



A REVIEW ON AI USING PHARMACY DISCIPLINE

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ABSTRACT

Artificial Intelligence (AI) focuses in producing intelligent modelling, which helps in imagining knowledge, cracking problems and decision making. Recently, AI plays an important role in various fields of pharmacy like drug discovery, drug delivery formulation development, polypharmacology, hospital pharmacy, etc.

Artificial intelligence (AI) has emerged as a powerful tool that harnesses anthropomorphic knowledge and provides expedited solutions to complex challenges. Remarkable advancements in AI technology and machine learning present a transformative opportunity in the drug discovery, formulation, and testing of pharmaceutical dosage forms. By utilizing AI algorithms that analyze extensive biological data, including genomics and proteomics, researchers can identify disease-associated targets and predict their interactions with potential drug candidates. This enables a more efficient and targeted approach to drug discovery, thereby increasing the likelihood of successful drug approvals. Furthermore, AI can contribute to reducing development costs by optimizing research and development processes.

KEYWORD: Artificial Intelligence, Type, Advantages, disadvantages,

Technology, Pharmacology, Pharmacokinetics, Pharmacodynamics, Pharmacovigilance, Machine learning, Future.

INTRODUCTION

• Artificial Intelligence

Artificial intelligence is a field of science concerned with building computers and machines that can reason, learn, and act in such a way that would normally require human intelligence or that involves data whose scale exceeds what humans can analyze.

AI is a broad field that encompasses many different disciplines, including computer science, data analytics and statistics, hardware and software engineering, linguistics, neuroscience, and even philosophy and psychology.

On an operational level for business use, AI is a set of technologies that are based primarily on machine learning and

deep learning, used for data analytics, predictions and forecasting, object categorization, natural language processing, recommendations, intelligent data retrieval, and more.

• How does AI work?

While the specifics vary across different AI techniques, the core principle revolves around data. AI systems learn and improve through exposure to vast amounts of data, identifying patterns and relationships that humans may miss. This learning process often involves algorithms, which are sets of rules or instructions that guide the AI's analysis and decision-making. In machine learning, a popular subset of AI, algorithms are trained on labeled or unlabeled data to make predictions or categorize information.

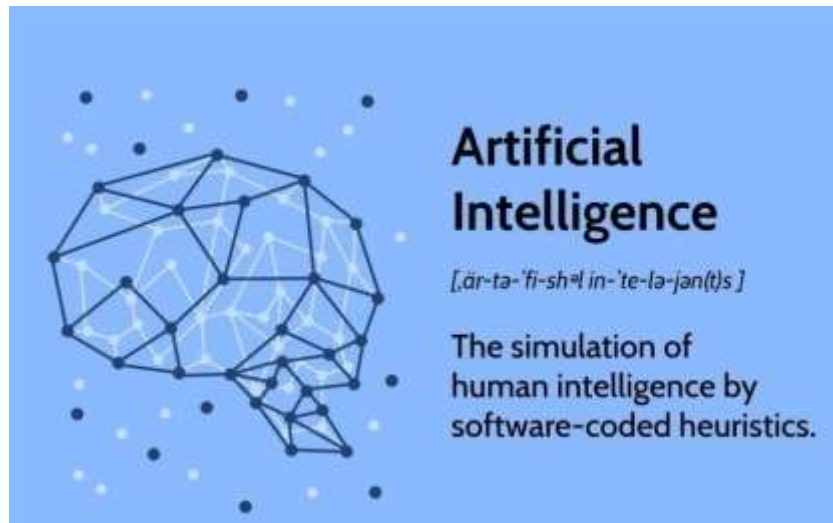


FIG: 1.

- **Types of Artificial Intelligence**

Artificial intelligence can be organized in several ways, depending on stages of development or actions being performed.

For instance, four stages of AI development are commonly recognized.

1. **Reactive Machines:** Limited AI that only reacts to different kinds of stimuli based on preprogrammed rules. Does not use memory and thus cannot learn with new data. IBM's Deep Blue that beat chess champion Garry Kasparov in 1997 was an example of a reactive machine.
2. **Limited Memory:** Most modern AI is considered to be limited memory. It can use memory to improve over time by being trained with new data, typically

through an artificial neural network or other training model. Deep learning, a subset of machine learning, is considered limited memory artificial intelligence.

3. **Theory of Mind:** Theory of mind AI does not currently exist, but research is ongoing into its possibilities. It describes AI that can emulate the human mind and has decision-making capabilities equal to that of a human, including recognizing and remembering emotions and reacting in social situations as a human would.
4. **Self Aware:** A step above theory of mind AI, self-aware AI describes a mythical machine that is aware of its own existence and has the intellectual and emotional capabilities of a human. Like theory of mind AI, self-aware AI does not currently exist.

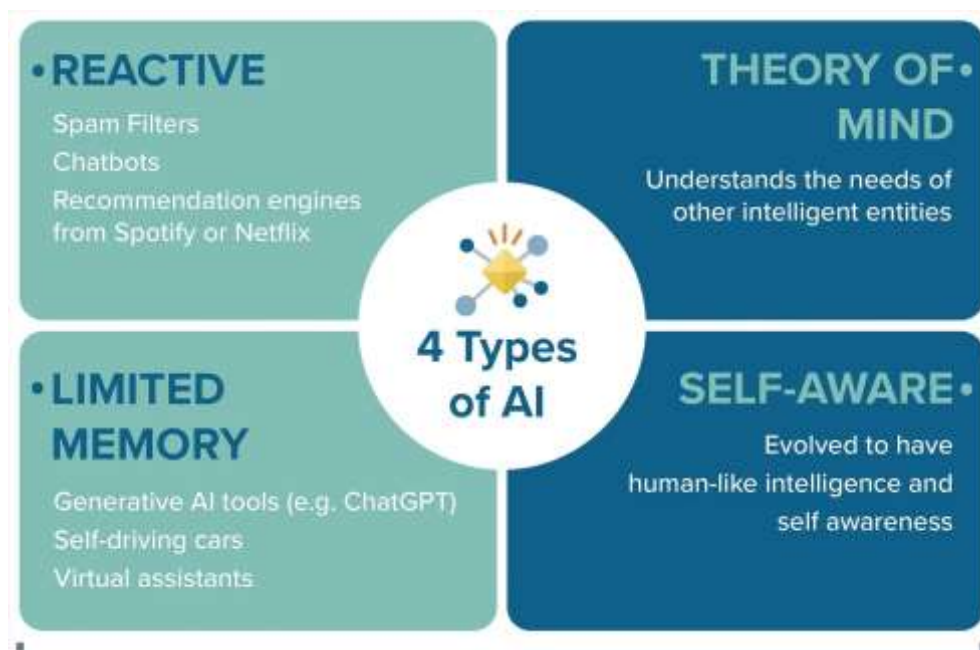


FIG: 2.



- **Advantages of AI technology**

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.

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.

Daily application: AI is very useful for our daily acts And deeds. For examples, GPS system is broadly Used in long drives. Installation of AI in Androids Helps to predict what an individual is going to type. It also helps in correction of spelling mistake

Digital assistants: Now-a-days, the advanced Organizations are using AI systems like ‘avatar’ (models of digital assistants) for the reduction of Human needs. The ‘avatar’ can follow the right Logical decisions as these are totally emotionless. Human emotions and moods disturb the efficiency Of judgement and this problem can be overcome by The uses of machine intelligence.

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 program. Trainee surgeons Can gather knowledge by the applications of AI Programs like various artificial surgery simulators (for examples, gastrointestinal simulation, hear Simulation, brain simulation,) etc.[2]

- **Disadvantages of AI technology**

Expensive: The launch of AI causes 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 machine consume longer time and huge Money.

No replicating humans: Robots with the AI technology Are associated with the power of thinking like human And being emotionless as these add some advantages To perform the given task more accurately without Any judgement. If unfamiliar problems arise, robots Cannot take the decision and provide false report.

No improvement with experience: Human resource Can be improved with experiences. In contrast, Machines with AI technology cannot be enhanced With experience. They are unable to identify Which individual is hard working and which one is Nonworking.

No original creativity: Machines with AI technology Have neither sensitivity nor the emotional Intelligence. Humans 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 machine

Unemployment: The widespread uses of AI technology In all the sectors may cause large scale unemployment. because of the undesirable unemployment, Human workers may lose their working habits and Creativity.[2]

PHARMACEUTICAL TECHNOLOGY

AI for Drug Discovery: AI has revolutionized drug research and discovery in numerous ways. Some of the key contributions of AI in this domain include the following:

.Target Identification: AI systems can analyze diverse data types, such as genetic, proteomic, and clinical data, to identify potential therapeutic targets. By uncovering disease-associated targets and molecular pathways, AI assists in the design of medications that can modulate biological processes.

Virtual Screening: AI enables the efficient screening of vast chemical libraries to identify drug candidates that have a high likelihood of binding to a specific target. By simulating chemical interactions and predicting binding affinities, AI helps researchers prioritize and select compounds for experimental testing, saving time and resources.

Structure-Activity Relationship (SAR) Modeling: AI models can establish links between the chemical structure of compounds and their biological activity. This allows researchers to optimize drug candidates by designing molecules with desirable features, such as high potency, selectivity, and favorable pharmacokinetic profiles.

De Novo Drug Design: Using reinforcement learning and generative models, AI algorithms can propose novel drug-like chemical structures. By learning from chemical libraries and experimental data, AI expands the chemical space and aids in the development of innovative drug candidates.

Optimization of Drug Candidates AI algorithms can analyze and optimize drug candidates by considering various factors, including efficacy, safety, and pharmacokinetics. This helps researchers fine-tune therapeutic molecules to enhance their effectiveness while minimizing potential side effects.

Drug Repurposing: AI techniques can analyze large-scale biomedical data to identify existing drugs that may have therapeutic potential for different diseases. By repurposing approved drugs for new indications, AI accelerates the drug discovery process and reduces costs.[4]

PHARMACOLOGY OF DRUG USING AI

- **Pharmacology Of Drug After Formulation**

Prediction of Drug Release through Formulation The prediction of drug release certainly has the potential for stable quality control. Drug release studies are performed through in vivo and in vitro methods, which are treated as fundamental technologies regularly evaluated or tested during product development. The release of the drug from oral solid dosage forms is based on the

contribution of critical material attributes along with the processing parameters. Some of the common factors affecting drug release include compaction parameters such as the pressure used for tablet hardness setting, geometric aspects of

the tablets, and drug loading characteristics. Many analysis techniques, including spectrophotometric analysis methods, have been implemented, or drug release studies are usually required for extensive analysis

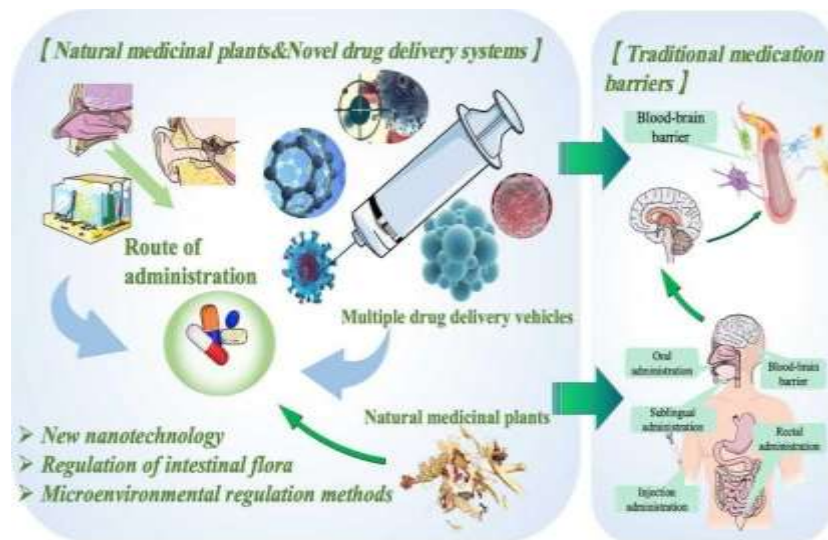


FIG: 3

- **Application of AI for the Detection of Tablet Defects**

The application of AI in the detection of tablet defects has revolutionized quality control processes in pharmaceutical manufacturing. AI algorithms and computer vision techniques are employed to analyze images of tablets, enabling the automated and efficient detection of defects such as cracks, chips, discoloration, or variations in shape and size. By training AI models on large datasets of labeled images, the system learns to accurately classify and identify different types of defects, achieving high levels of precision and recall. Conventional methods, such as X-ray computed tomography, have been used to analyze the internal structure of tablets, but they are still time-consuming and affect the demand for the rapid production of tablets. Deep learning is implemented along with X-ray tomography to detect tablet defects. Ma et al.

explored the application of neural networks for tablet defect detection with the help of image analysis completed through X-ray tomography. These researchers have manufactured several batches of tablets by using excipients such as microcrystalline cellulose along with mannitol. The prepared batches were analyzed with the help of the so-called image augmentation strategy. Three different models were used during the same research, including UNetA, which is applicable for the identification of distinguished characteristics of tablets from those of bottles. Module 2 was used for the identification of individual tablets with the help of augmented analysis. The internal cracks in the internal structure of the tablet were analyzed with the help of UNetB. Such UNet networks have been used to check tablet defects with better accuracy and thus provide ease of identification of defects with significant reductions in time, financial costs, and workload. This AI-

powered detection not only improves the speed and accuracy of defect identification but also reduces the dependence on manual inspection, minimizing human errors and subjective judgment. The real-time monitoring capabilities of AI systems ensure the prompt detection of defects, facilitating timely intervention and preventing the release of faulty tablets into the market. Ultimately, the integration of AI into tablet defect detection enhances product quality, increases productivity, and ensures the safety and efficacy of pharmaceutical products.[5]

AI FOR PHARMACODYNAMIC AND PHARMACOKINETICS

Drug development is a complex process that involves several stages, including drug discovery, preclinical studies, clinical trials, and regulatory approval. Pharmacokinetics and pharmacodynamics are crucial aspects of drug development, as they determine the optimal dosage, administration route, and safety of a drug in the body. Traditional experimental methods for pharmacokinetics and pharmacodynamics studies can be time-consuming and expensive and may not always provide accurate predictions of drug efficacy and safety.

Traditionally, pharmacokinetics and pharmacodynamics studies have been conducted using experimental methods such as animal studies and human clinical trials. These methods have critical challenges, such as ethical concerns, sample size, and interindividual variability. Furthermore, these studies may not always provide accurate predictions of drug pharmacokinetics and pharmacodynamics in humans. To overcome these limitations, computational models and AI methods have been developed to predict drug pharmacokinetics and pharmacodynamics in a faster, more cost-effective, and more accurate manner.



AI has shown tremendous potential in the fields of pharmacokinetics, pharmacodynamics, and drug discovery [With the advent of powerful computing and machine learning algorithms, AI has emerged as a valuable tool for predicting and optimizing drug pharmacokinetics and pharmacodynamics. Although the challenges of large data and reliable datasets are hard to ignore, AI can open new doors in PKPD studies and their impact on therapies.

• **AI Approaches in Polypharmacology**

Now a day, 'one-disease-multiple-targets' concept governs over the 'one-disease-one -targets' concept for the advanced realization of pathological process in various disorders at their molecular basis. The phenomenon of 'one-disease-multiple-targets' is known as polypharmacology.¹¹⁰ There are numerous and useful databases, for examples, PubChem, KEGG, ChEMBL, ZINC, STITCH, Ligand Expo, PDB, Drug bank, Supertarget, Binding DB, etc, which are accessible for the accomplishment of a variety of important and useful information related to the structure of crystals, chemical features, biological properties, molecular pathways, binding affinities, disease concern, drug targets, etc. AI also helps to discover the databases to sketch polypharmacological molecules/agents

• **Pre-Clinical Research**

New target discovery and toxicity prediction AI can contribute to address unmet medical needs by enhancing and accelerating identification of new molecular targets (genes or proteins). Access to large pharmacokinetics (PK) and pharmacodynamics (PD) datasets, from previous preclinical and clinical research (including from failed trials), is needed to develop and train effective and reliable algorithms that generate new stable molecules with real treatment potential. Lack of published PK/PD data, for competitive or proprietary reasons, is a significant hurdle to achieve full potential of AI in new drug discovery.

Several AI methodologies for safety prediction are described. In fact, software is available to predict drug toxicity based on target information. Efficient toxicity predictions have the potential to replace in vitro and animal models as the traditional pre-clinical approach. Additionally, the models can be used as risk-management and prioritization tools in development pipelines, by providing early indication of high-risk compounds flagged with significant safety concerns.

As in other AI fields, model interpretation can be challenging, especially given the high level of uncertainty in early phases of research. Understanding model features and underlying biological mechanisms is key for interpretability and confidence in predictions.

Clinical Trial Research

• **Protocol Design and Reporting**

AI systems extract valuable patterns of information to inform and enhance trial design. The SPIRIT-AI extension provides reporting guidelines for clinical trials evaluating interventions with an AI component.

These guidelines enhance transparency, consistency, and interpretability by improving protocol reporting and providing evidence-based recommendations for addressing essential elements.

• **Patient Selection and Recruitment**

AI-assisted techniques and digital transformation enable precise patient identification, optimize cohort composition, and enhance recruitment and retention rates in clinical trials. Automation and ML use large datasets, including electronic health records and omics data, to make intelligent predictions and streamline patient selection. This results in improved trial enrollment and retention, ultimately enhancing the efficiency of clinical trials.

• **Investigator and Site Selection**

AI technologies aid in selecting high-functioning investigator sites for clinical trials. They identify target locations, qualified investigators, and priority candidates while ensuring compliance with Good Clinical Practice requirements. AI also helps collect and collate evidence to satisfy regulators regarding study timelines, data quality, and integrity, improving the trial process.

• **Monitoring and Management of Clinical Trials**

AI algorithms analyze real-time patient data, ensuring trial integrity and identifying adverse events. Automation and ML optimize data collection, improve quality, and enable real-time monitoring for higher trial success rates. AI enhances patient monitoring, medication adherence, and retention through data automation, digital assessments, and real-time insights from wearable technology, enhancing engagement and retention.

• **Image Analysis and Biomarker Computation**

AI techniques enable automated and precise medical imaging analysis, facilitating the identification of patterns, abnormalities, and disease-specific biomarkers. Integrating AI with imaging biomarker analysis pipelines improves image-based evaluations' accuracy, consistency, and efficiency in clinical trials.

• **Intelligent Data Collection and Management**

AI streamlines data collection and management in clinical trials, accelerating the process. Collecting data through automated processes and utilizing this for AI algorithms minimizes errors, extracts relevant information from diverse sources, and data becomes efficiently structured and organized. Real-time access to data enhances analysis and decision-making, expediting trials and improving efficiency.^[6]

• **AI in Pharmacology**

In the application of machine learning, deep learning methods (e.g.convolutional neural network), and natural language processing AI has brought about a

groundbreaking transformation in various stages of drug discovery, development (including the discovery phase, clinical trial phase, and post-marketing surveillance) and precision medicine[7]

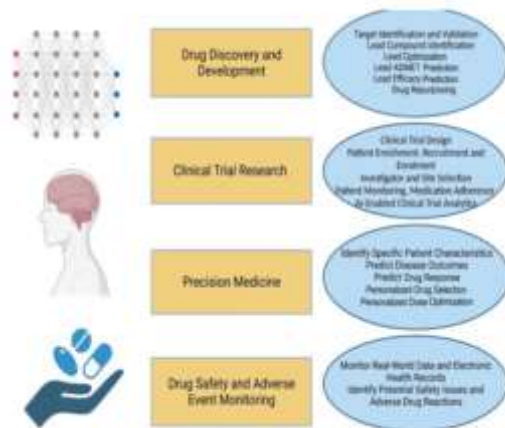


FIG: 4

Artificial Intelligence in Pharmacovigilance

• Artificial Intelligence in Pharmacovigilance

PV was designed mainly for patient safety who are limited exposed to treatment drugs during clinical trials and research. This makes it possible to observe drug profiles for a prolonged period and use. It also includes certain groups such as geriatric population, racial groups, pediatric population and pregnant women, and also the incomplete data from long-term drug exposure makes it mandatory to perform PV studies. The approval of life-saving drugs such as anticancer drugs, antitubercular, and antiretroviral drugs is based on fast track system so these drugs could be easily available for the patients and PV performs the assessment, communication of the risk, and effectiveness of these medications.

In developing countries, PV is still a new concept with low preference. Worldwide the countries are raising the issues in concern for the need of systems to monitor the safety of drug postmarketing.[8] Reporting of adverse drug reaction (ADR) is mainly done through spontaneous reporting or by pharmacoepidemiological methods that use systematic collection and analysis of adverse events (AE) associated with the use of drugs. It is also done by Adverse Drug Reaction Monitoring Centres and marketing authorization holder (MAH) industries to solve emerging problems, record signals, and communicate to minimize or prevent harm

Nowadays, drug safety is a major threat after launching the new drug to the market. During the clinical trial or after marketing, the major source of erosion is unpredictable toxicities that cause morbidity and mortality from normal dose of the drug. As per the record from 2008 to 2017, the Food and Drug Administration (FDA) approved 321 novel drugs. At the same time FDA, AE Reporting System has reported a total of >10

million AE reports in which 5.8 million were recorded as serious, and 1.1 million were death reports.

ADR data need to be collected by license holder that should be from pharmaceutical company and submitted to the local drug regulatory authority. The most important operation in PV industry is detection and reporting of ADRs, coding of AE in technical terms, preparing safety individual reports, assessment of seriousness, and relationship with suspected drug. All of these depend on the human interference, which is time-consuming; and hence, the detection of ADRs requires a new technology. A multinational pharmaceutical company in collaboration with a professional services company has developed an AI and ML system to facilitate the processing and maintenance of quality and compliance standards. The globally available data are so vast that it cannot be analyzed manually where AI becomes useful to track them. AI techniques play a significant role in the area of drug design and identification of AEs of pharmaceutical products.

Benefits of Artificial Intelligence in Pharmacovigilance

- The most important benefits of AI are reduced cycle times. Due to this method, the processing is spontaneous
- Improve the quality and accuracy of the information
- AI can handle or manage diverse types of incoming data formats
- It can be used for the identification of ADRs
- AI is useful to reduce the burden and time of case processing
- AI tools extract the information from the adverse drug event form and evaluate the case validity without the workforce.[8]

Machine learning

• Machine learning for target identification

The typical drug discovery requires identifying target proteins with casual aspects of pathophysiology and a plausible framework. Misunderstanding of target protein information may lead to modulation in the disease information, and in this sense, target selection is a mandatory step.

Evidence of successful drug response will be considered and subsequently, lead efficiency in the randomized clinical trial tends to the identification of prominent drug targets. The ML algorithm predicts the unseen biological happenings, events, and problems developed a computational model for predicting the morbidity and druggable genes on a genome-wide scale. That model has been widespread in reducing the laborious experimental procedures and identifying the putative molecular drug targets linked with disease mechanisms. Here, this classifier is modelled to uncover the biological rationale from a data-driven view. The main classification features are mRNA expression, gene essentiality, occurrence of mutations, and protein-protein network interactions.

The meta-classifier analysis results initiated from 65% of known morbid gene recovery and 78% of unknown druggable gene recovery. The decision tree (DT) and uncover rules inspect



the parameters that include the membrane localization and regulation of multiple transcription factors to identify biological traits [This can also exhibit understanding and designing the Biosystems principles by applying the reverse engineering methods. Volk et al. applied the ML methods to model the challenges at DNA, protein, specific pathway levels and process them for the genome and cellular communities. Jeon et al. stated and developed a Support Vector Machine (SVM) method to analyse the genomic variety and systematic data set to distinguish the protein based on homologs or likelihood for drug binding in breast cancer cases, pancreatic cancer, and ovarian cancers.

Momoshina et al. applied the same concept of identifying the drug target in the complicated disease by using the biomarker discovery approach in muscle tissue to detect the druggable targets considering the molecular basis of human ageing. In this approach, the SVM model is contracted with linear kernel and deep feature selection to find the gene of expression linked with ageing. This model also evaluates the gene expression samples from Genotype-Tissue Expression (GTEx) project and has obtained a 0.80 accuracy level[10.1]

• Machine Learning For Imaging Analysis

ML approaches are used in investigatory screens and automated or robotic image acquisition and investigations. For example, the potent inhibitors against the β_2 adrenoceptor target and radiological binding assay through novel molecules are screened based on ability to interfere with radiolabels ligand with binding affinity. This acute effect of small molecules may cause the alteration in the surface plasma resonance (SPR) detected in the receptors. This tendency allows the selection of small molecule inhibitors processed into the lead optimization stage. But this process is laborious and a long approach, and therefore, alternative methods such as phenotypic screening are highly focused.

At this stage, ML-based analytics are applied to identify complex phenotypes that have tended to increase the efficiency of the small molecule. Another technique, namely advanced imaging, is a mechanism applicable to finding the phenotypes and perturbation of small molecules, and this method is known to enhance prediction. More broadly, imaging can be composed of two camps:

1. Typically called phenotypic screening, which targets the predefined phenotypes of intracellular signalling molecules associated with the disease mechanism.
2. The various subcellular structures with antibodies, infective or chemical agents, and fluorescent dyes categorize their responses.[11.]

Artificial Intelligence Future

• AI today (and in the Near Future)

Currently, AI systems are not reasoning engines ie cannot reason the same way as human physicians, who can draw upon 'common sense' or 'clinical intuition and experience'. Instead, AI resembles a signal translator, translating patterns from datasets. AI systems today are beginning to be adopted by healthcare organisations to automate time consuming, high

volume repetitive tasks. Moreover, there is considerable progress in demonstrating the use of AI in precision diagnostics (eg diabetic retinopathy and radiotherapy planning).

• AI in the medium term (the next 5–10 years)

In the medium term, we propose that there will be significant progress in the development of powerful algorithms that are efficient (eg require less data to train), able to use unlabelled data, and can combine disparate structured and unstructured data including imaging, electronic health data, multi-omic, behavioural and pharmacological data. In addition, healthcare organisations and medical practices will evolve from being adopters of AI platforms, to becoming co-innovators with technology partners in the development of novel AI systems for precision therapeutics.

• AI in the long term (>10 years)

In the long term, AI systems will become more intelligent, enabling AI healthcare systems achieve a state of precision medicine through AI-augmented healthcare and connected care. Healthcare will shift from the traditional one-size-fits-all form of medicine to a preventative, personalised, data-driven disease management model that achieves improved patient outcomes (improved patient and clinical experiences of care) in a more cost-effective delivery system.[10]

CONCLUSION

The integration of Artificial Intelligence (AI) in the pharmacy discipline has revolutionized the field, transforming the way medications are discovered, developed, and delivered. AI's applications in pharmacy practice, research, and education have demonstrated significant potential in improving patient outcomes, streamlining clinical workflows, and enhancing the overall quality of care

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