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DRUG DEVELOPMENT: ROLE OF GENERATIVE ARTIFICIAL INTELLIGENCE

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ABSTRACT: This article explores the transformation of pharmaceutical research and development by the combination of digital twins and generative artificial intelligence (AI), especially in drug discovery. It highlights various cases that illustrate the increasing use of digital twins of biological systems alongside generative AI algorithms to speed up the identification of new drugs. This approach involves simulating vast chemical landscapes and predicting molecular properties, which facilitates the discovery of novel compounds that may have previously been overlooked. By leveraging computational models and machine learning, researchers can design targeted compounds, refine potential therapy candidates, and simulate their interactions within complex biological environments. This method accelerates the identification of promising drug candidates while predicting their efficacy and safety more efficiently, without extensive *in-vivo* testing. Furthermore, digital twins allow for a more personalized approach to drug development, enhancing the chances of success for specific patient groups. This cutting-edge methodology presents significant opportunities to streamline drug development processes, lower costs, and ultimately improve patient outcomes by delivering more effective treatments. However, the integration of these technologies also poses challenges, including the necessity for interdisciplinary collaboration and ongoing improvements in AI models, computational capabilities, and data integration. As the field progresses, further innovations will be essential to fully harness the potential of these technologies.

INTRODUCTION: Artificial Intelligence (AI) is a vibrant and fast-changing area of computer science focused on creating systems and machines that can perform tasks typically requiring human intelligence. These tasks include learning from experiences, understanding natural language, solving complex problems, making informed decisions, and adapting to new situations. AI aims not only to replicate human cognitive abilities but also to enhance them.

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It enables machines to perform tasks more quickly, accurately, and efficiently than humans in many cases. As artificial Intelligence technology progresses, it is transforming industries, society, and our interactions with technology, opening up new avenues for innovation and problem-solving. Artificial Intelligence is often viewed as a broad term that includes several subfields, each offering unique techniques and approaches to building intelligent systems.

Among these, two of the most significant and commonly used subfields are Machine Learning (ML) and Natural Language Processing (NLP). Machine learning (ML) is one branch of artificial intelligence (AI). This group of techniques includes reinforcement learning, unsupervised learning, and

supervised learning [2]. Natural language process [NLP], it is a process in which we know about the interaction between the people and the computers and see how they communicate by using, natural language. It makes it possible for machines to comprehend, decode [3].

Artificial Intelligence comes up with two Sub-fields:

1. Machine learning
2. Deep learning

Machine Learning [ML]: Machine learning program, is the process in which the, algorithmic program is collected for examine data, draw conclusions from it, and decide what to do next. The topic of machine learning is relatively new, incorporating techniques and algorithms that date back several decades, some as far back as the 1960s. The Naïve Bayes classifier and support vector machines are two examples of these traditional methods such as the Naïve Bayes classifier, which works on probabilistic models, and support vector machines (SVMs), known for their use in classification problems, are widely used in data analysis. Apart from classification, cluster analysis algorithms like K-means and tree-based clustering are also available [4]. Principal component analysis and tSNE, the two techniques used in machine learning, to decrease the dimensionality data and obtain a deeper understanding of its nature.

Deep Learning: A branch of artificial intelligence called "deep learning" uses artificial neural networks as its foundation. Deep learning can be considered a subset of machine learning, as it relies on data to train algorithms that learn patterns and solve complex problems. Deep learning and machine learning are often used interchangeably [5,] but they are distinct concepts. While both fall under the umbrella of artificial intelligence, deep learning specifically utilizes neural networks multi-layered algorithmic structures setting it apart from traditional machine learning approaches.

Areas of Application of AI:

Enhancing Drug Development: AI is being used by the pharmaceutical sector to expedite the discovery and development of new drugs. Conventional drug development is an expensive and time-consuming procedure [6]. AI accelerates this by predicting the efficacy of specific drug candidates and refining their chemical properties for optimal performance. This not only accelerates development but also reduces costs and improves the likelihood of success in clinical trials [7].

AI for Diagnosis: In the area of diagnostics, artificial intelligence has made one of the biggest contributions to healthcare. Deep learning algorithms and other AI-powered tools are remarkably accurate in analyzing medical images. AI systems, for example, can find anomalies in MRIs, CT scans, and X-rays; these algorithms frequently spot problems that the human eye could miss. When it comes to early diagnosis of diseases like cancer, when early intervention can greatly increase survival chances, this technology is especially helpful [8].

Drug Development: The meticulous, multi-phase process of drug development aims to find, test, and introduce novel pharmaceutical products to the market. Enhancing patient outcomes and developing medical therapies depends on this process. An examination of the drug development process identifies numerous critical phases, including regulatory approval, preclinical research, clinical trials, and drug discovery [9].

Phases of Discovery: The process starts with the discovery stage, during which researchers find possible therapeutic options. This phase entails learning about the biology of a disease and locating targets, or particular bodily molecules that a medication may interact with. To identify potential molecules, methods such as genetic investigations, computer-aided drug design, and high-throughput screening are frequently used [9].

Preclinical Investigations: Upon identification, candidates undergo preclinical research. To assess the compounds' safety, effectiveness, and pharmacokinetics (the way a drug is absorbed, distributed, metabolized, and eliminated), laboratory and animal studies are conducted during this phase [7]. The goal of preclinical research is to establish if a medication is safe enough to test humans.

Clinical Investigations: There are several stages to conduct clinical trials:

Phase I: Safety, dosage, and side effects are tested on a small number of well-trained volunteers or patients

Phase II: Involves a broader patient population to evaluate the safety and effectiveness of the medication.

Phase III: Enlarges the trial to include a larger patient population in order to verify efficacy, track side effects, and evaluate the medication against standard therapies. To determine the drug's therapeutic value and guarantee its safety for general usage, these trials are crucial for determining the drug's therapeutic value and ensuring its safety for general use [8].

Regulatory Acceptance: A drug developer submits a New Drug Application (NDA) or Biologics License Application (BLA) to regulatory bodies, such as the European Medicines Agency (EMA) or the U.S. Food and Drug Administration (FDA), after completing successful clinical trials. Complete clinical trial data are included in the application. Regulatory bodies examine the application, inspect the manufacturing facilities, and approve the drug for marketing if it satisfies all requirements [9].

After-Market Monitoring: Phase IV, also known as post-market surveillance, involves monitoring how well the medication works in the general population, spotting any uncommon or long-term side effects, and ensuring continued safety [10].

AI in Drug Development: The process of developing new drugs is being changed by artificial intelligence (AI), which is making it quicker, more economical, and more efficient. Drug discovery is typically a drawn-out, costly process with a high failure rate. Artificial intelligence (AI) uses cutting-edge algorithms and machine learning approaches to analyze large datasets, find promising drug candidates, and forecast the safety and efficacy of those candidates. Early on in the drug discovery process, artificial intelligence plays a major role in drug development [19]. AI is capable of sorting through enormous volumes of biological data to find interesting molecular structures and forecast how they will interact with particular targets. This expedites the process of identifying promising medication candidates and thereby lowers the time and expense involved in this stage.AI models mimic drug behavior in biological systems during preclinical research. Here, we talk over integration areas, methods and tools for enforcing AI, continuous difficulties, and solutions [15].

Artificial intelligence (AI) has been used more and more in many spheres of society, most notably the pharmaceutical business. The use of AI in the pharmaceutical industry is highlighted in this review, with applications ranging from drug development and discovery to drug repurposing, increasing pharmaceutical productivity, and clinical trials [19, 20]. These applications not only expedite target achievement but also lessen the workload for humans. We also talk about recurring issues, methods, and cross-talk between the AI tools and strategies.

AI in Drug Screening: It takes more than a decade to discover and develop a drug, and this costs about US$2.8 billion on average. Nevertheless, in the field of therapeutic molecules, nine out of ten never pass phase II of clinical trials and regulations [31, 32]. According to the synthesis feasibility of the techniques involved, numerous algorithms such as Nearest-Neighbor classifiers, RF, and extreme learning machines, as well as DNNs and SVMs, are employed for VS and are also capable of estimating in vivo activity and toxicity [31, 33]. Bayer and Roche, along with IT companies, are among many biopharmaceutical industry players working to build programs for the discovery of treatments for conditions like heart disease and immunopathology [19].

Estimating the Physical and Chemical Characteristics: The pharmacokinetic properties and the family of target receptors of the drug depend on certain physicochemical characteristics of the drug, such as solubility, partition coefficient, degree of ionization, and intrinsic permeability [34]. Various AI-dependent software and models can be used for prospective and predictive analysis of physicochemical properties. For instance, during compound optimization, large datasets are generated for use in training machine learning (ML) programs. These are used in conjunction with molecular descriptors, such as SMILES strings, potential energy measures, electron density of the molecule, and the coordinates of the atoms in 3D,

to design feasible molecules through deep neural networks (DNN) that will forecast their properties Zang *et al.* successfully designed a QSPR framework to identify six physicochemical properties of environmental chemicals from the EPA, known as the EPI Suite [35]. The ADMET predictor and ALGOPS program reveal that the developed neural networks are accurate in predicting the lipophilicity/solubility of different compounds [36].

Prediction of Bioactivity: Bioactivity can be predicted using the properties of the compound within the protein binding site. The potency of the drug molecules in relation to the intended protein or receptor is crucial in determining the efficacy of the drug. Drug molecules that do not interact with or bind to the protein being targeted cannot produce the therapeutic effect. Sometimes, developed drug molecules may bind to undesired proteins or receptors, leading to toxicity. Thus, drug-target binding affinity (DTBA) is crucial for predicting the interaction between the drug and target [42]. On the other hand, similarity in interaction refers to the likeness between a drug and its target, suggesting that they may interact with similar targets. There are web applications that can be used to predict drug-target interactions, where the 'r' value ranges from 0 to 1. Among them are Chem Mapper and the Similarity Ensemble Approach (SEA) [43].

Previous ML-based models, such as the Kronecker-regularized least squares (Kron RLS) approach, compare protein molecules and drug molecules to establish the DTBA. "Similarly, SimBoost uses regression trees to estimate DTBA and incorporates features and interaction similarities [46]. Taking this into account, drug features can be specified using SMILES, LMCS (Large Molecular Complexity Scoring), extended connectivity fingerprints, or a combination of these parameters. DL approaches have been found to perform better than ML because the techniques used do not require structural information of the protein. Some DL methods used to measure DTBA include DeepDTA, PADME, WideDTA, and Deep Affinity [46].

The Impact of AI on the Drug Discovery Process: A further critical application domain for AI techniques in drug discovery involves the design of novel compounds with set properties and activity. Traditionally, drug design approaches generally detect existing compounds. Conversely, methods that use [AI] make it possible to create novel compounds with specified properties, and activities quickly and effectively. A deep learning algorithm has recently been taught with a data set of drug compounds featuring known attributes to suggest new therapeutic chemicals,[10] that have prized characteristics demonstrating the capabilities of these techniques in promptly and effectively designing new drug candidates.

DeepMind made, arguable, the most enormous contribution to AI research in the field of biology with the invention of AlphaFold the software platform that will advance the ability of our understanding towards the biology [19]. This is a very strong algorithm that uses protein sequence data together with AI to predict the three-dimensional structures of these proteins. In the field of de novo drug design, ML techniques are being used together with molecular dynamics simulations in such a manner that the efficiency and accuracy of the methodologies are improved. The combination of these methodology is under investigation in order to make the most of synergies that exist between them. DL and IML methods also power this effort. Researchers are using the power of MD, and AI to design the drugs better and also more effective than before.

The concept of rational drug design is defined as the act of modifying existing molecules to achieve specific properties and recognition. Recently, DeepMind developed AlphaFold, a revolutionary software application that enhances biological knowledge. In contrast, the AI-based method allows the design of the new molecules with potential properties and biological activity at a high speed and increased efficiency.

The applicability of these techniques in designing new drug candidates in a short duration is well reflected from the above said exercise where deep learning algorithm was trained with a dataset of compounds and their properties and later used for designing new therapeutic molecules having certain properties like solubility and activity. Recently, DeepMind has produced AlphaFold that is a revolutionary software application to enhance biological knowledge which has brought a

significant impact on the AI-related research. It is a powerful tool that can forecast the matching three-dimensional structures of the proteins by the protein sequence data and artificial neural network. This was expected to revolutionize medication discovery and individualized treatment in the domain of structural biology. In the area of structural biology and the biological sciences more broadly, in terms of utilizing AI, AlphaFold is probably a big leap forward.

Machine learning (ML) strategies, together with molecular dynamics (MD) simulations, are currently being used in order to improve speed and reliability in the de novo drug discovery field. With a view to fully leverage these approaches, the option of combining them is being considered under what is referred to as the strategy merge [20]. This endeavor also includes an interpretation of deep learning and other specific machine learning algorithms. This way, AI and MD enable researchers to build medications more effectively and efficiently than they could before [21].

Successful Drug Discovery Projects that Involved the Use of AI: Numerous case studies prove the effectiveness of the AI model in the framework of drug discovery. For example, Gupta, R., *et al* [21] have recently described the use of AI techniques in the identification of new drugs for the therapy of cancer. These scientists employed a fairly large set that included 166 substances that are reactive to cancer and their corresponding biological activity profile to create an algorithm based on deep learning. Thus, new compounds that hold great potential for cancer treatment in the future were developed, which means that this technology is capable of identifying new treatments.

A new approach proving that ML can be used to identify small-molecule inhibitors of the MEK protein has been presented several weeks ago. MEK itself can be looked upon as a target for cancer therapy but it has been quite challenging to work with efficient inhibitors. In this case, ML was able to uncover the newer inhibitors for this protein [22]. Another example is the use of artificial neural networks to screen more inhibitors of beta-site APP cleaving enzyme 1 (BACE1); an enzyme associated with Alzheimer's disease [23].

Despite the fact that the cases where AI has been applied to drug design are limited, it is clear that it works efficiently in the search of new antibiotics. A competition of over 100 million molecules was evaluated by an innovative machine learning algorithm that identified antibiotic sorts that are rather powerful – including one that fights many bacteria [25,] including unmanageable ones and tuberculosis.

In the past two years, a novel approaching of using AI to search for drugs to combat against Covid-19 has been explored. Computer-aided reasoning has been applied to analyze large databases of potential compounds to identify those that have the highest likelihood of treating the virus. There are many techniques that have, in some cases, identified potential medications much more quickly than could possibly be achieved through the traditional methods [26, 27, 28, 29, 30, 31]. Some other examples which show how such AI based techniques can hasten the drug discovery process as well as help to synthesize better drugs [3, 32, 33, 34, 35, 36, 37].

AI in Pharma Industry: The increasing complexity of manufacturing processes and the growing demand for efficiency and improved product quality are driving modern manufacturing systems to embed human knowledge into machines, transforming manufacturing practices [88]. The application of AI in manufacturing has the potential to boost the pharmaceutical industry. Tools like CFD use Reynolds-Averaged Navier-Stokes solvers technology to study how agitation and stress levels affect different equipment (e.g., stirred tanks) automating many pharmaceutical operations. Similar systems, such as large eddy simulations and direct numerical simulations, utilize advanced techniques to resolve complicated flow challenges in manufacturing [85].

A new computer program supports digital automation for the production and synthesis of molecules, considering a variety of chemical rules and are programmed with the Chemical Assembly scripting language. The synthesis and manufacture of sildenafil, diphenhydramine hydrochloride, and rufinamide have seen yields and purity on par with manual synthesis thanks to its use by scientists [89]. Technologies powered by AI can project the finish of granulation in granulators that have capacities

between 25 and 600. AI technology and neuro-fuzzy logic identified key factors in their responses [90 91]. Scientists have used DEM a lot in the drug industry it has been used to study color separation in a double mixer, the effects of blade speed and shape changes, and tablet movement during coating. They've also used it to figure out how long tablets spend under the spray [85]. AI tools like neural networks and fuzzy models have looked at how machine settings relate to the problem of sticking trying to cut down on tablets sticking during production. Parts of the problem about tablets sticking during production have been addressed by AI tools like neural networks and fuzzy models, which had studied how machine settings are relevant to this issue. These tools are the meta-classifier and tablet- classifier, it uses AI to verify whether your output is finally good [93]. They can identify potential pitfalls in the making of that tablet. There is a patent application pending for such an invention that could determine what strength of drug combined with which patch type might work best in any given patient. Part of the solution is a computer that inputs patient information and creates just the right patch for them [94].

AI in Quality Control and Quality Assurance: Making the requested product from raw materials involves balancing various factors. Quality control checks on products, plus keeping consistency from batch to batch, need human intervention [93]. This approach might not work best in every situation showing why we need to put AI into action at this point. This prompted the FDA to revise Current Good Manufacturing Practices (cGMP) by introducing a 'Quality by Design' approach to define key processes and critical requirements that determine end quality of pharmaceutical product. Decision trees were prepared using primary data, being the combination of manual activity with artificial intelligence algorithm by Gams *et al* [85]. They turned these into rules for drivers to examine helping guide future product cycles. Goh and team looked at the dissolution profile, which shows how consistent theophylline tablets are from batch to batch. They used an ANN to predict the dissolution of the tested formula achieving an error rate of 8%. AI may be applied to law in-line production process for the requested quality of product as well. This type of ANN-based monitoring uses a UBG snap-drying process with a tone-adaptive elaboration setting, as well as original search and reverse accumulation. For control purposes in practice, this can be used as a way to predict the temperature and cutlet texture at a later time point ($t+\Delta t$) for a fixed set of operating conditions [96].

An Electronic Lab Tablet which reads an automated data entry platform can then under tight control guards maximize protection for the product a repeating analysis--smart ways like these should mean good-housekeeping holds up pretty well! Furthermore, discovery techniques-based data mining and visualization to Total Quality Management 990 [97]. And intelligent opinions, and eventually building new technology into those two things - these system intelligence-controlled decisions quality control precious [99].

AI in Clinical Trial Design: Clinical trials Clinical trials of a new investigational medicinal product take an average of six to seven years to scientifically establish its safety and efficacy in treating a specific illness in people, not to mention the large sum of money required. However, only one in ten of the molecules that go through these trials manage to get clearance, an outcome that is staggering for the business. Such failures could be attributed to poor patient selection, absence of technical standards, and poor facilities [100]. However, by employing the AI system, such problems are considerably reduced because there is tremendous digital medical data available at the moment. Recruitment of patients occupies a third of the trial's time [101].

The selection of the right patients is a key determinant of the success of a clinical study, because it avoids roughly 86% of failure scenarios [102]. By means of patient-specific genome–exposome profile analysis, the AI is capable of recruiting only the particular diseased population in the [phase II and phase III clinical trial]. It can contribute to the premature division of the landscapes of therapeutic targets in the chosen patients by design [19, 101]. Other AI based approaches such as predictive machine learning and other forms of reasoning help in preclinical molecular discovery and also lead optimization such that the resultant drugs are more likely to pass clinical trials with respect to the chosen patient

population [101]. Patient dropout is identified as a major reason for failure in 30% of clinical trials because the number of patients to be recruited is increased to meet the required number in order to complete the trial thus incurring a lot of time and money. This can be prevented when patient is closely observed and can be helped to observe the planned protocol for the research trial [102]. Patients that are diagnosed with schizophrenia are commonly prescribed antipsychotic medications and so Ai Cure developed mobile applications that ensure that the identified patients take the required doses as required by the Phase II trial. This led to a 25% compliance percentage among the patients so that the clinical trial was successfully accomplished [19].

Artificial Intelligence in the Management of Pharmaceutical Products:

Marketing Positioning through AI: Any business strategy for an organization that is looking to develop a unique brand must include market positioning, which is the process of endowing a product with a personality in the market to attract customers [103, 104]. This marketing approach was taken up by the producers of original Viagra aiming at treating other life issues alongside erectile problems among men. The platform that technology and e-commerce provide has made it easy for companies to have its organic recognition as a brand name in public domain [106]. Businesses use search engines as one of the technology platforms to take center stage in online marketing. Businesses are always looking for ranking their websites higher than those of their competitors so that they can establish their brand first. There were also other tools like; particle swarm optimization algorithms, and statistical analysis techniquesis introduced by Kennedy and Eberhart in 1995 coupled with (NNs) that helped to understand markets better. This way, it is possible to accurately predict consumer demand and provide a basis for a marketing plan of a product [107].

AI-Based Advanced Applications:

AI-based Nanorobots for Drug Delivery: AI-based cutting-edge applications, such as nanorobots for drug delivery, involve nanorobots with integrated circuits, detectors, power sources, and data backup systems. AI technologies maintain these components [117, 118]. Engineers program them to avoid collisions, identify targets, detect and attach, and leave the body. New nano/microrobots can navigate to specific areas based on body conditions like ph. This improves their effectiveness and reduces side effects. To develop implantable nanorobots for drug and gene delivery, scientists must consider drug adaptation long-term release [119]. AI tools like; integrators and, neural networks fuzzy logic control the drug release. Doctors use microchip implants to program drug release and locate the implant within the body.

Artificial Intelligence used for Forecasting Synergism/Antagonism alongside Combination Drug Delivery: AI in combination drug delivery and symbiosis/antagonism prediction Many drug combinations get approval and hit the market to treat complex conditions, like TB and cancer, because they can boost each other for faster healing [120, 121]. Picking the right drugs that work well together means testing lots of drugs, which takes a long time; for example, cancer treatment often uses six or seven drugs together. ANNs logistic regression, and network models help screen drug combos and make treatments more effective [120,122].

Rashid and his team created a system to find the best drug combo to treat multiple myeloma that doesn't respond to bortezomib. They looked at 114 FDA approved drugs. Their model said decitabine (Dec) and mitomycin C (MitoC) work best as a pair, while Dec, MitoC, and mechlorethamine make the top three-drug mix [121]. Combo drug delivery can work even better with info on how drugs help. Li and his team designed a synergistic drug combination model, made possible through RF, to predict synergistic combinations of anticancer drugs. The approach was successful in predicting 28 synergistic anticancer combinations based on gene expression profiles and various networks. In their report, Mason and colleagues discussed three examples of these combinations, though the remaining ones may still carry importance [123].

The advent of AI in Nano-medicine: The advent of AI in nanomedicine Nanomedicines are those forms of medicines that employ drug and nanotechnology together to alleviate, treat or diagnose and monitor complex diseases like HIV,

cancer, malaria, asthma or other inflammatory diseases. Due to the improved efficiency and effective treatment as a result of nanoparticle modified drug delivery systems, this mode of delivery has recently gained prominence in therapeutics and diagnostics [121, 124]. There are several challenges in formulation development [125]. Perhaps here astonishment might lie because of AI and nanotech together. Clothes employ any stage of contacts of the field to spot regions with certain properties that could induce the formation of cluster shapes [83]. Coarse-grained simulation provides aid to the estimation of drug encapsulation in the dendrimers and the estimation of drug – dendrimer interaction alongside chemical computation. The influence of surface chemistry on the internalization of nanoparticles into cells could also have been investigated by using computer programs such as LAMMPS and GROMACS 4 [83]. This increased silicasome intake three- to four-fold because iRGD enhances silica some transcytosis, hence leading to better treatment outcomes and increased overall survival [124].

AI's Pharmaceutical Market: AI's pharmaceutical market, pharma companies increasingly look at AI as a means to reduce the costly burden of VS along with its high failure rates. The AI market that was valued at US$ 200 million in, (2015) reached (US$700 million in 2018). It is expected to increase by 40% from 2017 to 2024, meaning that it is bound to make radical changes in pharmaceuticals and medical sectors. Most pharmaceutical firms have invested in AI and are still investing. They have also partnered with AI startups to provide essential healthcare technologies.

Constant Challenges to the use of AI: The effectiveness of artificial intelligence depends on the volume and quality of available data, as data is essential for training these systems effectivity. If a company is in need of access to data from a number of database providers, then it will have to pay more, and for correct result prediction, the data also needs to be reliable and of high quality. Other challenges that further impede the full-scale implementation of artificial intelligence in the pharma sector include a lack of trained personnel to run the AI-based platforms, small organizations having small budgets, fears that such replacement will lead to a loss of jobs, skepticism regarding data emanating [6]. With time, some of the jobs in clinical trials, manufacturing process, and, supply chains, and research of medication and sales will become automated; however, all those jobs fall into the category of "narrow AI," which simply means for the AI to be appropriate for a particular task, it needs to be trained on a huge amount of data first. Hence, for this AI platform to be developed, implemented, and run successfully, the requirement for human intervention becomes necessary. But since the reins of all the mundane tasks have already been taken over by AI itself, leaving space for human intelligence to be applied to higher insights and creative expression, the fear of unemployment might not have been that real after all.

Yet, certain pharmaceutical companies have embraced advancements in AI technology, with estimates of US$2.199 billion in revenues to be earned from AI solutions by the pharmaceutical industry by the year 2022 with investments of US$7.20 billion over more than 300 deal strategies that were undertaken from the year 2013 to the year 2018. Post-deployment, pharmaceutical companies often remain uncertain about the extent to which AI can address the concerns it was implemented for and the limits of its capabilities [127]. To properly capitalize on the AI platform, appropriate resources inside an organization, such as successful data scientists, suitable software engineers, if possible, with fundamentals of AI knowledge and clear understanding business objectives and R weekends of the firm.

CONCLUSION AND FUTURE DIRECTIONS: The advanced capabilities of AI aim to reduce the challenges faced by pharmaceutical firms, which impact the entire product life cycle and medication development process. This could be one of the reasons for the rise in start-ups within this domain. The increasing cost of drugs and therapies is one of the major challenges currently faced by the healthcare sector. Therefore, society needs to adopt an entirely new approach to address this challenge [23]. AI-enabled production of pharmaceutical products allows for drug personalization based on each patient's specific needs by adjusting the dosage, release parameters, and other critical factors [128]. State-of-the-art AI-based technologies will further accelerate product market entry,

improve product quality, enhance production safety, and reduce costs. These are the advantages that have accorded importance to automation. A major concern regarding the adoption of AI innovations is the potential job losses and the strict regulations surrounding AI integration. However, these innovations are not designed to displace humans but to simplify and optimize work processes [129]. AI can accelerate and streamline the identification of hit compounds, propose synthesis pathways, predict the required chemical structures, and provide better insights into drug-target interactions and structure-activity relationships (SAR). AI can significantly enhance drug development, optimization, and integration into appropriate dosage forms additionally; AI enables timely decision-making, accelerates high-quality production, and ensures batch-to-batch consistency. Comprehensive market analysis and prediction enabled by AI can validate product safety and efficacy during clinical trials while optimizing market placement and pricing strategies. AI is not yet fully commercialized, and while it must overcome several obstacles before widespread adoption, it is highly likely that the pharmaceutical sector will find it indispensable in the near future.

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