

Smart Molecules, Safer Patients: The Dual Promise of AI in Modern Pharmacy

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ABSTRACT

Artificial Intelligence and Machine Learning are transforming pharmaceutical sciences by addressing two critical challenges: the slow, expensive process of drug discovery and the limitations of traditional pharmacovigilance. This project explores AI applications across both domains. In drug discovery, deep learning accelerates target identification, generative AI designs novel molecules, and predictive models optimize ADMET properties early, compressing development timelines and reducing costs. In pharmacovigilance, natural language processing extracts safety signals from unstructured clinical narratives, machine learning enhances signal detection in spontaneous reporting databases, and predictive models enable personalized adverse event risk assessment. Key challenges include data quality, model interpretability, regulatory uncertainty, and workforce readiness. The Pharmacy Council of India's 2025 curriculum revision mandating AI education for pharmacy students underscores the technology's growing importance. This project concludes that AI is not replacing pharmaceutical expertise but amplifying it, demanding that future pharmacists possess both domain knowledge and computational literacy.

Keywords-: Artificial Intelligence, Machine Learning, Drug Discovery, Pharmacovigilance, Deep Learning, Natural Language Processing.

INTRODUCTION-:

The Latin word "vigilare" (which means "maintain watch") and the Greek word "pharmakon"(which means drug) were combined to create the English phrase "pharmacovigilance." The World Health Organisation (WHO) created the pharmacovigilance (PV) initiative for worldwide drug monitoring in 1961. PV is the term used to describe the science and methods used in the detection, assessment,comprehension, and mitigation of pharmaceutical side effects as well as any other potential drug-related problems. The processing of the massive amounts of data that PV collects every day is a difficult task on a global scale.

Pharmacovigilance, the science of monitoring, assessing, and preventing adverse drug reactions (ADRs), is critical for ensuring the safety of the patient. Traditional pharmacovigilance methods, reliant on manual signal detection and spontaneous reporting systems, often struggle to keep pace with global data's sheer volume and complexity. Emerging technologies like artificial intelligence (AI) and machine learning (ML) are transforming this landscape, enabling more efficient, accurate, and proactive drug safety monitoring. AI-driven signal detection leverages advanced algorithms to mine vast datasets, identifying safety signals that may remain hidden in traditional systems. Studies highlight how AI enhances early detection of ADRs, enabling quicker regulatory responses [1]. Powered by ML models, predictive analytics further anticipates potential safety concerns, reducing the risk of widespread harm.Integrating real-world data (RWD) sources like social media and online health forums has expanded pharmacovigilance horizons. Language models excel in extracting relevant ADR signals from unstructured text . Additionally, AI-driven automation streamlines case processing, while ML algorithms enhance risk assessment strategies.However, challenges persist, including data quality issues, algorithmic biases, and regulatory uncertainties. Addressing these limitations is crucial for harnessing AI and ML's full potential to revolutionize pharmacovigilance As the pharmaceutical industry develops, maintaining the safety of medications that are on the market becomes critical to protecting public health. The foundation of medication safety monitoring has traditionally been traditional pharmacovigilance techniques, which rely on clinical trials, spontaneous

reporting systems, and regulatory reporting Finding the “needles in the haystack,” or safety signals that need escalation and triage, is a critical task for PV, and

it requires making sense of vast and heterogeneous amounts of data. Many have hypothesized that these similar technologies could be applied to address the fundamental issues with PV in light of the emergence of artificial intelligence (AI) and machine learning (ML) during the

past ten years in numerous fields of science and medicine. These techniques were initially used for human safety data in the early 1990s, and since the 2000s, their application has grown steadily. The objective of this review is to systematically identify works that characterize the present status of machine learning in PV by using ML, generally defined, for safety data. It also aims to shed light on how recent developments in AI and ML might be applied to enhance different aspects of pharmacovigilance. The studies and procedures that deal with the detection, assessment, understanding, and prevention of side effects or all other problems related to drugs is referred to as pharmacovigilance, or PV, in line with the World Health Organization (WHO) (U.S. FDA). Adverse drug reactions are reported worldwide in a variety of handwritten, unstructured, and multilingual formats; on average, many companies receive over 3 lakh ADRs each year. Human error is possible with manual processes, and project prices are going to increase overall.

➤ **Artificial Intelligence:-**

Artificial Intelligence (AI) refers to the ability of computer-based systems to perform tasks that usually require human intelligence, such as learning from experience, identifying patterns, understanding language, and supporting decision-making. In recent years, AI has gained increasing importance in healthcare, particularly in areas where large volumes of data need to be processed efficiently and accurately. Pharmacovigilance is one such field where AI is emerging as a valuable supporting tool. In pharmacovigilance, AI is mainly applied to the management of Individual Case Safety Reports (ICSRs). An ICSR is a standardized document used to record information related to adverse events, product-related problems, and consumer safety reports in line with regulatory requirements. Traditionally, ICSR processing involves manual steps such as data entry, medical review, coding, and causality assessment, which are time-consuming and may lead to inconsistencies. Machine learning techniques help automate these activities, enabling faster processing and improved consistency while reducing the overall workload on pharmacovigilance professionals.

AI also supports the identification and analysis of adverse drug reactions by examining data from various sources, including spontaneous reporting systems, electronic health records, and patient-reported information. Natural language processing allows AI systems to understand and extract relevant details from unstructured text, such as clinical narratives and free-text safety reports. Through advanced pattern recognition, AI can assist in signal detection, prediction of potential drug side effects, identification of drug-drug interactions, and recognition of patient populations at higher risk of experiencing drug-related toxicity. Despite its advantages, the use of AI in pharmacovigilance presents certain challenges. Data privacy

and security are major concerns, as AI systems rely on access to sensitive health information. In addition, the reliability of AI tools depends heavily on the quality of the data.

➤ **HISTORY :-**

Allen Newell, Herbert A Simon developed the Logic Theorist. It was born in 1956 that Dartmouth College had organized the famous conference. It has been forecasted that the revenue from the AI market will be increasing by as much as ten-fold between the years 2017 and 2022. The natural language processing market, which has several applications including text prediction, and speech and voice recognition has been said to achieve a growth of 28.5% in the year 2017. Worldwide revenue from big data and business analytics was US\$ 122 billion in the year 2015 and it is expected that the figures will rise to more than US\$ 200 billion by the year 2020. Artificial intelligence has a rocky history spanning back to the 1950s. For a long time, it was seen as a field for dreamers, but that started to change in 1997 when IBM's Deep Blue computer was able to defeat chess champion Garry Kasparov. By 2011, IBM's new Watson supercomputer was able to win the US\$1m prize in the US game-show Jeopardy. Since then, Watson has expanded into healthcare and drug discovery, including a partnership with Pfizer in 2016 to accelerate drug discovery in Immuno-oncology. While the FDA launched its Emerging Drug Safety Technology Program (EDSTP) in 2024 to support AI adoption, globally harmonized regulatory standards are still emerging. AI models depend on high-quality data; if training data is biased, the predictive models will reflect those biases. The need for explainable AI (XAI) is critical; stakeholders need to understand how AI arrives at a decision, ensuring human oversight remains integral to the process.

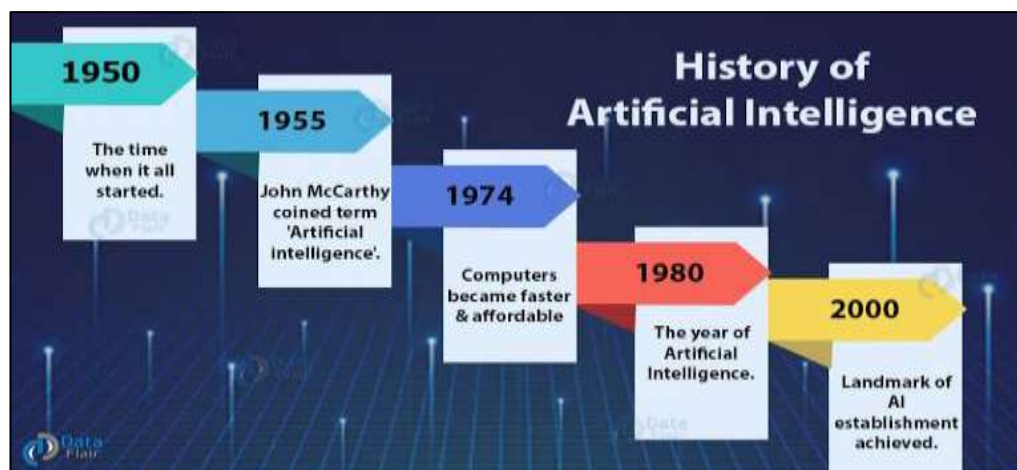


FIGURE 1 - REVOLUTION OF ARTIFICIAL INTELLIGENCE

➤ ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND MACHINE LEARNING -:

Artificial Intelligence (AI) and Machine Learning (ML) are transforming the drug discovery landscape by shifting the paradigm from labor-intensive trial-and-error to data-driven predictive modeling. Traditionally, developing a single drug can take 10–15 years and cost approximately \$2.6 billion, with a 90% failure rate in clinical trials. AI-driven approaches aim to shorten this timeline by 1–2 years and significantly reduce early-stage. Artificial intelligence (AI) and machine learning (ML) are transforming pharmaceutical development by accelerating drug discovery—through molecular design and target identification—and enhancing pharmacovigilance (PV) via real-time safety monitoring, automated adverse drug reaction (ADR) detection, and natural language processing (NLP) of safety reports. These technologies reduce development costs, predict toxicity, and enable personalized medicine.

2.1 AI DRUG DISCOVERY-:

Artificial Intelligence (AI) in drug discovery refers to using computer systems that can learn, analyze data, and make predictions to help find new medicines faster and more efficiently. Simple idea Traditionally, discovering a drug takes 10–15 years and costs billions. AI helps reduce this time by analyzing huge biological and chemical data much faster than humans.

2.2 AI MACHINE LEARNING -:

AI and machine learning (ML) in pharmacovigilance (PV) refers to the use of advanced algorithms, including Natural Language Processing (NLP) and deep learning, to automate the detection, assessment, and reporting of adverse drug reactions (ADRs) from vast, diverse data sources. These technologies, also known as automated safety surveillance or intelligent drug monitoring, transform PV from manual, reactive processes to proactive, real-time safety management by analyzing structured and unstructured data like electronic health records (EHRs) and social media.

2.3 Aims and Objectives-:

This project aims to comprehensively examine and document the applications, methodologies, challenges, and future trajectories of AI and ML technologies in pharmaceutical sciences, with specific focus on drug discovery and pharmacovigilance

Primary Objectives-:

1. To systematically review current AI/ML methodologies employed across the drug discovery pipeline, from target identification through lead optimization.
2. To analyze AI-driven approaches for adverse drug reaction detection, signal generation, and safety surveillance in pharmacovigilance.
3. To evaluate the integration of structured and unstructured data sources using advanced natural language processing techniques.
4. To identify technical, regulatory, and ethical challenges limiting broader AI/ML adoption in pharmaceutical applications.

5. To propose recommendations for effective implementation of AI technologies in pharmaceutical research and education.

2.3 Significance of the Study:-

The Pharmacy Council of India's revised B.Pharm syllabus (PCI-2025) has formally recognized the transformative potential of AI by integrating AI and Python programming into the undergraduate curriculum across drug discovery, pharmacology, manufacturing, and healthcare analytics. This curricular reform reflects the industry's urgent demand for pharmacy graduates equipped with computational competencies enabling them to operate effectively in data-driven pharmaceutical environments. This project responds directly to this educational imperative by providing a comprehensive resource that bridges pharmaceutical domain knowledge with computational methodologies. The findings will serve as foundational reference material for pharmacy students navigating the intersection of traditional pharmaceutical sciences and emerging AI technologies.

2.4 Scope and Limitations:-

This project focuses on AI/ML applications in small-molecule drug discovery and post-market pharmacovigilance. Biologics, gene therapies, and medical devices, while increasingly relevant, fall beyond the primary scope. Methodological emphasis is placed on supervised and deep learning approaches with demonstrated pharmaceutical applications. Temporal scope is constrained to developments from approximately 2015-2026, reflecting the period of most rapid advancement in deep learning architectures and their pharmaceutical deployment. Geographic scope encompasses global pharmaceutical research with particular attention to regulatory frameworks in the United States (FDA), European Union (EMA), and India (CDSCO).

> ARTIFICIAL INTELLIGENCE TOOLS USED IN DRUG DISCOVERY:-

Deep learning is a part of machine learning, having the capability to extract a greater level of features through utilization of multiple layers from input data. Deep learning is an immense field that is creating massive premiums nowadays. Recently, deep learning techniques have been used in many research fields and have achieved higher profitability in business strikes. In general, deep learning is the same neural network architecture that consists of several layers, and data can be transformed between these layers. It's still a significant popular expression, but the innovation behind it is genuine and very refined. So, models in deep Learning can be developed through a strategy called greedy layer-by-layer. In this review, Deep learning algorithms have presented numerous models like DNN, CNN, RNN, GNN in drug discovery areas.

1.Convolutional Neural Networks (CNNs):- Originally developed for image analysis, CNNs have been adapted for molecular graph representation, enabling direct learning from chemical structures. In pharmacovigilance, CNNs process adverse event data achieving 85% predictive accuracy compared to 78% for logistic regression and 80% for support vector machines.

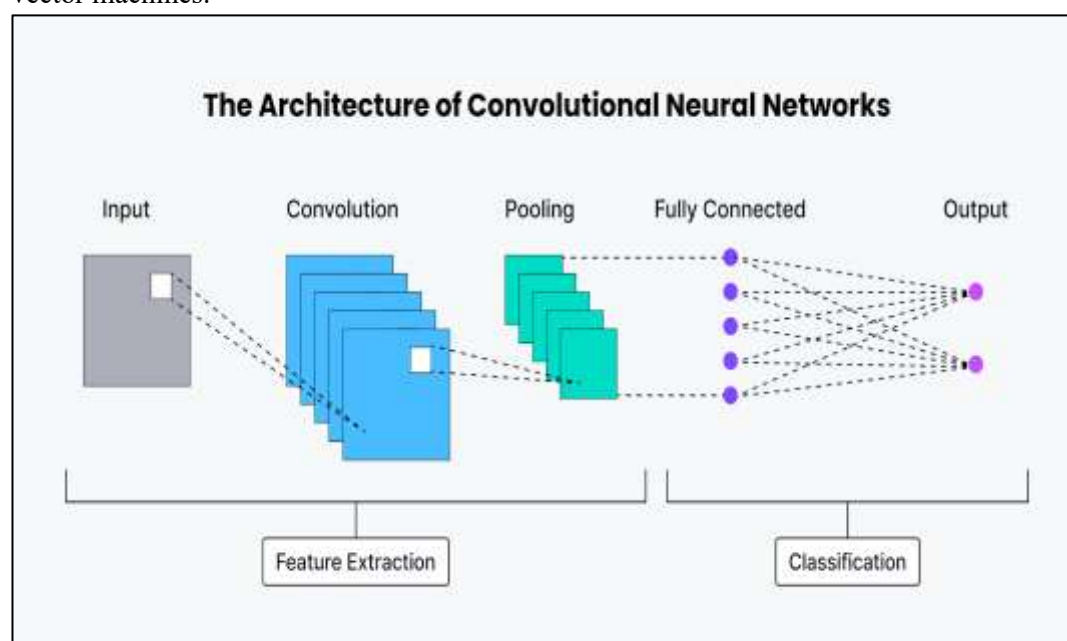


FIGURE 2 - CONVOLUTIONAL NEURAL NETWORKS

2.Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM)-: These architectures process sequential data, proving valuable for SMILES string generation in de novo molecular design and temporal pattern analysis in longitudinal patient records.

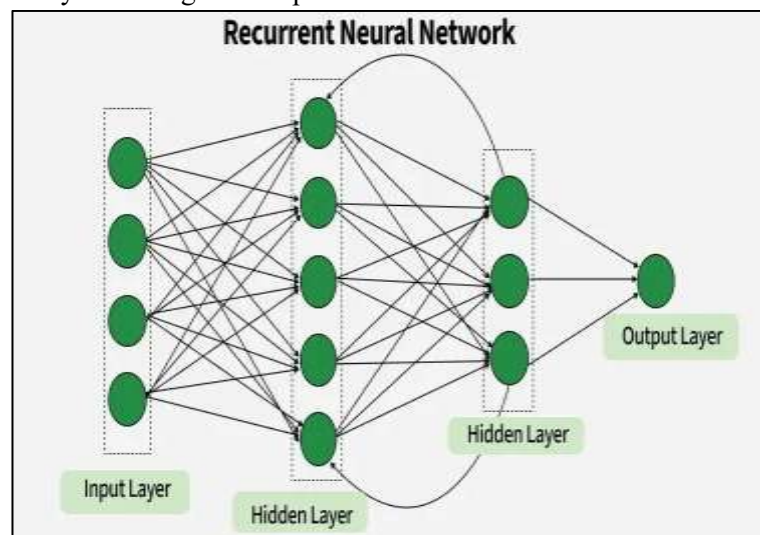


FIGURE 3 - RECURRENT NEURAL NETWORKS

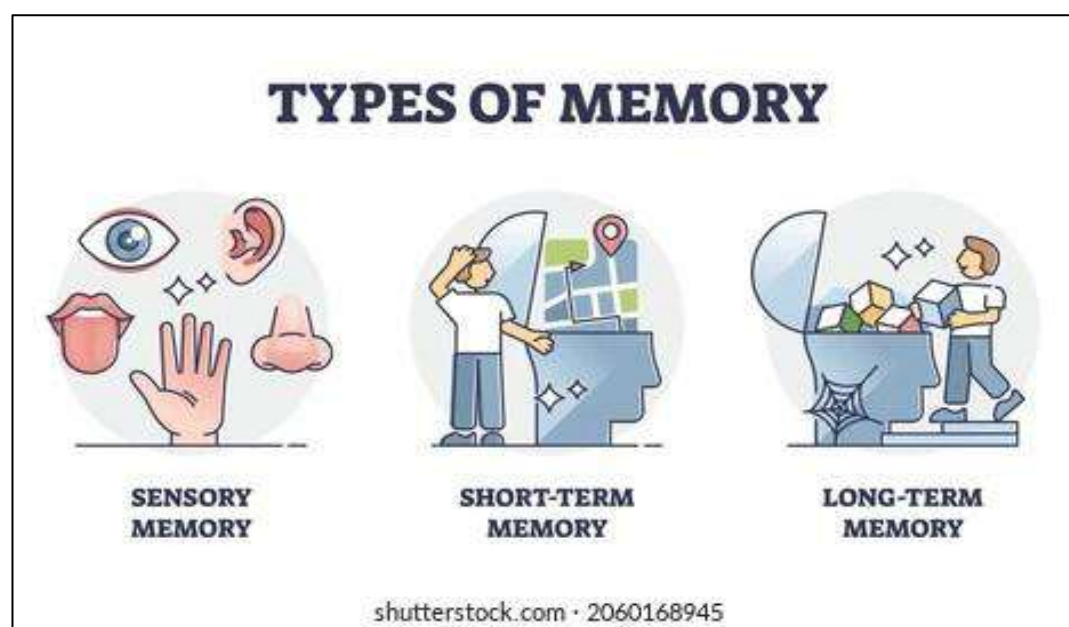


FIGURE 4 - LONG SHORT TERM MEMORY

3.Transformer Models: The attention-based architecture underlying BERT (Bidirectional Encoder Representations from Transformers) and GPT (Generative Pre-trained Transformers) has revolutionized natural language processing. In pharmaceutical contexts, these models

extract adverse event information from clinical narratives and enable high-throughput screening of biomedical literature.

4.Graph Neural Networks (GNNs)-: Specifically designed for graph-structured data, GNNs excel at modeling molecular structures where atoms represent nodes and chemical bonds represent edges. These architectures demonstrate superior performance in predicting protein-ligand binding affinities and molecular properties.

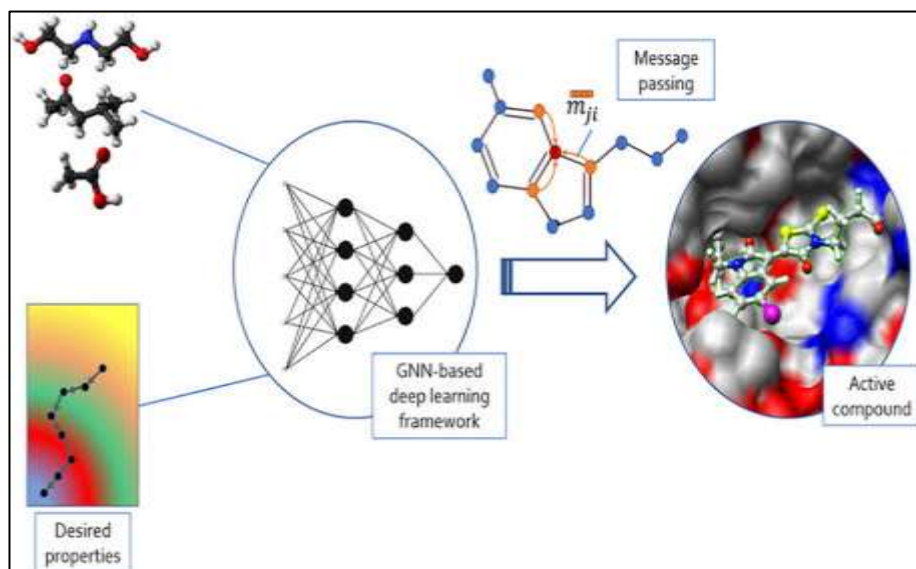


FIGURE 5 - GRAPH NEURAL NETWORKS

➤ ARTIFICIAL INTELLIGENCE MACHINE LEARNING IN DRUG DISCOVERY:-

❖ INTRODUCTION :-

Pharmacovigilance, the science of detecting, assessing, and preventing adverse drug reactions (ADRs), is crucial in ensuring drug safety, especially post-marketing. As the pharmaceutical industry evolves, the sheer volume and complexity of data have made traditional methods of monitoring drug safety insufficient. It is where artificial intelligence (AI) and machine learning (ML) are stepping in, offering transformative solutions to address existing challenges and enhance drug safety monitoring. Below, we explore how AI/ML reshapes pharmacovigilance through advanced signal detection, predictive analytics, and In innovative applications.

September 2015, the Google search trend showed that after the introduction of ML, AI was the most searched term. Some describe ML as the primary AI application, while others describe it as a subset of AI. AI is an umbrella term where computer programs are able to think and behave as humans do, whereas ML is beyond that where data are inputted in the machine along with an algorithm like Naive Bayes, decision tree (DT), hidden Markov models (HMM) and others, which helps the machine to learn without being explicitly programmed. Later, with the development of neu-ral networks, machines could classify and organize inputted data that mimics like a human brain, which further shows advancement in AI. Around the twentieth century, Igor Aizen-berg and his colleagues, while talking about the artificial neural network (ANN), brought up the term “deep learning” for the first time. DL is a subset of ML, which itself is a subset of AI, and thus, the evolution goes like AI>ML>DL. ML either uses supervised learning, where the model is trained to use labeled data, which means that the input has been tagged with corresponding preferred output labels or uses unsupervised learning, where the model is trained to use unlabeled data but looks for recurring pat-terns from the input data. Others are semi-supervised learning that uses the combination of both supervised and unsupervised learnings; self-supervised learning, which is a special case, uses a two-step process where unsupervised learning generates labels for unlabeled data and its ultimate goal is to make supervised learning model; reinforcement learning is a type of ML which improves its algorithm over time with the help of a constant feedback loop and lastly DL where there are many layers of ML algorithms which is called as a brain-inspired family of algorithms which mim-ics human brain but requires high computational power for training and big data to succeed.

1.Target identification:-

The target identification for NCE's is an extreme task due to lack of knowledge on their off-targets such as enzymes, ion channels, proteins, or receptors. The binding site recognition for the NCE's is another key task for computational/bioinformatics experiments where more than one active site has existed in the protein. In the above cases, the predefined most popular web servers (FTMap), as well as specific modules such as "Sitemap" developed with the help of algorithms, can define the preferential binding site to speed up the drug discovery process. A few other online programs like GHECOM, POCASA, Pocketome, SURFNET, ConCavity, LIGSITE, Q-SiteFinder, Fpocket, and PASS predict the feasible binding sites located within the provided protein templates. Whereas, the metaPocket 2.0 program utilizes the above platforms to afford the most reliable ligand binding sites present on templates. Further, AI

models like FD/DCA can also predict the druggable sites in the provided biological macromolecules. Recently, the DeepDTnet as a new target identifier in drug repurposing has been tested. The DeepDTnet strategy is developed by amalgamating the multi-disease cellular targets, pathogenic genes (genomics), and drugs (chemical spaces) being utilized for their treatment.

1.1 Prediction of protein folding:-

Patients who experienced illnesses can be recognized through protein dysfunctions. Here, active molecules can be recognized through a structure-based drug design approach. Time and cost consumption should be required for 3D structural processing, and it is also important to be aware of what algorithms are used to predict the 3D structure of proteins. Because of the essence of the large amount of protein sequence data, it creates a problematic issue in making 3D structure accuracy for de-novo prediction.

1.2 Prediction of protein-protein structure:-

PPIs are essential for biological processes and infections PPI can be characterized as 'it performs similar to networks for mathematical representation of physical contacts between cell proteins. Composed contacts between binding regions in proteins have specific biological importance. Also, it obtains the experimental and bioinformatics strategies from PPI's database. PPI interface is also referred to as a collection of multiple residues. In this way, it turns into a new class for drug targets that are different from mainstream pharmaceutical targets like ion channels, coupled receptors, G-protein, etc. It used two techniques i.e., fragment docking and direct coupling analysis for detecting druggable PPI sites. Fragment docking named "iFitDock", utilized for

checking druggable hot spots(problem areas) in the PPI interface. Further improvement for candidate binding locales needs to integrate similar small hot spots. At last, based on the evolutionary conservative level, the scoring function must be located to provide the finest protein-protein binding spots. The PPI interface objective was to improve computational methodologies for locating the best hot spots and significant structure of small modulator targets in the PPI interface.

1.3 Prophecy of protein-protein interactions:-

The Protein-Protein Interactions (PPI) is one of the major biological phenomena through which the basic units of the body (cell) transports the signals, ions, substrates, and energy production components that need to improve the pharmacological responses needed by the body. In another circumstance, the PPI plays a critical role in the pathogenesis of the disease such as various types of cancer, especially colorectal carcinoma. The development of colorectal carcinoma in humans is purely dependent on lifestyle as well as hereditary means. However, the time and cost for experimental prediction of PPI are considered as rate limiting barriers. In this regard, the different databases hosted the web servers (few are publicly available) framed by targeting PPI which are prevailing as preliminary PPI identification tools to accelerate the medicinal chemistry research

2.Hit discovery:-

The Hit discovery process is advanced in success which has been taken in drug discovery. In this procedure, small molecules are considered as hits for target binding to identify the best-altered functions. The detection of hits by diverse algorithms is currently prevailing as a robust technique in the current drug discovery paradigm. An application of multivariate parameters (K-nearest neighbors (K-NN) and support vector machine(SVM)) on highcontent screening (HCS) analysis in one such method produced a variety of hits against neurological complications.

2.1 Drug repurposing:-

DeepDTnet's training parameters outperform other existing target identification techniques and rely on a minimum quantity of FDA-approved drugs (732 drugs) to produce beneficial therapeutic effects (human retinoic acid receptor orphan receptor gamma t-ROR- γ t) of the existing topoisomerase inhibitor Topotecan (TPT). The deepDTnet strategy also transfers several FDA drugs with different chemical scaffolds against GPCR with new targeted pharmacological actions. The deepDTnet algorithm is considered to be much more advantageous than NetLapRLS and KBMF2K methods as well as Naive Bayes, SVM, KNN,

and Random Forest algorithms. "Repurpose" refers to "reprocess/reused/recycle". Drug Repurposing is characterized as 'locating new indications for drugs which are as of now in the existence stage'. Because it reduces time and is hazardous. significant reason for utilizing the drug repurposing concept in drug discovery, because it is exceptionally supportive to have multiple targets in each drug which corresponds to various impacts. In this way, it provides high diversity in drug-disease relationships. Example: Few drugs extend their life expectancy such as "Metformin" which is an approved medicine to deal with diseases like "type 2 Diabetes". In repurpose, essential elements are utilized. Drug targets and disease genes are other elements utilized in drug repurposing.

2.2 Virtual screening:-

It is an AI strategy utilized in the drug discovery process for locating small molecules to distinguish bound structures for a drug target. In drug development, virtual screening also utilized software as well as algorithms to recognize hits from private chemical collections for retrieving unique hits inefficiently. After identification of new hits, a further step needs to purify compounds with unfavorable scaffolds (framework). And furthermore incorporates few strategies like docking based, similarity searching, pharmacore-based, and machine learning methods. Based on the above techniques, classification has taken two strategies i.e., structure-based and ligand-based virtual screening.

2.3 High throughput virtual screening and scoring in molecular docking techniques:-

Routine techniques used after target identification are high through virtual screening (HTVS) and molecular docking techniques embedded in free energy perturbations, sampling, and scoring algorithms. The knowledge of the active site for the protein/receptor where the ligand would bind to mimic/antagonize the physiological role which is an essential task to initiate the HTVS protocol. Similarly, the ligand-based virtual screening (LBVS) considered as another basic method relies on the Physico-chemical properties of chemical databases.

➤ Activity scoring:-

In virtual scoring, the scoring function is a fundamental component in molecular docking for assessing binding affinities towards target. In machine learning, mapping ability features can yield great accomplishment to extract physical, geometric, and chemical features to retrieve scores. Based on scores, data driven black box models which are considered to predict interactions in binding affinities and furthermore avoiding few concepts in docking like physical function are very hard to study. Random Forest and SVM concepts identified with AI utilization for better performance in the scoring function. For instance, an SVM model can be utilized instead of a linear additive method related to the energy terms concept. Since an SVM can characterize the relationship between experimental binding affinities and own energy terms i.e., can be extracted from the docking program eHiTS. Thus, data gives better execution in scoring power and screening power. Thus, the point in activity scoring was, choosing few features among protein-ligand interaction for predicting binding affinities with help of the CNN model, so it increases information scoring function but it upgrades the predictive capabilities.

3. Hit to lead:-

It is also referred to as lead generation in the beginning phases of drug discovery. It locates small molecules referred to as hits from the High Throughput Screen (HTS) through deficient optimization to locate promising lead compounds. The practical interface of the hit to lead optimization approach integrated with chemical synthesis as well as mapping algorithm "design layer"/Random Forest regression applied to create new biologically active chemical spaces through the utilization of existing kinase inhibitor libraries.

3.1 QSAR:-

QSAR analysis was used in the hit-to-lead optimization process to find potential lead compounds from the hit analogs with the prediction of bioactivity analogs. And primarily utilized in mathematical concepts to study quantitative mapping with physicochemical or structural objects and biological activities. QSAR analysis taken apart in foundation of mathematical models, selection and making the progression of molecular descriptions, evaluation and interpretation methods, utilization techniques

3.2 De novo drug architecture:-

De novo Drug Architecture progressed unique chemical structures by adjusting or balancing the target interest. To introduce a new molecule from scratch using a popular De novo model called the fragment-based approach. If at this point there are impracticalities and complexities in the molecular structure, the risk arises in the development of the structure and becomes difficult in the assessment of bioactivity. Deep learning models utilized powerful knowledge and generative capabilities to introduce a new structure with appropriate properties. In the De novo drug design process, the deep learning models act as autoencoders to generate an appropriate format for new chemical entities (NCE's). Therefore, an embedding of an autoencoder with multilayer perceptron classifier is also a value-added technique in the generation of NCE's with predefined physicochemical properties. The syntax of the drug/chemical structure is produced in SMILES format which might be difficult to understand in many circumstances and grammar variational autoencoder (VAE) overcomes this problem to accelerate the process.

4. ML in e-Resources for drug discovery:-

The AI and ML algorithms prevailed as the main computational scoring functions for evaluation when a predicted value was added as a parameter, which is involved in the basic drug discovery paradigm, illustrated in 6 The detailed applications of the ML algorithms specified in the e-resource are described in the following sections.

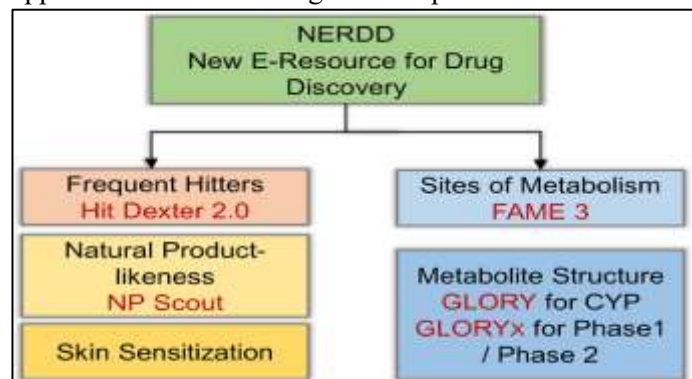


FIGURE (6):- ML in e-Resources of drug discovery platform

4.1 ML in Pan-assay interference screening (PAINS):-

The precise information about hits can be obtained from primary or secondary biological screening assays of purchasable/commercially available databases which were the most important parameters before starting medicinal chemistry projects. Thus, elimination of the compounds has been exhibited in different cellular biological assays considered as pan-assay derived hits could reduce the cost and time of the medicinal chemists. The pan assay information can be accessed from the PAINS database on request. Therefore, the Hit Dexter 2.0 web server has been launched compiled from Pubchem library and screening assays. The Hit Dexter 2.0 could be initially utilized to know the biological properties of the newly designed compound and thus anyone can easily eliminate the panassay interfering compound at the initial stage itself.

4.2 ML in drug metabolite and metabolic site prediction:-

The identification of metabolic sites for any kind of drug or new chemical entity is very essential before its administration into the human body. The prediction of drug metabolism can be done by animal models (preclinical studies) which is a rate-limiting step as well as costly and it is mandatory to retrieve therapeutic approval of new chemical entities. The site of metabolism can be predicted by several modules among "ADMET Predictor" of SimulationsPlus tools that have gained attention and are pure works on the models compiled

by artificial intelligence algorithms. The FAME3 is one of the online servers which predicts the region for the given drug/compound which undergoes metabolism validated databases gathering phase-1/phase-2 metabolic parameters associated with several databases validated by comparing with Matthews correlation coefficient (MCC).. It is also important to have an overview of the chemical modification of drugs/NCE's which undergo metabolism and thus can be used in calculating dosage regimen, dosage frequency, toxicity, and other beneficial side effects. The online services such as GLORY/GLORYx provides the precise information about the possibilities of new metabolites and their relevant formation data with respect to

mitochondrial cytochromeP450 enzyme and conjugations.

4.3 ML in skin sensitivity parameter prediction:-

The prediction of skin sensitivity is one of the essential criteria for assessing safety parameters of the new drugs/compounds and it is patient to patient specifications. In this regard, the AI models such as Random Forest based MACCS (RF_MACCS) and support vector machine (SVM) based PaDEL (SVM_PaDEL) algorithms trained with approximately 1400 ligands linked with local lympho node assay (LLNA) information.

4.4 ML in natural product identification:-

The ML trained with 265000 natural product isolates and synthetic libraries validated by MCC is being used as a basic predictive model NP Scout online server will reveal the probable identity of the newly discovered analogs. The application of NP Scout in the prediction of sources for the query molecule might provide information about their natural product sources and could become a part of natural product-based drug discovery.

➤ Future Perspectives:-

1. Emerging Technologies:-

- i) **Quantum Machine Learning:** Potential for exponential acceleration of molecular simulations.
- ii) **Multimodal Foundation Models:** Unified models processing chemical, biological, and clinical data.
- iii) **Autonomous Laboratories:** Fully closed-loop discovery systems with minimal human intervention.
- iv) **Digital Twins:** Patient-specific models predicting individual drug responses.

2. Educational Transformation:-

The Pharmacy Council of India's 2025 syllabus revision mandating AI and Python programming in B.Pharm curricula signals a fundamental shift in pharmaceutical education. Future pharmacists require:

- i) Computational thinking and programming literacy.
- ii) Understanding of AI/ML capabilities and limitations.
- iii) Ability to critically evaluate AI-generated insights.
- iv) Skills in data curation and analysis.

3. Collaborative Models:-

Effective AI deployment requires multidisciplinary collaboration:

- i) Pharmaceutical scientists providing domain expertise.
- ii) Data scientists developing algorithms.
- iii) Clinicians validating clinical relevance.
- iv) Regulators ensuring safety and efficacy.
- v) Patients contributing real-world data and perspectives.

4. Personalized and Precision Medicine:-

AI's ultimate promise lies in truly personalized therapeutics—drugs and dosing regimens optimized for individual patient characteristics based on integrated analysis of genomic, clinical, and lifestyle data.

CONCLUSION:-

AI and Machine Learning are fundamentally reshaping pharmaceutical sciences. In drug discovery, AI accelerates target identification, designs novel molecules, predicts ADMET properties, and enables drug repurposing, cutting development time from years to months while reducing costs. In pharmacovigilance, AI enhances signal detection, extracts safety data from unstructured clinical text, predicts adverse events, and automates case processing—improving patient safety surveillance significantly. Despite challenges like data quality issues, model interpretability, regulatory uncertainty, and workforce skill gaps, the integration of AI into pharmaceutical research and safety monitoring is inevitable. The Pharmacy Council of India's 2025 curriculum revision mandating AI and Python training reflects this reality. The future lies in multidisciplinary collaboration—pharmacists, data scientists, clinicians, and regulators working together. For pharmacy students, combining domain knowledge with AI literacy is no longer optional but essential. Ultimately, the goal remains unchanged: delivering safer, more effective medicines to patients faster than ever before.

RESULT AND DISCUSSION:-

1. Why Do These Results Matter ?

The findings demonstrate that AI is not merely theoretical but delivering measurable improvements. Acceleration from years to months in drug discovery directly addresses the industry's unsustainable cost trajectory. In pharmacovigilance, AI detection of safety signals earlier than traditional methods has direct patient safety implications.

2. Key Observations

- 1) Integration is critical: Best results emerged when AI combined multiple data types. (chemical, biological, clinical, textual)
- 2) Human oversight remains essential: AI outputs require expert validation; the technology amplifies rather than replaces human judgment.
- 3) Explainability gap persists: While CNNs, RNNs, GNNs, LSTM complete transparency remains elusive for complex deep learning models.
- 4) Data quality dictates performance: Models trained on biased or incomplete data produce unreliable predictions.

3.Implications for Pharmacy Practice

- 1) Pharmacists need AI literacy to critically evaluate AI-generated insights.
- 2) Curriculum reforms (PCI-2025) are timely and necessary.
- 3) Interdisciplinary collaboration between pharmacists and data scientists is essential.
- 4)Regulatory frameworks must evolve to keep pace with technological advancement.

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