand S PhD, Hons C, Balmith M PhD; Evolution of Drug Development and Regulatory Affairs: The Demonstrated Power of Artificial Intelligence; Clinical Therapeutics; Volume 46; Issue 8; Pages e6-e14; 2024
14. Scott A, Burkhalter D, Calado G, Dakrouni S; Artificial Intelligence Applied to clinical trials: opportunities and challenges; Health and Technology; Volume 13 ; pages 203–213; 2023.



15. Shanbhag T, Shenoy S (2020); Pharmacology for Medical Graduates (Fourth Edition); Elsevier.
16. Bin Zhang, Lu Zhang, Qiuying Chen, Zhe Jin, Shuyi Liu & Shuixing Zhang; Harnessing artificial intelligence to improve clinical trial design; Communications Medicine; 2023
17. <https://www.fda.gov/patients/drug-development-process/step-4-fda-drug-review#:~:text=Directions%20for%20use-,FDA%20Review,FDA%20official%20makes%20a%20decision.>
18. Stasevych M and Zvarych V; Innovative Robotic Technologies and Artificial Intelligence in Pharmacy and Medicine: Paving the Way for the Future of Health Care—A Review; Big Data and Cognitive Computing; Volume 7; Issue 3; 2023
19. Kaminski R; AI in Pharma. What Does Artificial Intelligence Bring to the Pharmaceutical Industry?; 2021.
20. Ali K, Mohin SK, Mondal P, Goswami S, Ghosh S, Choudhuri S; Influence of artificial intelligence in modern pharmaceutical formulation and drug development; Future Journal of Pharmaceutical Sciences; Article number 53; 2024
21. Impact of Artificial Intelligence in the Pharmaceutical industry: How is AI transforming the pharmaceutical industry?; <https://intone.com/impact-of-artificial-intelligence-in-the-pharmaceutical-industry/>
22. Kone S; Role of AI in Quality Assurance; 2024; <https://techfysolutions.com/blog/role-of-ai-in-quality-assurance/>
23. Zheng Y, Rowell B, Chen Q, Kim J, Kontar R, Yang X, Lester C; Designing Human-Centered AI to Prevent Medication Dispensing Errors: Focus Group Study With Pharmacists; Journal of Medical Internet Research; 2023; Volume 7.
24. Chalasani H, Syed J, Ramesh M, Patil V, Kumar P; Artificial intelligence in the field of pharmacy practice: A literature review; National Library of Medicine; 2023; 10.1016/j.rcsop.2023.100346
25. Saha G; Transforming pharmaceutical manufacturing: The AI revolution; European Pharmaceutical Review; 2024