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Artificial Intelligence in Drug Discovery and Drug Design

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ABSTRACT
Overthepasttenyears,artificialintelligencehasrevolutionisedthefieldofdrugresearch. The process for discovering new drugs could be completelytransformed by artificial intelligence, which could provide increased speed, accuracy, and efficiency. The process for discovering new drugs could be completely transformed by artificial intelligence, which could provide increased speed, accuracy, and efficiency. Numerous uses of artificial intelligence, including virtual screening and drug design, have been employed in drug development. AI methods are brokendown into learning paradigms and modelarchitectures. The surveyed publications are arranged chronologicallyto illustratethe evolution ofAI indrug discoveryover time in terms of technical advancement. We anticipate that this survey offers an in-depth examination of artificial intelligence in drug discovery. This development is being motivated, among other things, by the increasing use of machine learning, and specifically deep learning, in many scientific domains and by advancements in computer hardware and software. Medicinal chemistry has benefited from the beginning scepticism that has begun to fade over the use of AI in pharmaceutical development. A number of methodological advancements, including hybrid de novo design, message-passing models, spatial symmetry-preserving networks, and other cutting-edge machine learning paradigms, are probably going to become standard practicesandaidinansweringsomeofthetrickiestproblems.Thecreationofmodelsandopen data sharing will be essential to the advancement of drug discovery using AI. There is a growingpotentialforthediscoveryofseveralnovelmedicationsasaresultoftheadvancement of artificial intelligence in the pharmaceutical sector. Human illness rates are rising dramatically, but there areveryfew medications available totreatorcurethem. However, the pharmaceuticalindustry'sandartificialintelligence'scombinedeffortswillpreventthissortof situation in the future by accelerating the discovery of medications with better clinical outcomes. AI-based drug development techniques are being used by several pharmaceutical companies to treat a variety of illnesses, including diabetes, Parkinson's disease, Alzheimer's disease, OCD, and more Technology may significantlyassist in resolving a number of issues and limitations with the conventional drug development process.

KEYWORDS: Artificial Intelligence, Machine Learning, Deep Learning, Drug Discovery, Drug Designing, Computational Drug Design, Pharmaceutical Research, Virtual Screening, Molecular Docking, Quantitative Structure-Activity Relationship (QSAR)

We have highlightedthe range ofapplications ofartificialintelligence (AI) inpharmaceutical sciences, including extensive possibilities for drug discovery and development.

Objectives

ArtificialIntelligence(AI)seekstoautomatehuman-performedrepetitivetasksandprocedures in order to boost productivity, lower mistake rates, and free up human resources for more intricate andimaginativeprojects.

Artificialintelligence(AI)modelsarebuilttoevaluated ataandforecastorpredictfuturetrends or events. This talent is used to make educated decisions in a variety of industries, including finance, weather forecasting, and healthcare. Applications like picture identification, natural language processing, and anomaly detection are made possible by AI algorithms' exceptional ability to identify patterns and trends in massive datasets. By identifying the best answers to challenging issues, artificial intelligence (AI) is used to optimise systems and processes. This covers route planning, scheduling, logistics, and resource allocation. AI makes experiences more individualised byevaluating user information and preferences to create customised recommendations.

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I. INTRODUCTION

Drug discovery advancements have fundamentally altered medicine, turning once-fatal illnesses into a sort of prescribed therapy regimen. The development and testing of new pharmaceuticals has been made easier, which has contributed to the improvement of medicine. Theadvancement ofmedicinehas beenfacilitatedbytheeaseofdevelopingandtestingnovel medications.Anewdrug'sdevelopment cantakemorethantenyearsand costsanIntroducion average of 2.6 billion US dollars. Furthermore, less than 10% of drugs that begin Phase I clinical trials successfully reach the market [1,2]. The process of developing a new drug is particularly time-consuming and costly since it involves numerous in vitro, in silicon, and in vivo experiments that typically take four years on average. Preclinical, pharmacokinetic, pharmacodynamic,andtoxicologicalresearcharealsoincludedinthisprocess.Drugscreening is a processthat involves a series ofexperiments and characterizations onthe further possible drug.synthetic intelligence Artificialintelligence(AI),also knownasmachine intelligence, is thesimulationofhumanintellect,wherebyacomputerreplicatesthecognitivebehaviour linked to the human brain during learning and problem-solving [3], using tools and software thatenableautonomousdecision-makingforcertainobjectivesbylearningfromandanalysing incoming data [4]. The terms artificial intelligence and machine learning have different meanings. A subfield of computer science that combines engineering and statistics, artificial intelligence employs models or algorithms to accomplish tasks and produce actions like decision-making and prediction. Drug candidates' potential toxicity has also been predicted using AI-based techniques [5].

PurposeofAI

1. Utilisingreal-timedatacollecting,amobileplatformcanenhance medicaloutcomesby making patient recommendations.
2. Thecapacitytoassessvastpatientdataanddetermineavailabletreatmentsviaacloud- based technology is known as personalised medicine.
3. Drugdevelopment:Pharmaceuticalfirmsareexperimentingwiththemostcutting-edge technologies to reduce the expensive and time-consuming process of drug research in collaboration with software businesses [29].
4. Numerousacquisitionstomeetthe initialdemandsofmajor biotechcorporations, new startups are fusing artificial intelligence and healthcare.

ArtificialIntelligencewithin thePharmaceuticalSector

Data digitization in the pharmaceutical sector has increased dramatically in recent years. However, digitization has made it more challenging to gather, examine, and integrate such knowledgetosolvecriticalclinicalissues[6].Knowledgerepresentation,problemsolving,and a basic machine learning model (ML) are only a few of the methodological domains that are included inartificialintelligence(AI). Whenearlierneuralnetworkimplementations,suchthe Perceptron, were introduced, they appeared to be a promising solution to these problems. A notableexample fromthisera isa1992 paper byWeinstein et al. that used neuralnetworksto explain the mechanism ofaction ofcancer treatment [7]. Unsupervised machine learning can provideresultsliketheidentificationofdiseasetargetsandsicknesssubtypesbyusingfeature- finding algorithms and grouping [8].

Limitationsofexistingdrugdiscovery techniques

Using these methods, a vast number of possible medication molecules are examined to find those that have the necessary qualities. But these techniques may be expensive, time- consuming, and frequently produce inaccurate findings [9]. They may also be constrained by the availability of appropriate test substances and the capacity to precisely forecast how they willbehaveinthebody[10].Theseissuesmayberesolvedbyavarietyof AI-basedalgorithms, suchasreinforcementlearning,supervisedandunsupervisedlearningtechniques,evolutionary algorithms,andrule-basedalgorithms.Forexample,thesealgorithmscanmoreaccuratelyand efficiently forecast the efficacy and toxicityofnoveltherapeutic molecules than conventional methods[11,12].Additionally,noveltargetsfordrugdevelopment,suchasparticularproteins orgeneticpathwaysimplicatedinillnesses,canbe foundusingAI-basedalgorithms[13].This has the potential to broaden the scope of drug discovery beyond the constraints of more traditional methods and ultimately result in the creation of new and more potent drugs [14]. Despite their historical

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relative success, traditional pharmaceutical research methods are constrained by their reliance on trial-and-error testing and their incapacity to precisely anticipate the behaviour of novel, potentially bioactive chemicals. Conversely, artificial intelligence (AI)-based methods can increase the efficacy and precision of drug discovery procedures, resulting in the creation of more potent drugs.

ArtificialIntelligenceApplications

Although ligand and/or structure-based approaches are the most well-known methods for creating unique molecular profiles with efficient pharmacological potency and qualities, computer-assisteddenovodrugcreationisadifficultprocess[15,16].MakinguseofAIWhen combined with single-cell biology information, artificial intelligence (AI) and machine learning can lead to previously unheard-of results in drug development and discovery by improving biomarker prediction and finding high-quality, disease-associated targets for new drug candidates [17]. AI in medication development and research can increase a drug's metabolism and excretion, improving a medicine's safety and efficacy in both humans and animals. In order to eliminate hazardous compounds fromour bodies and stoptheir build up, which may lead to metabolic disorders and damage to the liver and kidneys, regulation of metabolism andexcretionis essential.In particular,drug metabolism alsoaffectsmultidrug resistanceincancertreatmentandviraldiseases.AI'susefulnessinanticipatingthemetabolism and excretion of medications has been demonstrated by recent studies [18].

TheuseofMLtoforecast thetoxicityandeffectivenessofdrugs

To determineacompound'spossibleeffectsonthehumanbody, traditionaldrug development processesfrequentlyrelyonlabour-intensiveandtime-consumingexperiments.Theprocedure canbetime-consumingandexpensive,andtheoutcomesarefrequentlyambiguousandhighly variable. These restrictions can be solved by AI methods like machine learning. Machine learning algorithms areableto detect patternsand trends ina vast quantityofdatathat human researchers could miss. Recently, a dataset of recognised medicinal molecules and their associated biological activity was used to train a DL algorithm [19]. Then, the algorithm demonstrated a high degree of accuracy in predicting the activity of new chemicals. After extensive training utilising vast databases of known hazardous and non-toxic chemicals, notablecontributionstothepreventionofthetoxicityof possibletherapeuticcompounds have also been reported [20].

The detection of drug-drug interactions, which occur when several medications are used for the same or different conditions in the same patient and result in changed effects or bad responses, is another significant application of AI in drug development. Throughthe analysis of massive datasets of known medication interactions and the identification of patterns and trends, AI-based techniques can identifythis. A machine learning systemhas recently solved this by successfully predicting the interactions of novel medication pairings [21]. AI plays a significant role in personalised medicine by helping to discover potential drug-drug interactions, which makes it feasible to create individualised treatment regimens that reduce the chance of negative side effects.

CasestudiesofeffectivedrugdiscoveryinitiativesusingAI

As a result, new compounds with great promise for treating cancer were found, proving that thisapproachiscapableoffindingpromisingnewtherapeuticpossibilities.Ithasrecentlybeen shown that machine learning can be used to find small chemical inhibitors of the MEK22 protein. Although MEK is a target for cancer therapy as well, finding efficient inhibitors has been difficult. For this protein, the ML system was able to find new inhibitors. As further instance involves the applicationof machine learning algorithms to identify new inhibitorsof beta-secretase, an enzyme implicated in the progression of Alzheimer's disease [22]. The aforementioned instances show how using AI to pharmaceutical research might enhance the forecasting of possible therapeutic compounds' toxicity and efficacy. This can expedite the drug discoveryprocess and allow for the production of safer and more effective drugs.

What roleforAIto improvemedicinalchemistry

Accesstosizabledatasetsfortrainingandtechniquesthatfacilitateanalysisandinterpretation are essentialfor the success of AI and machine-learning technologies in medicinalchemistry. TomisquoteMcAfeeandBrynjolfsson, it seemsplausiblethat "medicalchemistswho useAI will replace those who don't," rather than "AI replacing medicinal chemists." Predicting the toxicity and efficacy of possible therapeutic

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molecules is one of the main uses of AI in medicinal chemistry. Traditional drug development methods frequently depend on labor- intensive and time-consuming experiments to evaluate a compound's possible effects on the human body.

Artificial intelligence (AI) has become ubiquitous in many fields, such as research and the pharmaceutical business, where it has beeneffectivelyapplied to find novelchemicalentities with desired features. AI algorithms' application to drug research offers amazing potential as wellasdifficulties. ArtificialIntelligence isused inmanyareasofchemistrytoimproveR&D andoperatingprocedures.AIistypicallyappliedincom putationalchemistry,spectroscopyand analysis, materials design, reaction optimisation, drug discovery, and process control and optimisation.Cliniciancancreatetherapiesbasedono utcomeswiththeaidofclinicaldecision support systems. Additionally, it isemployed inmedical imagingto analyseMRIs, CT scans, X-rays, and other picturesfor lesionsorother radiological findings in humans. Cliniciancan createtherapiesbasedonoutcomeswiththeaidofclinic aldecisionsupportsystems.Additionally, it isemployedinmedicalimagingtoanalyseMRIs,CTsca ns,X-rays,andother picturesforlesionsorotherradiologicalfindingsinhum ans.Artificialintelligence(AI)hasthe potentialto completelytransformmedicine byimproving our knowledge ofhealthand illness andexpandingourcapacityfordata-drivendecision-making."AIwon'treplacedoctors,"stated Carolyn Meltzer, MD, dean of USC's Keck School of Medicine.

Ethicsin theapplication ofAIinthepharmaceuticalsector

The potential for AI to be used to make judgements about which pharmaceuticals to create, which clinical trials to run, and how to sell and distribute drugs is a major concern. These decisionsmighthaveanimpactonpeople'shealthandw ell-being.ThepossibilityofbiasinAI algorithms is another major worryas it might lead to unjust treatment ofparticular groupsof peopleandunevenaccesstomedicalcare.Concernsabo utjoblossesfromautomationarealso raised bythe applicationof AI inthe pharmaceuticalsector. Furthermore, concerns regarding datasecurityandprivacyarebrought upbytheapplicationofAI inthepharmaceuticalsector. Sensitivepersonaldata maybeaccessedormisusedsinceAIsystems dependonvast volumes ofdatatooperate.Boththereputationoftheorganisation sinvolvedandindividualpeoplemay suffergreatlyfromthis.Sensitivemedicaldatamustbeg atheredandusedinawaythatrespects people's privacy and conforms with applicable laws. In order to apply AI ethically in the pharmaceutical sector, these issues must be carefully considered and addressed. This might involvetakingstepslikemakingsureAIsystemsaretrai nedonrepresentativeandvarieddata, auditing and evaluating AI systems on a regular basis to check for bias, and putting in place stringent data protection and security procedures.

The core principles of reinforcement learning include decision-making within a specific environment and taking appropriate action to maximise effectiveness.

Morethan800 cancer treatments and vaccines are currently being tested, according to a2015 study by Pharmaceutical Research and Manufacturers of America. This could advance the science of genetically based personalised medicine by producing new compounds that could develop into new treatments, discovering or repurposing existing drugs that might be more effective when used alone or in combination, and other areas where AI is being widely incorporatedforease, automation, and betterresults. Inorderto improveradiationtreatments, UniversityCollegeLondonHospital(UCLH)andGoo gle'sDeepMindHealtharecollaborating todevelopmachinelearning algorithms thatcan distinguish between malignantandhealthy tissues. AI is also being used to provide customised treatments for more accurate disease assessments in clinical trial research, radiology, and radiotherapy.

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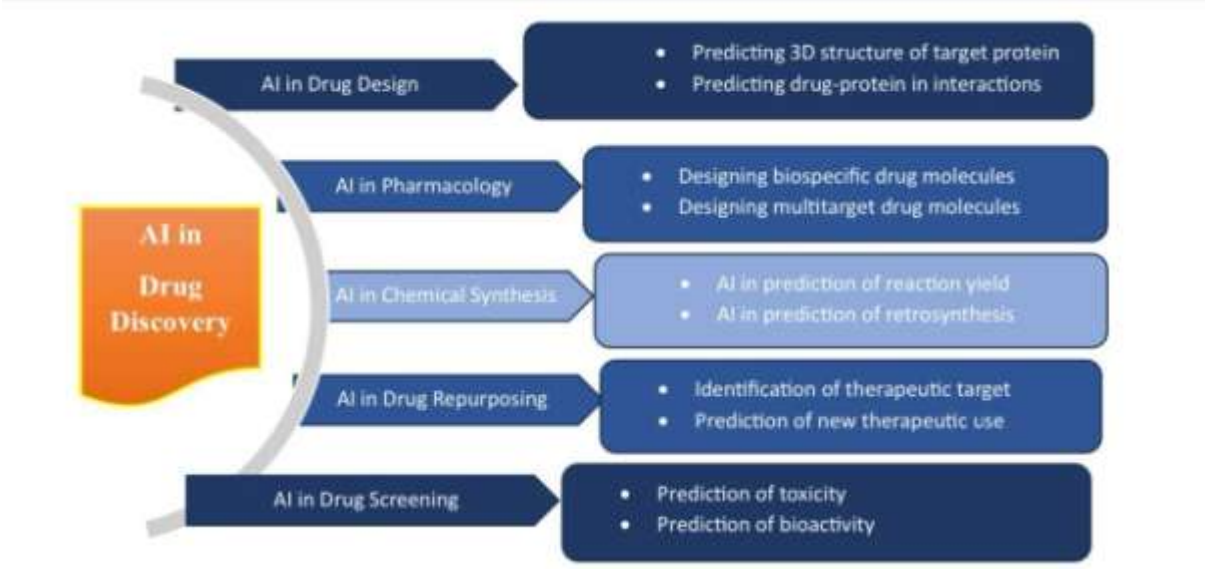

AIinsynthesisofdrug

Aftermoleculesareidentified,themostimportantanddifficultstepistosynthesisethe chosen compounds, which is often done by the process of retrosynthesis [23]. Using a set of criteria programmed into the computer, the Synthia programme, formerly known as Chematica, may proposepossiblesynthesisingpathsforeighttargetsthatare significant formedicine. Itisalso said to be helpfulinthe synthesisofmaterialsthathaven't been made before and to be able to provide substitute synthetic processes for products that are patented.
The Reinforcement Learning for Structural Evolution approach, which uses generative and predictive DNNs to produce new molecules, was used to explore de novo drug production.

AIforDrugDiscovery

Target Identification: Artificial intelligence (AI) systems have the capacity to assess many forms of data, such as clinical, proteomic, and genomic data, in order to pinpoint possible targetsfor treatment. AI aids in the development ofdrugs that controlbiologicalprocesses by revealingtargetsandmolecularpathwayslinkedwithillness. Targetidentificationanddisease modellingareessentialfirstphasesinthedrugdiscovery processthathaveabigimpactonhow well drugsaredeveloped.Moderndrugtargetdiscoveryisincreasinglyrelyingonartificial intelligence(AI)duetoitsbenefitsinanalysingvastdatasetsandintricatebiologicalnetworks.
Wecovertheuseofartificialintelligence(AI)generated syntheticdatafortargetidentification, theapplicationofdeeplearningmodelsfortargetdiscovery,andthevalidationofAI-identified targets through experiments. Target selection heavily relies on novelty as well as druggability and toxicity. Selecting innovative targets against high-confidence targets comes with a trade-off. A new era in AI- driven drug development has begun with the entry of numerous AI-derived medications into clinical trials in recent years. The most important first steps in drug discovery are disease modelling and target identification, which affect the likelihood of success at every stage of drug development. Conventional target identification is a laborious procedure that typically beginsinanacademicatmosphereandtakesyearsorevendecades. Artificialintelligence(AI) is becoming increasingly important in the identification of therapeutic targets in modern medicine because of its benefits in analysing big datasets and complex biological networks.
Weexaminecurrentdevelopmentsintargetdiscovery, emphasisinginnovationsinAI-powered therapeutic target investigation. We also touch on the significance of choosing targets with a mix between novelty and confidence. We address the existing constraints and possible opportunities as more AI-identified targets are being confirmed through experiments and as more AI-derived medications are approaching clinical trials.

Virtual Screening: Virtual Screening AI enables the effective screening of large chemical libraries

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to find therapeutic candidates that have a high likelihood of binding to a particular target. AI helps scientists prioritise and choose which compounds to test in experiments by modellingchemicalreactionsand forecastingbindingaffinities, whichsavestimeand money. Millions of lives could have been spared by SARS-CoV-2-targeting medications during the COVID-19 pandemic, and in order to prepare for future epidemics, it is now imperative to discover inhibitors of coronavirus reproduction. In order to identify inhibitors of the SARS- CoV-2 major protease in ultra large chemical libraries, we investigated two virtualscreening techniques.First,235millionvirtualmoleculesfromav ariedlibrarywerescreenedagainstthe activesiteusingstructure-baseddocking.Ethanomicand bindingtestswereperformedonone hundred of the best-ranked compounds. Second, docking millions of complex molecules and testing 93 compounds experimentally directed the optimisation of a fragment found by crystallographic screening. In the first library screen, three inhibitors were found, and five of thechosenfragment elaborationsexhibited inhibitoryeffects. Thegreatest healthcrisisofthis generationhasbeenbroughtonbythesevereacuterespir atorysyndromecoronavirus2(SARS- CoV-2), which has already claimed over 5 million lives globally. (1) Despite encouraging COVID-19 immunisation campaigns, antiviral medications will probably be essential for managingtheinevitablecoronavirusoutbreaksinthefu ture.SinceSARS-CoV-2variationsfor which vaccinations are less effective have already surfaced, antiviral medications are clearly requiredtosupportvaccinesinthelongrun.Comparabl etoordinarycoldviruses,SARS-CoV- 2 is anticipated to persist in spreading and pose a significant risk to our community. In this case, antiviral medications are required for both the treatment of infected patients and the preventative treatment of high-risk populations.

StructureActivityRelationship: Structure-ActivityRelationship(SAR)modelling:Artificial Intelligence can create associations between a compound's molecular make-up and its biological effectiveness. This allows scientists to build compounds with desirable properties, suchasincreasedpotency,selectivity,andgoodpharma cokineticprofiles,inordertomaximise the potential oftherapeutic candidates. The difficulties in processing and analysing SAR data may be solved by artificial intelligence. AI methods like deep learning and machine learning can be used to automatically extract useful information from SAR data. One of the biggest obstacles to the timely collecting of comprehensive environmental data on each compound is the sheer amount of synthetic organic compounds that are now in production. The idea of structure-biodegradability relationships, or SBR, has been used to explain why organic compounds in the environment vary in their persistence. Earlier attempts usually involved usingacomplicated"universal" inoculum, usuallyderived frommultiplesources,to studythe degradation of a homologous series of structurally related substances under the same conditions. Using this method, it was possible to determine how the positions and types of substituentsaffectedtheapparent biodegradabilityofvariouschemicalclasses. This led to the identification of broad themes, such as the general conferment of persistence under aerobic conditionsbyhalogens.ThispaperintroducestheChem SARweb-basedpipeliningframework forcreatingsmallchemicalSARclassificationmodels. ChemSARcanbeusedto validateand standardise chemical structure representation, compute 783 1D/2D molecular descriptors and ten commonly used fingerprint types for small molecules, filter features, generate predictive modelsthroughajobsubmissionprocessthatisstep-by-step,interpretmodelsintermsof feature importance and tree visualisation, and generate reports. The outcomes can be downloaded as local files and shown as excellent plots.

DE-NovoDrugDesign: Byutilisinggenerativemodelsand reinforcementlearning,artificial intelligence algorithms can suggest new chemical compounds that bear similarities to pharmaceuticals. AI broadens the range of chemical possibilities by incorporating data from experimentalstudiesandchemicallibraries,whichmak esiteasiertodiscoverground-breaking treatment ideas. There are two main de novo drugdesign methodologies: structure-based and ligand-based design. Receptor three-dimensional structures are often obtained using electron microscopy, NMR, or X-raycrystallography. The jobofcreating new medications is difficult and complex, made more so bythe continuallychanging needs in global health. One method that shows promise for quickening and improving this process is de novo drug design. A paradigm change has been sparked by the recent development of Generative Artificial Intelligence

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(AI) algorithms, which enable the quick and semi-automate generation and optimisation of drug-like compounds. The influence of de novo drug creation is examined in this review, which also highlights the promising development of Active Learning (AL) and bothconventionalandrecentlyproposedgenerativealgorithms.Itlaysparticularfocusontheir use in the development of cancer drugs, where there is a pressing demand for innovative therapeutic agents. The possible fusion of these AI technologies with well-established experimentaland computationaltechniquesportends.

Althoughartificial intelligence (AI) has the potential to have a big impact on de novo drug discovery, it's crucial to take a balanced approachto both its present status and its future possibilities. To fullyrealise AI's promise in this subject, it is imperative that the issues listed in this review be addressed. Although we expectAItoenhancetheefficacyandefficiencyofdrugdevelopment,it'scriticaltounderstand that these developments will be slow and dependent upon overcoming substantial obstacles.

AlthoughtheuseofAIinmedicationcreationseemstohaveabrightfuture,therearestillmany unknowns in this field. Advances in algorithmic complexity and range of applications are expected, although they will probably encounter difficulties in overcoming the existing constraints. It is envisaged that AI will both complement and improve conventional drug creation techniques as the area develops. Notwithstanding, this progression necessitates a meticulousanddeliberatemethodology,guaranteeingthat emergingtechnologiesareresilient, dependable,andgenuinelyadvantageousinthepursuitofinnovativetherapeuticremedies.

Notable modifications in drug design have been brought about by AI approaches, including increased algorithmic efficiencyand the discovery ofnovel chemical spaces. It's important to remember that these developments are still in their early phases. Although the use of AI in medicationcreationseems to have a bright future, there are stillmanyunknowns inthis field.

Advancesinalgorithmiccomplexityandrangeofapplicationsareexpected,althoughtheywill probablyencounter difficulties in overcoming the existing constraints. It is envisaged that AI willbothcomplementandimproveconventionaldrugcreationtechniquesastheareadevelops.

Notwithstanding, this progression necessitates a meticulous and deliberate methodology, guaranteeingthatemergingtechnologiesareresilient,dependable,andgenuinelyadvantageous in the pursuit of innovative therapeutic remedies.

OptimizingDrugCandidate: Artificialintelligencealgorithmspossesstheabilitytoevaluate and improve medication candidates by taking into account multiple aspects, including pharmacokinetics,safety,andefficacy.Withtheuseofthiscomputationalmethod,researchers can optimise therapeutic compounds to maximise their efficacy and reduce the possibility of adverse consequences. Drug candidates' physicochemical characteristics, such as their solubility,bioavailability,andtoxicity,canbepredictedbyAIalgorithms.Byconcentratingon compounds with a higher possibility of success, this helps to optimise drug development by cutting costs and time. Artificial intelligence (AI) in medicine refers to the application of AI techniques,algorithms,andtechnologiesinhealthcare. Itentailstheanalysis,decision-making, and execution of tasks that are typically carried out by human healthcare professionals using computer systems and specialised software. By utilising ML, NLP, and other AI techniques, medical AI seeks to increase the precision, efficacy, and efficiency of medical diagnosis, treatment, and patient care. Medical image analysis, medication discovery, customised treatment planning, illnessdiagnosisandprediction,virtualhealthassistants,electronic health recordmanagement,andpatientmonitoringarejustafewofthemanyfieldsinwhichartificial intelligence (AI) is being applied. AI systems can help healthcare personnel make more informeddecisions, identifypatterns, and forecast patientoutcomesbyanalysing largevolumes of patient data and medical literature. This can improve patient care and medical results. Artificial intelligence (AI) in medicine is developing quickly and having an impact on fields including remote patient monitoring, virtual health aides, and medication discovery. It is anticipated that the application of AI-driven technologies would enhance medical diagnosis,illnessprevention,andtreatmentresults,ultimatelyresultinginahealthcaresystemthatismore patient-centric and effective. Along with individualised treatment plans, virtual health assistants, and diagnostic support, drug discovery and development fall within the field of virtualapplications. ApplicationsofvirtualAI help medicalpersonneldiagnose patients more

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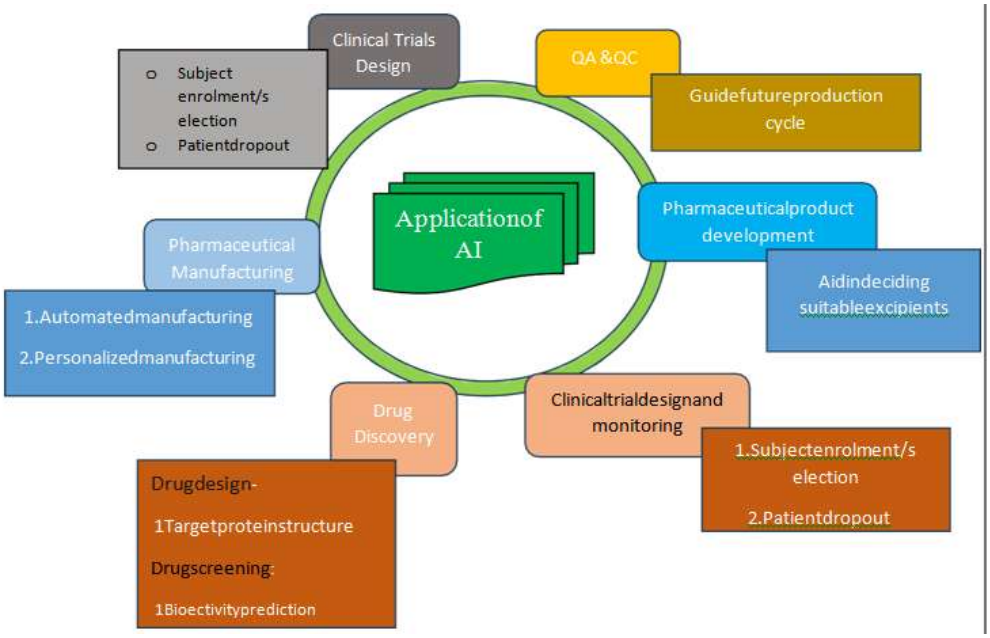
quicklyand accurately. Medicalimaging data,including X-rays, CT scans, and MRI pictures, canbeanalysedbyAIalgorithmstofindanomaliesandh elpinearlydiseaseidentification[6]. Thiscapacityresultsinafar lowerpossibilityofmisdiagnosisandimprovespatient outcomes. Artificial intelligence (AI) is powerful because it can process and analyse vast amounts of medical data and identify trends that people might not see right away. AI can assist in enhancing the precision of diagnoses and creating individualised treatment regimens in this way. DL algorithms, in particular, can spot irregularities or possible

Drug Repurposing: One prominent use of AI in drug research is the identification of authorised medicationswiththerapeutic potentialforvariousdisordersthroughtheanalysisof large biological data. AI lowers costs and speeds up the drug research process through this repurposing process. AI lowers costs and speeds up the drug research process through this repurposing. When it comes to serious, common conditions for which there are still few effective treatments, drug repurposing to find novel therapeutic applications for already-approvedmedicationsisanappealingalternativetothee xpensiveandtime-consumingprocess ofnewdrugdevelopment alone. Inmanyrespects,COVID-19hasbeenseenasagenerational problem. However, it also acts as a spark for group efforts, creativity, and learning. Among these advancements are the realisation of artificial intelligence's (AI) full potential for drug developmentandthestructuredeterminationofunkno wnproteins.AImaybeusedtoanticipate the structure of infectious proteins, find medications that would work well to target these proteins, and suggest novel chemical compounds for additional investigation as possible therapeutics.AIandmachinelearning(ML)enabletheq uickdevelopmentofnewmedications as wellasthe repurposing ofold ones. The searchfor new or authorised antiviralmedications thatcouldsuppressSARS-CoV-2wasdoneusingalgorithms.Thisstudyprovidesanove rview of the AI and ML techniques being employed.



Designingnewmolecules&planningsynthesiswith AI

The generating model and the activity prediction model excluded experimentally verified actives, however the model produced structures of which >95% were projected to be active. Although the task of predicting dopamine activity is rather simple, this study showcased the capacityto producemoleculesonitsownandthengainknowledge byevaluatingthemagainst a model for prediction. The most suspicion regarding artificial intelligence

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in medicinal chemistry pertains to the planning of chemical synthesis. This is understandable given that: retrosynthesis is a highly regarded, creative process requiring a great deal of chemical knowledge; and automated rule-based methods for forward reaction prediction lack the chemical intelligence required to provide reliable results and a wide coverage. The development of DNN techniques for synthesis prediction may provide an upgrade [25]. The next crucialstepinunderstandinghowAImaybenefit medicinalchemistryandtoconcentrate AI innovation is the experimentalvalidation of AI on actualdrug development projects, both incompetitionwithandenhancingtraditionalhuman-ledprocedures.Duringthisphase, fundingandresourcesmustbeallocated,especiallytoth equickproductionofchemicalsfound byAIdesign.Althoughthereisanexcellent argument beingmadeforusing AIineveryphase of drug discovery, lead generation is the area we are currently concentrating on. In order to create predictive models, we use our extensive historical collection of pertinent physicochemical, absorption, distribution, metabolism, and excretion (ADME), and in vitro toxicological data. In this phase, the optimisation of molecules is primarily driven by in vitro properties.Combiningthisadvancementinautomated chemicalsynthesisplanningwithothers might potentially reduce the time needed to synthesise target compound clusters from any locationinchemicalspace. ThroughthisparadigmAI explorationcanbepropelledbyenough datatomakefurtherdesigniterationswithhighconfiden ce.Notablerecentadvancementshave been made in automating chemistry [26]. Despite our suggestion that a far larger effort be placed on tackling the difficulties of automating three-to five-step synthesis encompassing significant medicinal chemistry reaction classes, considering the enormous breadth of drug-likeandchemicalsynthesisreactionspace[27].Itisreas onabletobelievethatpeoplewillwish tomaintaincontroloverthecompoundsthatentersynth esis, ascompoundsynthesis isstillthe step that determines the rate at which in vitro properties are optimised. In contrast, Delaney's study implies that existing medicaland agriculturalinitiatives are functioning atthe levelofa self-avoiding stroll, with the exciting prospect that having algorithms in control now may actuallybemoreefficient [28].Perhapswhilewedon'tthinkmanyprojectswould beprepared to give up this much control right now, the research shows that system control of medicinal chemistry may be feasible and perhaps beneficial if automated synthesis can be widely implemented

Artificialintelligenceandstructure-basedmodellingusingQSAR

In the more than 50 years since its start, QSAR/QSPR modelling has advanced significantly [42]. These computer models have had a significant impact on drug development, as demonstrated by their ability to accurately predict biological activity and pharmacokinetic parameters, such as toxicity, distribution, metabolism, and excretion [43,44]. The structural characteristicsofmolecules(suchaspharmacophoredistribution,physicochemicalproperties, and functionalgroups)areoftentranslated into machine-readable numbersusingtheso-called molecular descriptors for ligand-based QSAR/QSPR modelling [45]. Many current concepts, suchasself-organizingmaps,recurrentsystemsforsequenceandtime-seriesanalysis, autoencoders, and deep and adaptive networkdesigns, were invented during the first boomof artificial neural networks in chemoinformatics in the 1990s [46,47]. Deep networks' most significant discoverymayhavecomefromtheir2012victoryinthe MerckMolecular Activity Challenge[48]. Deeplearningtechniquesprovide severalbenefits, albeit there issomedebate about whether the latter kind of models perform better than other strategies (such as gradient boosting machines) [49]. whenthe same collectionofdescriptors is used [50]. Applying deep architecturestomultitasklearning[51,52]presentsano therpotentialbenefit.Multitasklearning seeks to identify a shared internalrepresentation that serves a group ofrelated endpoints; this is not to be confused with multi output learning, which does not specifically utilise related information between the tasks to be learned. Multitask learning may make better use of correlated data in typical situations when a chemical library is not fully evaluated on all endpoints of interest and without the requirement for previous imputation, since drug development is a multiparameter optimisation issue [53]. Aiming to link a collection of predetermined chemical descriptors to observable endpoints, the concept of multi-output QSAR modellinghasbeeninvestigatedpriortotheincreasingu seofdeeplearningtechniques [54,55].

Preclinicaldrug researchwithartificialintelligence

Preclinical research focuses on studies related to toxicity, pharmacokinetics, and non-clinical

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pharmacology. Toxicologicaland pharmacokinetic research depend on a drug's ADMET and physicochemical characteristics [30,31]. The costly drug development phase will fail due to the inappropriate qualities of drug candidates [32]. Assessing the pertinent qualities of medication candidates early on helps reduce the failure rate and loss of clinical trials.

1. Predictionofphysicochemicalproperties:

The success of a medicine entering the market will be greatly influenced by the ADMET qualitiesofadrugcandidate,whichcanbedirectlyinfluencedbyitsphysicochemicalfeatures [33,34]. The aqueous solubility of a molecule is influenced by the ionisation constant (pKa), the fundamental parameter that underlies features like solubility and the octanol–water distribution coefficient(logD).Thismighthaveanimpacton thedrug formulation process.

Furthermore, the charge state of the compounds has a significant impact on the ADMET of compounds at various pH levels [35]. The promising properties of lead compounds, even though they may not always translate into successful drug designs, serve as a source of inspiration for drug design. Nevertheless, because it is difficult to measure the physical propertiesofsmallmoleculesdirectly,accuratepredictionoftheirpropertieshelpsrefinesmall molecules' structural optimisation until the desired properties are achieved. Certain physicochemicalfeatures, suchlipophilicity[36], or watersolubility[37], aretheemphasis of certain methods for predicting the physicochemical properties of molecules, whilst other methodspredictmanyphysicochemicalpropertiessimultaneously[38].Oneofthemodelsused an NLP technique to create embedding vectors based on small molecule SMILES for the second challenge, which involved predicting aqueous solubility. These vectors were then fed into the transformer model to predict molecular water solubility [39].

2.ForecastingfeaturesassociatedtoADMET

The majority of clinical trial failures are frequently attributed to insufficient ADMET drug studies rather than a lack of specific efficacy. The "absorption, distribution, metabolism, excretion(ADME)" portionofADMET frequently establisheswhether a medicationwillfind itswaytothetargetproteininvivoaswellaswhichproteinwillcarryorprocessthemedication [40,41].Intheearlystagesofdrugdiscovery, hundredsofcompoundsareawaitingevaluation for potential ADMET characteristics; it would be costlyand time-consuming to confirmeach onethroughlengthyanimaltrials. Asaresult,therehas beenwidespread adoptionofusing AI to quickly and reliably predict the ADMET characteristics of medications.

Diagnosisofdiseasesusing AI

AI is completely changing how medical professionals recognise, treat, and manage illnesses. Inordertoidentify diseasesintheirearlystages,AIalgorithmscanquicklyexaminehuge databasesofclinicalsymptomsandlaboratorytestfindings.Earlyidentificationenables promptcontainmentandintervention efforts tostop thespreadof thedisease.Thissection focusesonthelatestdevelopmentsinthedetectionofbothcommunicableillnessesmade possiblebyAI.AI-powereddiagnostictoolscanidentifyinfectiouspathogenswithahigh degreeofsensitivityandaccuracy,whichreducesthelikelihoodofmakingthewrongdiagnosis and performing unnecessary medical procedures. This leads to better outcomes for patients.

Pulmonaryhypertension:

Acomplicatedcardiovascularconditioncalledpulmonaryhypertensionistypified byelevated pressure in the pulmonary arteries, which reduces blood flow to the lungs. Early detection of hypertension is essential for early intervention to avoid negative consequences. Chest X-ray photographs of patients with various forms of pulmonary hypertension as well as healthy individualsareusedtotrainthemodel.TheAUROCisestimatedtobe0.945.Theirmodelwas able to achieve an accuracyof86.14% in distinguishing between various forms ofpulmonary hypertension.

Alzheimer’sdisease:

Alzheimer's disease (AD) is a type of brain neurodegenerative illness. The difficulty in diagnosing AD is one reason whythere isn't a simple, affordable screening technique for the disease. The diagnosis of AD frequently depends on invasive testing that are usually only performed in specific clinical situations. Early AD detection was made easier by a technological advancement in imaging, specifically fluorine-18-fluorodeoxyglucose positron emission tomography(PET) ofthe brain. The AI model created for this work is referred to as "end-to-end" as it includes every step of the procedure,

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beginning with the analysis of unprocessed speech recordings and ending with AD predictions. Because the AI system handles feature extraction and pre-processing inside a single framework, this method does away with the need for separate human stages.

Cancer:

The primary procedures for cancer diagnosis are those using clinical imaging. A online tool called "AI Dermatologist" uses deep learning to identify skin cancer from photos. The user's uploadedphotographcanbeusedbytheprogrammetodiagnoseskincancer.Evenonthebasis ofasymmetry,boundaries,colour,diameter,andchangesovertime,itmaydistinguishbetween benignandmalignanttumours.TheAIdermatologist'ssensitivityinidentifyingmalignantcells frombodyscans was 87%. Usually, microscopic analyses of the tissues are used to make the first diagnosis of skin cancer. In order to identify the optimal model architectures for decipheringvariouspatternsandcharacteristicsfromradiologicalpictures,thetoolis continuously being developed. The development of Next Generation Sequencing (NGS) technology has produced extensive information on individual genomes and allowed for the collecting of enormous volumes of data. It might take a few days or weeks. Deep learning modelsandotherAI-basedmodelshaveopenedanewareaofstudyintoturningthis"bigdata" into fresh and relevant knowledge. Numerous aspects of genomic analysis, including gene annotation, genotype-phenotype correlations, consanguinity disorders, mutation studies, cancer detection, biomarker discovery, gene function prediction, and variant calling, have benefited from the application of AI technology.

Artificial intelligence (AI) is a fascinating and promisiield of study that has the potential to revolutionisethedrugdevelopment process. This isduetothe increased interest and attention from researchers, pharmaceutical firms, and regulatory agencies, as well as the potential advantages of AI.

Futuredirectionsand challenges:

A number of massive compound data sources have been created as a result of the rapid emergenceofquickerandmoreaffordabletechnologyandadvancesinprocessingpower.This requiredtheapplicationofmanyAIandmachinelearningtechniquesatdifferentphasesofthe drugdiscoveryprocessinordertoextractmedicinalknowledgefrommassiveamountsof"big" data. Designing and finding novel compounds, as well as further optimising them, has been spurred bythe insights gained fromusing these AI algorithms in big data. Byautomating and personalising the procedure and confirming the importance of big data, this method has advanced the drug discovery process. Along with a boom in startups and AI-based research and development firms, artificial intelligence is having an increasing impact onthe academic andpharmaceuticalsectors.Inordertofindpreclinicalcandidates, anAI-basedcomputational pipeline can screen virtual chemical libraries more quickly than the conventional high throughput screening methods. In addition to drug screening, artificial intelligence (AI) techniques are used in a variety of phases of the drug discovery cycle, including patient recruitment and surveillance, physical property prediction, bioactivity, toxicity ofthe compounds, ADME characteristics, and protein structure prediction. Aside from the diverse uses of AI-based technology, there are still certain obstacles and restrictions that must be addressed. The success of artificial intelligence (AI) technologies depends on how easilyand frequently people can access data. Better data curation and administration, as well as user-friendlyonlineportals,arenecessarytomeetthevarious "V"aspectsofbigdata,whichinclude volume, velocity, variety, and volatility. To extract meaningful information, trustworthy and well-curated data is therefore necessary. The absence of sufficient curated data and data accessibility can prove to be a barrier, despite the fact that AI technology is gradually revolutionisingthedrugdevelopment processthroughquickerdrugdesignmethodologiesand lower failure rates. Additional stages in rate limiting include the challenge of quickly and continuouslyupdatingthesoftwarethatisnowaccessibleinaccordancewiththeformatofthe generated data and the most recent algorithm. Furthermore, it is difficult to find qualified workersforthefull-fledgedoperationofAI-baseddrugdiscoverysystems. Certainfeaturesof machine learning techniques, such predicting conformational changes in proteins and the binding affinity between medicinal molecules and targets, continue to be thoroughly investigateddespitetheirwidespreaduseandadvancements.Deeplearningisonlyconstrained by the quantity and quality of the data since it needs vast amounts of data. Therefore, a more effective strategy for resolving this issue may be the quick transfer of learning technology development. Even

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if these cutting-edge methods demonstrated excellent performance and prediction accuracy, deep learning is still a "black box" method whose exact mechanism of problem-solving is still unknown. Furthermore, even though artificial intelligence (AI) technologies and massive data sources have greatly accelerated the medication discovery process, trials must still be completed before the treatments are authorised. Notwithstanding thesedrawbacks,artificialintelligence(AI)hasrevolutionisedthefieldofdrugdiscovery,and given its growing popularity, it will probably soon establish itself as a vital instrument in the pharmaceutical industry's quest for new medications and their targets [56].

II. RESULT& DISCUSSION

Predicting the toxicity and efficacy of possible therapeutic molecules is one of the main uses of AI in medicinalchemistry. Conventionaldrug development methods frequentlydepend on labor-intensiveandtime-consumingexperimentstoevaluateacompound's possibleeffectson the human body. AI is used in drug discovery to optimise leads, identify targets, and plan clinical trials. It contributes to more effective and efficient drug discovery by accelerating overall drug development, identifying prospective therapeutic targets, and predicting drug attributesthroughtheanalysisofenormousdatasets. AI canbeusedto anticipateprotein-drug interactions, virtually screen and optimise molecules, and evaluate their bioactivities. AI can assistinvirtualscreeningbycreatingpredictivemodelsthatcanrecognisesubstancesthathave ahighlikelihoodofattachingtoatargetprotein.Predicting thetoxicityandefficacyofpossible therapeutic molecules is one of the main uses of AI in medicinal chemistry. Traditional drug development methods frequentlydepend on labor-intensive and time-consuming experiments to evaluate a compound's possible effects onthe human body. Artificial intelligence (AI) has become ubiquitous in manyfields, suchasresearchand the pharmaceuticalbusiness, where it hasbeeneffectivelyappliedtofindnovelchemicalentitieswithdesiredfeatures.AIalgorithms' application to drug research offers both incredible prospects and difficulties. The Artificial Intelligence for Structure-Based Drug Discovery programme facilitates knowledge sharing between scientists in the industrywho want to use machine learning techniques that leverage molecular structure to produce better drugs and researchers at Stanford University who are developing novel machine learning methods.

These data are utilised for the system's subsequent training, the availability of a significant volume ofdatais essentialto AI's overalleffectiveness. Abusiness may have to paymore for access to datafrommanydatabase providers, and for accurateresult prediction, the datamust also be dependable and of good quality. The lack of trained personnel to run AI-based platforms,smallbusinesses'limitedfunding,concerns aboutAIreplacinghumansandcreating job losses, scepticism about the data generated by AI, and the "black box" phenomenon (i.e., theconclusionsdrawnbythe AIplatform)areadditionalobstaclespreventingthe full-fledged adoption of AI in the pharmaceutical industry. But, considering that AI is already replacing monotonous tasks and freeing up human intelligence to be employed in the development of more complex insights and creative endeavours, the worry of unemployment may be unfounded. Pharmaceutical companies want clarity on the ability of AI technology to solve issues when it is put into practice as well as knowledge of the realistic objectives that can be met. The full potential of the AI platform may be utilised by highly qualified data scientists, software developers with a solid understanding of AI technology, and a clear grasp of the business aim and R&D goal of the enterprise.

The development of AI and its amazing tools continuously tries to lessen the difficulties experiencedbypharmaceuticalfirms,whichhasanimpactonboththemedicationdevelopment processandtheproduct'sentirelifetime.Thiscouldaccountfortheriseinthenumberofstart- ups in this industry. The rising cost of medications and treatments is only one of the many complicated issues the healthcare industry is currently facing. As a result, society needs to makesomeverybigadjustmentsinthisarea.ArtificialIntelligence(AI)canbeusedin pharmaceutical manufacturing to create customised drugs with the right dose, release parameters, and other necessary elements based on each patient's needs. The rising cost of medicationsandtreatmentsisonlyoneofthemanycomplicated issuesthehealthcareindustry is currently facing. As a result, society needs to make some very big adjustments in this area. ArtificialIntelligence (AI) canbe used inpharmaceutical manufacturing to create customised drugs with the right dose, release

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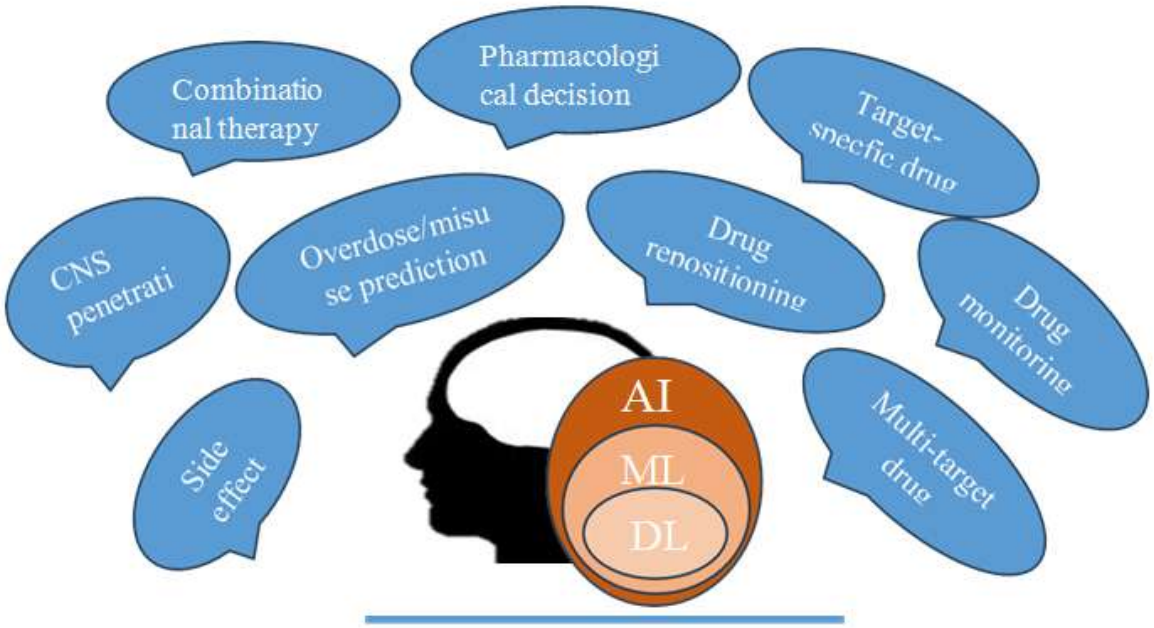
parameters, and other necessary elements based on each patient's needs. The primary concern surrounding the integration of these technologies is the potentiallossofjobsandthestringent lawsrequiredto integrateartificialintelligence. Butthe goalofthesetechnologies isn'tto fullyreplacepeople;rather,they're just meantto maketasks easier. Artificial Intelligence (AI) has the potential to facilitate the identification of hit compounds quickly and easily. It can also suggest synthesis pathways for these molecules, forecast thenecessarychemicalstructure,and provide insightsondrug-target interactionsand their SAR. AI can also significantly aid in the optimisation and continued integration of the developed medication in the appropriate dosage form. Furthermore, AI can facilitate prompt decision-making, which can expedite the production of higher-quality products and ensure batch-to-batch consistency. By conducting thorough market research and prediction, AI can also help determine the product's safety and effectiveness in clinical trials and guarantee appropriate pricing and positioning inthe marketplace. While there aren't anymedicationson the market right now that were created using AI-based techniques, and there are still some obstaclestoovercomebeforethistechnologyiswidelyused,itisexpectedthatAI in the near future turn into a priceless instrument in the pharmaceutical sector.



III. CONCLUSION

Thepharmaceuticalindustryhasexperienced enormousprogressinanumberofcriticalsectors sincetheintroductionofartificialintelligence.Artificia lintelligenceplaysakeyroleinfinding viable therapies for life-threatening and chronic illnesses including diabetes, Parkinson's disease, Alzheimer's, OCD, and others that were previously difficult to treat with current methods. AnAI-basedstrategyisalso particularlyhelpfulin COVID-19epidemic, where it is essentialto findanddevelopdrugsmorequickly.Inthenear future,almost allpharmaceutical businesses will surely work with an AI-based company, which will drive the pharmaceutical sector to unprecedented heights. We believe that interpretable AI tools and active learning algorithms will play a major role in the next ten years of AI-based drug development. These tools will gradually improve workflow and generate interpretable concepts that scientists can track, assess, and understand throughout the entire drug development process. Empirical implementations of AI/ML demonstration are essential for revolutionising the drug research and development process pipeline and enhancing human decision-making capabilities. Deep learning in AI has been widely used to speed up the identification of important drugs using Computer-Aided Drug identification (CADD) techniques. I've quickly reviewed the most currentresearchfindingsinthefieldofartificialintellige nce'sapplicationtothedrugdiscovery and development process in this mini-review. The availability of high-quality data, the resolution of

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ethical issues, and the understanding of the limits of AI-based methods are all necessaryfortheeffectiveapplicationofAIindrugdiscovery.Promising approaches for getting beyond the difficulties and restrictions of AI in drug discovery include the use of explainable AI, data augmentation, and integration with conventional experimental techniques.

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