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ARTIFICIAL INTELLIGENCE USED IN THE PHARMA FIELD – ON REVIEW

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ABSTRACT

The advent of artificial intelligence (AI) has catalyzed a profound transformation in the pharmaceutical industry, ushering in a paradigm shift across various domains, including drug discovery, formulation development, manufacturing, quality control and post-market surveillance. The comprehensive review examines the multifaceted impact of AI-driven technologies on all stages of the pharmaceutical life cycle. It discusses the application of machine learning algorithms, data analytics, and predictive modeling to accelerate drug discovery processes, optimize formulation development, enhance manufacturing efficiency, ensure stringent quality control measures, and revolutionize post-market surveillance methodologies. By describing the advancement, challenges, and future prospects of harnessing AI in the pharmaceutical landscape, this review offers valuable insights into the evolving dynamics of drug-development and regulatory practices in the era of AI-driven innovation.

Key words: Artificial intelligence, Machine learning, pharmaceutical industry, Drug discovery, Drug manufacturing, Supply chain management.

INTRODUCTION

Artificial Intelligence (AI) is a stream of science related to intelligent machine learning, mainly intelligent computer programs, which provides results in the similar way to human attention process. This process generally comprises obtaining data, developing efficient systems for the uses of obtained data, illustrating definite or approximate conclusions and self-corrections/adjustments. In general, AI is used for analyzing the machine learning to imitate the cognitive tasks of individuals. AI technology is exercised to perform more accurate analysis as well as to attain useful interpretation. In this perspective, various useful statistical models as

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well as computational intelligence are combined in the AI technology.

The progress and innovation of AI applications are often associated to the fear of unemployment threat. However, almost all advancements in the applications of AI technology are being celebrated on account of the confidence which enormously contributes its efficacy to the industry. Recently, AI technology becomes a very fundamental part of industry for the useful applications in many technical and research fields. The emergent initiative of accepting the applications of AI technology in pharmacy including drug discovery, drug delivery formulation development and other healthcare applications have already been shifted from hype to hope. The uses of AI model also make possible to predict the in vivo responses, pharmacokinetic parameters of the therapeutics, suitable dosing, according to the importance

of pharmacokinetic prediction of drugs, the uses of in silico models facilitate their effectiveness and inexpensiveness in the drug research. There are two key classes of AI technology developments. The first one comprises the conventional computing methodologies including expert systems, which are capable of simulating the human experiences and illustrating the conclusions from the principles, like expert systems. The second one comprises the system, which can model the mode of brain functioning employing the artificial neural networks (ANNS). In specific, various ANNs like deep neural networks (DNNs) or recurrent neural networks (RNNs) control the evolutions of AI technology. In Merck Kaggle11 and NIH TOX21 challenge, DNN issues show the greater predictivity than the baseline machine learning methodologies. The machine learning employs suitable statistical methodologies with the capability to learn with or devoid of being unequivocally programmed. In addition, de novo design promotes the invention of newer drug molecules with regard to optimal or desired qualities. In the current review article, the uses of AI in pharmacy, especially in drug discovery, drug delivery formulation development, polypharmacology and hospital pharmacy are discussed. (Al Kuwaiti A, et al. 2023; Al Kuwaiti A, et al. 2023).

Classification of AI

AI can be classified into two different ways: according to caliber and their presence. According to their ability, AI can be categorized as

- i) Artificial Narrow Intelligence (ANI) or Weak AI: It performs a narrow range task, i.e.,
- ii) Artificial General Intelligence (AGI) or Strong AI: It performs all the things as humans and also known as human level AI. It can simplify human intellectual abilities and able to do unfamiliar task.
- iii) Artificial Super Intelligence (ASI): It is smarter than humans and has much more activity than humans drawing, mathematics, space, etc. According to their presence and not yet present, AI can be classified as follows:

Type 1: It is used for narrow purpose applications, which cannot use past experiences as it has no memory system. It is known as reactive machine. There are some examples of this memory, such as a IBM chess program, which can recognize the checkers on the chess playing board and capable of making predictions.

Type 2: It has limited memory system, which can apply the previous experiences for solving different problems. In automatic vehicles, this system is capable of making actions, but these records are not stored permanently.

Type 3: It is based upon “Theory of Mind “. It means that the decisions that human being make are impinged

by their individual thinking, intentions and desires. This system is non-existing AI.

Type4: It has self-awareness, i.e., the sense of self and consciousness. This system is also non-existing AI. (Albayrak Ünal O, et al. 2023)

Advantages of AI technology

The potential advantages of AI technology are as follows:

- i. Error minimization: AI assists to decrease the errors and increase the accuracy with more precision. Intelligent robots are made of resistant metal bodies and capable of tolerating the aggressive atmospheric space, therefore, they are sent to explore space.
- ii. Difficult exploration: AI exhibits its usefulness in the mining sector. It is also used in the fuel exploration sector. AI systems are capable of investigating the ocean by defeating the errors caused by humans.
- iii. Repetitive tasks: In general, human beings can perform single task at a time. In contrast to the human beings, machines are capable of performing multi-tasking jobs and can analyze more rapidly in comparison to the human beings. Various machine parameters, i.e., speed and time can be adjusted according to their requirements.
- iv. Medical uses: In general, the physicians can assess the condition of patients and analyze the adverse effects and other health risks associated with the medication with the help of AI programs like various artificial surgery simulators (for examples, gastrointestinal simulation, heart simulation, brain simulation, etc.)
- v. No breaks: Unlike human beings who have the capacity of working for 8 h/day with breaks, the machines are programmed in such a way that these are capable of performing the work in a continuous manner for long hours devoid of any kinds of confusions and boredom.
- vi. Increase technological growth rate: AI technology is widely used in most of the advanced technological innovations worldwide. It is capable of producing different computational modeling programs and aims for the invention of the newer molecules. AI technology is also being used in the development of drug delivery formulation.
- vii. No risk: In case of working at the risky zone like fire stations, there are huge chances of causing harm to the personnel engaged. For the machine learning programs, if some mishap happens then broken parts can be repairable.
- viii. Acts as aids: AI technology has played a different function by serving children as well as elders on a 24x7 basis. It can perform as teaching and learning sources.

- ix. Limitless functions: Machines are not restricted to any boundaries. The emotionless machines can do everything more efficiently and, also produce more accurately than the human beings.

Disadvantages of AI technology

The important disadvantages of AI technology are as follows:

- i. Expensive: The launch of AI caused huge money consumption. Complex designing of machine, maintenance and repairing are highly cost effective. For the designing of one AI machine, a long period of time is required by the R&D division. AI machine needs updating the software programmes, regularly. The reinstallations as well as recovery of the machines consume longer time and huge money.
- ii. No replicating humans: Robots with the AI technology are associated with the power of thinking like human beings emotionless as these add some advantages to perform the given task more accurately without any judgment. If unfamiliar problems arise, robots cannot take the decision and provide false report.
- iii. No original creativity: Machines with AI technology have neither sensitivity nor the emotional intelligence. Human have the ability to hear, see, feel and think. They can use their creativity as well as thoughts. These features are not achievable by the uses of machines.
- iv. Unemployment: The widespread uses of AI technology in all the sectors may cause large scale unemployment. As because of the undesirable unemployment, human workers may lose their working habits and creativity. (Alowais SA, et al. 2023; Badwan BA, et al. 2023)

The role of AI in pharmaceutical formulation optimization and development

Pharmaceutical formulation development is a crucial step in drug discovery and development. Pharmaceutical experts can manipulate crucial characteristics of new medications, such as enhanced bioavailability and targeted distribution, by designing drug formulations. The conventional method for drug formulation relies on a repetitive trial and error process, which requires a significant amount of resources and time-consuming studies conducted in laboratories and living organisms. The introduction of AI into pharmaceutical formulation development has streamlined this process for a more efficient, precise, and cost-effective approach. The application of AI in pharmaceutical formulation can be categorized into three groups, namely, conventional dosage forms, advanced oral drug delivery, and micro/nanoparticles for drug delivery. (Bannigan P, et al. 2023)

Clinical trials

Artificial Intelligence in telepsychology [E-therapy]

AI may be able to extract a meaningful relationship. This can also be applied to the disease's diagnosis, course of treatment, and mitigation. Many of the more recent method utilized in the emerging field of computational understanding have the potential to be applied in nearly all branches of medical science. The challenges of learning, analyzing and applying a wealth of knowledge must be overcome in order to solve the complex clinical problems. The advancement of AI in medicine has aided clinicians in resolving challenging clinical issues. The biological nervous system serves as the foundation for the artificial neural network (ANN). A network of linked computer processors, resembling neurons, conducts concurrent data processing.

In 1974, Paul Werbos introduced a novel method known as "Back propagation learning" featuring and effective learning algorithm. Artificial neural networks have found applications in fields like image diagnosis, data interpretation, and waveform analysis. Fuzzy logic is a discipline concerned with reasoning, and inference that can comprehend and apply real world phenomena.

Artificial intelligence in radiooncology

It effectively enhances plan quality, consistency, and reduces error rates. The treatment process can be categorized into three segments: automated rule application, modeling of previous clinical knowledge, and multi-criteria optimization. The treatment planning system can analyse a patient's anatomy and physiology and replicate the reasoning process typically used in manual treatment planning. Radiomics can be applied to predict outcomes and assess toxicity in individual patients receiving radiation therapy.

Artificial intelligence in ophthalmology

Retinal high-resolution imaging has made it possible to assess human health in a remarkable way. An ophthalmologist or retina specialist can create a personalized therapy plan and implement an ever-improving learning healthcare system using just one retinal photograph and high-definition medications.

Artificial intelligence in oncology

AI has become increasingly important in the fields of cancer diagnosis and treatment due to its wide range of applications. A multilayer perception neural network was trained with gene expression data to predict the lymphoma subtypes of non-Hodgkin lymphoma. 12 Lymphoma subtypes make up the output layer of the neural network, while 20,863 genes make up the input layer. The results showed that 58 genes have high accuracy survival predictions, 10 of which were linked to poor survival, and 5 of which were favorable. Artificial

intelligence has made assays for classification and further clinical application more economical, efficient and repeatable. AI reduces time while maintaining high accuracy in the diagnosis of cancer.

AI has shown great promise in the last ten years for the diagnosis of breast cancer. Utilizing a combination of quantitative and qualitative MRI features, assisted techniques can be used to predict treatment response in patients with breast cancer, even prior to the initiation of neoadjuvant chemotherapy (NAC). AI based software can assist radiologists in their clinical work by helping them differentiate between benign and malignant breast lesions and by lowering the likelihood that false negative mammograms will be interpreted.

Artificial intelligence in chronic pain management

Based on computer programming techniques, various computerized therapies are available. The patient may follow recommendations for one medication and perform their own biopsy. Regular monitoring is necessary for chronic diseases and artificial intelligence (AI) can be used to create virtual medical assistants to help with this monitoring.

Artificial intelligence-enhanced drug screening

Testing compounds against samples of diseased cells is a common step in the lengthy drug discovery process. Further analysis is needed to identify compounds that are biologically active and worthy of further investigation. New and efficient medications can be made available sooner thanks to computers significantly faster discovery of new data sets than traditional human analysis and laboratory.

Advance techniques

- A. Robot pharmacy: Robotic technology is used by UCSF Medical Center to track and prepare medications with the goal of enhancing patient safety. They claim that the technology has flawlessly prepared 3, 50,000 doses of medication.
- B. MEDI Robot: The acronym for medical and engineering designing intelligence is MEDI. AI instruments Tanya Beran, an Albertan professor of community health science at the University of Calgary, oversaw the project that resulted in the development of the pain management robot.
- C. TUG robots: Aethon TUG robots are made to move through hospitals on their own and deliver supplies, meals, medications, specimens and heavy items like trash and linen. (Chaudhary S, et al. 2023; Dinh H. 2024)
- D. Erica robot: Professor Hiroshi Ishiguro of Osaka University in Japan is the creator of the new care robot Erica. It was created in cooperation with Kyoto University, the Advanced Telecommunication Research Institute International (ATR) and the Japan

Science and Technology Agency. Its facial features are a mix of European and Asian and it speaks Japanese.

Propose Emerging Therapeutic Approaches

Verge is addressing the primary issues in drug discovery through automated data collection and analysis. On the human brain, concentrating especially on the preclinical stage.

Synthesis of Innovative Peptides

The Irish start up Nerites uses artificial intelligence (AI) and other cutting-edge technologies to make it easier to find new, healthier ingredients and foods that are more robust.

Care and Supervision of Uncommon Diseases

AI developments and a resurgence of interest in treating rare diseases. Over 350 million people worldwide suffer from more than 7,000 rare diseases at the moment. Nevertheless, there is hope for patients suffering from uncommon illness as Heal, a biotech company based in the UK, has managed to obtain \$10 million in series funding to employ artificial intelligence in creating novel medications for uncommon ailments.

Medication Adherence and Measurements

To strength medication adherence and increase drug trial vigilance, Abbvie teamed up with Acura, a company-based in New York. More specifically, the patients use their smart phones to record themselves swallowing a pill and the AI powered platform verifies that the right person did, in fact, swallow the prescribed medication. Bayer uses Pharmacovigilance Artificial intelligence (PVAI) from Genpact to monitor medication adherence and identify possible side effects much earlier.

Benefits of Artificial Intelligence Technology's

The prophecy benefits of Artificial Intelligence technology are as follows:

1. Accuracy Improvement: Artificial intelligence aids in reducing mistakes and enhancing precision, resulting in increased accuracy.
2. Challenging expedition: Artificial intelligence demonstrates its practicality in the mining industry, as well as finding application in fuel exploration. AI technologies have the capability to explore the ocean by overcoming human-induced errors.
3. Artificial intelligence Assistants: AI system like "avatars" or model of digital assistants, are being used by sophisticated organization these days to reduce the need for human labor. The efficiency of judgment is disrupted by human emotions and moods, but machine intelligence can help solve this issue.

4. **Clinical Applications:** With the aid of an AI program, doctors can generally evaluate their patient's conditions and analyses any side effects or other health risks related to their medications.
5. **Assistants and Relief:** AI technology serves individuals of all ages, children and the elderly, round the clock, taking on roles as educational resources for teaching and learning.

Vision of Artificial Intelligence

When it comes to pharmaceuticals, there are a lot of unmet needs. In healthcare, a revolution is taking place. A Johnson & Johnson representative said in a statement that “artificial intelligence is giving to discover new treatments and techniques faster than we would have thought possible just a decade ago.” In the pharmaceutical field, efforts are underway to leverage AI to predict the timing and locations of potential epidemic outbreaks with a reasonable level of accuracy. Within the healthcare sector, AI is being employed to proactively avoid medical mistakes and lower the frequency of hospital readmissions.

The future of AI in the pharmaceutical industry

The future of AI in the pharmaceutical industry is brimming with potential; it is poised to revolutionize drug discovery, pharmaceutical product development, industry management, regulatory affairs, and PMS. AI algorithms can analyze vast amounts of biological data to identify potential drug targets and accelerate drug discovery. AI-driven simulations can be implemented in drug development to predict the interactions between compounds and biological systems, facilitating more efficient and cost-effective clinical trials.

Over a thousand research articles and reviews have been published in the last 5 years on the use of AI in pharmaceutical applications. This indicates the value of enhancing and accelerating current research processes and protocols. As technology continues to advance, the integration of AI into various aspects of the pharmaceutical industry will undeniably drive innovation, improve patient outcomes, and reshape the future of healthcare. (Drug Discovery News. 2024)

Challenges and opportunities AI in pharma

Artificial intelligence brings both challenges and opportunities to the pharmaceutical industry. In one sense, AI accelerates drug discovery, improves clinical trials, and optimizes supply chains, resulting in greater efficiency and innovation. However, it also poses challenges that bring along significant hurdles and limitations, such as:

- *Lack of transparency
- *Lack of data availability

*Biases in data

*Data Inability

Therefore, AI-based models should be used in combination with traditional experimental methods to ensure the safety and efficiency of drugs. (Gruber A, et al. 2024)

Application of AI Poly-pharmacology

In disease-related molecular networking, poly-pharmacology is the strategic creation of a therapeutic molecule with the innate capacity to interact with numerous targets or pathways (put, “one disease-multiple target”). One can use this method to create a more effective and less hazardous therapy than currently available one. Several well-known databases that offer details on biochemical pathways, binding strengths, pharmacological goals, and physiological effects are PubChem, ChEMBL, drug bank, and binding DB. The AI system can use this data to probe and discover potential poly-pharmacological drugs selectively. One can use the range of available applications, improved computer capacity, and developments in AI technology to change the drug development process. (Kalaivasan R, et al. 2024)

Quality control and quality assurance

Developing a pharmaceutical formulation within the given timeframe while ensuring quality necessitates a meticulous and scientifically-driven approach to navigate the intricate process successfully. Gathering information involves capturing data about operations, and equipment. Various knowledge applications are utilized, such as heuristics, decision trees, correlation, and first-principal models. This information and knowledge inform the decision-making process for production, selection of excipients, and determination of equipment size. Consequently, AI and its networks, technologies, and tools ensure higher product quality, less waste, and increased profit for manufacturing company. Quality-by-Design (QBD) method ensures the improved quality of the generated goods. This approach makes it easy to comprehend the crucial elements in the pharmaceutical production process that might have an impact on the final product's quality. (Kamya P, et al. 2024)

Product development

The pharmaceutical sector focuses on accelerating pharmaceutical product development, cutting production costs, and enhancing process design for confirming an active medication. An example of a decision-support tool is the rule-based expert system, which represents domain knowledge as a collection of rules structural as IFTHEN statements. These rules utilize input data to assist in addressing specific problems. Each rule consists of two components: the IF

part, which establishes an assumption (such as medication insolubility), and the THEN part, which defines the corresponding action to be taken (such as using a soluble filler to address the solubility issue). This knowledge is subsequently applied to facilitate the development of the formulation. The design of later iterations of PFES involves three levels: physical, task, and control. Expert systems in formulation development have several benefits, such as ensuring a consistent process for regulatory compliance, aiding in novice and professional training, reducing product development time and cost, and freeing up experts to focus on innovation. AI has the potential to address certain challenges associated with controlled and conventional drug delivery systems, including issue such as systemic toxicity, narrow therapeutic ranges, and dose adjustments during long-term therapy. Microchips are employed to manage medication administration, lower systemic toxicity, narrow the therapeutic window, and reduce adverse effects. AI has made significant advancements in enhancing the efficacy, safety, and adherence of patients by innovating implanted drug delivery devices capable of regulating drug release timing and concentration. It is crucial to monitor glucose levels in diabetic patients and provide insulin regularly to treat the condition. The combination of glucose sensors, mathematical models, and control algorithms holds promise for facilitating this objective. Conventional therapeutic methods that have been utilized over time face certain limitations, which can be overcome by integrating information technology, wireless communication, and ANNs into standard therapeutic procedures. (Knox C, et al. 2024; Nitheezkant R, et al. 2024)

Pharmaceutical manufacturing

The FDA recommends a non-stop processing strategy to limit the variation of final products and patient outcomes. One can use various process analytical technology (PAT) tools, efficient and cost-effective to control uninterrupted production. Through automated ML, using AI conjunction with PAT can improve the process overall and help regulate the production process.

Predicting the mode-of-action of compounds using AI

The prospect of an AI platform that can predict drugs' on-and off-target effects as well as in vivo safety profiles prior to synthesizing has medicinal chemists, in particular, thrilled. The existence of such platforms reduces the amount of time, money, and attrition rates needed to create new medications. Among these

platforms are Deep Tox, which predicts the toxicity of new drugs, and PROCTOR, which assesses the probability of toxicity during clinical trials.

As a substitute for chemo-proteomics, SPIDER, a novel AI tool, was recently created to promote natural products for drug development. The platform expected that 5-lipoxygenase (5-LO) would be modulated allosterically and reversibly by lapachone. An alternative AI methodology, known as read-across structure-activity relationships (RASAR), has demonstrated the ability to effectively forecast the toxicity of unfamiliar compounds. (Vora LK, et al. 2023)

CONCLUSION

During past few years, a considerable amount of increasing interest towards the uses of AI technology has been identified for analyzing as well as interpreting some important fields of pharmacy like drug discovery, dosage form, designing, pharmaceutical industry, polypharmacology, hospital pharmacy, etc., as the AI technological approaches believe like human beings imagining knowledge, cracking problems and decision making. The uses of automated workflows and databases for the effective analyses employing AI approaches have been proved useful. As a result to the uses of AI approaches, the designing of the new hypotheses, strategies, prediction and analyses the various associated factors can easily be done with the facility of less time consumption and inexpensive. In conclusion, the function of AI in pharmaceutical formulation and development is rapidly expanding, bringing a host of benefits to the industry. The prospects for AI in pharmaceutical formulation and development are up-and-coming. As AI continues to evolve and improve, it is predictable to show an even more significant function in drug development to show an even more significant function in drug development, aiding researchers in identifying new drug targets, drug interactions, and patient populations most likely to benefit from treatment. So, the role of AI in pharmaceutical formulation and development has already proven to be transformative and is expected to continue to revolutionize the industry in the coming years.

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