Artificial Intelligence Enabled Early Drug Discovery and Pre-Clinical Testing: A Paradigm Shift Towards Automation

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Abstract: Artificial intelligence (AI) is rapidly transforming the process of drug discovery and development and supporting all the stages involved in bringing a potential drug to the market. Currently, more than 30 drug molecules developed by using AI are in various stages of drug development. Artificial intelligence usage has an important part in reducing the time and costs associated with bringing new drugs to market. This article highlights the latest AI advancements and patents in the field of drug discovery and the preclinical stage of drug development. However, there are many ethical concerns which are associated with the use of AI in multiple stages of drug development, and they must be addressed.

Keywords: artificial intelligence (AI), early drug discovery, drug screening, machine learning (ML), preclinical drug development, and animal testing

1 Introduction

Each year, regulatory health authorities approve multiple drugs for human use. Fifty new drugs were permitted for human consumption by the US Food and Drug Administration (US FDA) in 2024 [1], and the European Medicines Agency (EMA) recommended 114 medicines for marketing authorisation [2].

From the process of screening to market a new drug, it takes approximately 14.6 years [3] and costs an average of US$2.6 billion [3, 4]. The various stages in the drug development process include early drug discovery, animal or pre-clinical testing, clinical trials [5], regulatory drug reviews and approvals, and post-marketing surveillance [5]. The overall rate of success in the multi-stage drug development process is 10%–15% [6, 7, 8, 9,10].

The overall reasons for the high drug failure rate include poor physical and chemical properties, high toxicity, and insufficient efficacy [10, 11, 12]. A 2021 study by Chahal [13] highlighted that the majority of drug development applications rejected by regulatory health authorities were due to deficiencies in scientific content [13]. Furthermore, only 8% of new compounds entering clinical trials secure regulatory approvals [14]. By using AI-assisted methods, these challenges can be overcome.

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As per the McKinsey report [15], the use of AI in various ways can fast-track the process of screening to market a new drug. This is primarily due to its ability to increase productivity through expediting the identification of compounds that could potentially lead to novel drugs, a fast-track process of development, and regulatory approvals. Unquantifiable benefits to human health and well-being are anticipated from the upcoming generative (Gen) AI-driven life science revolution [15]. The creation of a drug using AI technology is a groundbreaking achievement for the pharmaceutical industry. The first medication (INS018-055), created by using AI, entered Phase 2 clinical trials in 2023 [16, 17] for idiopathic pulmonary fibrosis [16, 17]. Currently, more than 30 drug molecules are being developed using methods involving AI.

This article highlights the latest developments, including patented AI tools in drug discovery and preclinical testing.

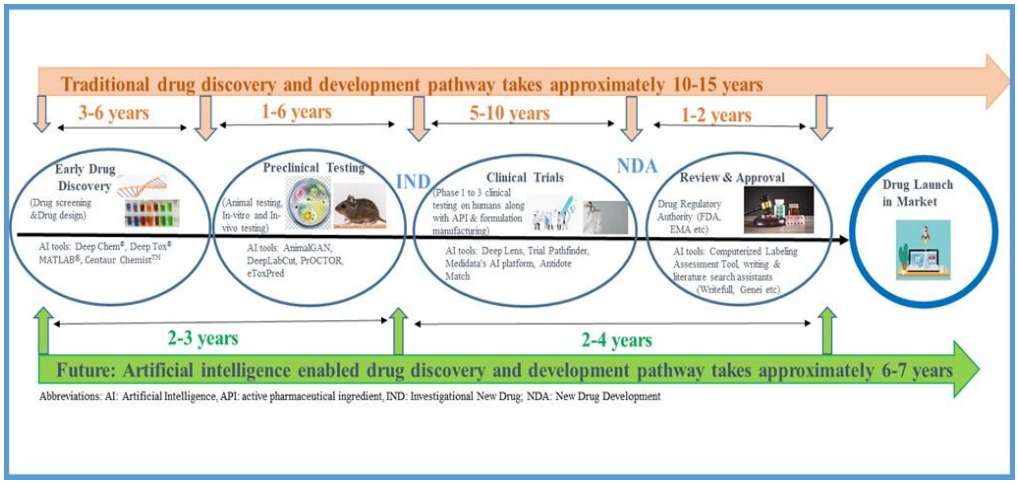


Fig 1: Drug Discovery and Development Timeline

2 Early Drug Discovery

The process of drug discovery starts with drug screening, which involves a search for therapeutic targets [20], typically proteins, linked with a specific disease state [18, 19, 20]. This process varies based on the molecular mechanisms and the type of drug being developed [18, 19, 20]. Initially, a million compounds are screened, and hundreds are evaluated for lead identification and optimization [19], ultimately yielding one or two promising molecules [6]. However, only 10% of small molecules in industry progress to become potential drug candidates, often failing for various reasons [6]. The reasons for failure in the early drug discovery process include, but are not limited to, unpredictable assays, multiple failures during high-throughput screening (HTS) [7], undesirable behaviour and side effects of compounds in various pharmacological assays, production of toxic compounds, and unattractive pharmacokinetic (PK) or pharmacodynamic (PD) profiles [6, 7].

The use of AI can speed up the initial drug development process by the provision of more accurate and effective results of massive data [21, 66]. As per the McKinsey report [15], the potential effect of Gen AI tools on research and early discovery of drugs is expected to be more than thirty percent higher than manual drug evaluation [15]. This includes:

- A greater than 2-fold increment in the activities of models of chemical compounds [15]

- A four-fold faster identification of new leads [15]

- A three-fold acceleration in large-molecule design [15]

Artificial intelligence can find lead molecules [22] and their PK and PD parameters, thereby saving time, resources, and costs [23, 24]. Additionally, AI can identify drug-drug interactions between novel drug pairs [24, 25].

Table 1 provides various AI organization's software tools and platforms employed in early drug delivery [23, 26]. Some examples of recent patent applications in early discovery of drugs are presented in Table 2.

Table 1: Artificial Intelligence Tools Applications in Early Drug Discovery

S.No	AI organisations/ AI Software and Program	Functionalities	Applications
1.	COMSOL Multiphysics® simulation software [27]	Various processes and devices used in pharmaceuticals can be modelled by COMSOL [27, 28]	Drug release from a biomatrix (identification of composition, geometry, affinity, and degradation). Rate constants of the DNA degradation process reactions using chemical modelling. Develop dose-planning methods [27, 28]
2.	SCHRODINGER Suite (LiveDesign for material science) [29]	Provides a computational platform for molecular design and discovery [29]	Instantly calculate physicochemical properties for thousands of compounds [29]
3.	DeepChem [30]	A library for drug discovery [3] and computational chemistry [3, 30]	DeepChem for machine learning in healthcare, and from different data modification and creation techniques to molecular fingerprints [30]
4.	GROMACS [31, 32]	A molecular simulation package [31, 32]	Designed for simulations of various macromolecules. It enables fast calculations that could be performed for various interactions [31, 32]
5.	MATLAB® and SimBiology® [33]	Biological data analysis tools [33]	Model simulations for humans based on data from preclinical studies. Helps in making predictions on the *in vivo* behaviour of potential drug candidates [33]
6.	IBM Watson's AI platform [34]	Pfizer collaborated with	Help find new drug targets, new antimicrobial peptides, new polymers,

S.No	AI organisations/ AI Software and Program	Functionalities	Applications
		IBM Watson for the use of machine learning (ML), natural language processing (NLP), and cognitive reasoning technology in immuno-oncology [34]	combination therapies, and patient selection strategies [34]
7.	BioXcelerate AI's PleioGraph [35]	PleioGraph leverages ML algorithms to analyse biological data [35]	Help drug developers assess the various interactions between genes and proteins. This helps to identify the cells that lead to various diseases [35]
8.	Drug design platform by NUMERATE [36]	Transforming the design of drugs by utilising algorithms and cloud computing methods [36]	Help in the generation of new small molecule leads that can target various diseases [36]
9.	Centaur Chemist™ [37]	AI-based drug discovery platform [37]	Help optimise and speed up novel lead structures of potential drug candidates for cardiovascular and oncological diseases [37]
10.	TorchDrug [38, 39]	A pyTorch-based flexible structure [3] for drug discovery models [3, 38, 39]	Help in the prediction of various properties, design, molecular representations, and retrosynthesis of drug molecules [38, 39]

Table 2: Patented/Filed Applications Using AI in Early Drug Discovery

S.No	Applicant	Patent/Application No.	Patent	Potential Applicability
1.	Preferred Networks Inc	US20200387831A1 [40]	Help in predicting how drug candidates will interact with other targets than the selected target [40]	Virtual screening of chemical compounds [40]
2.	Spring Discovery Inc	US10886008B2 [41]	It utilises ML algorithms to predict the biological age of samples for drug discovery [41]	Identification of an anti-ageing agent in

S.No	Applicant	Patent/Application No.	Patent	Potential Applicability
				drug discovery [41]
3.	RO5 Inc	US20230325687 [42, 43]	This system uses ML algorithms and comprises neural networks trained to reconstruct known ligand-receptor pairs, such that novel and unique molecules are discovered [42, 43]	Prediction of ligand-receptor binding poses and their affinity [42, 43]
4.	Spring Discovery Inc	US20240079085 [44]	A machine-learning model to determine one or more phenotypes of a cell. It is based on high-feature-density biological images of the cells [44]	Identification of compounds corresponding to the identified phenotype [44]
5.	ViQi Inc	US20240029403 [45]	A machine learning based model brings automated high content screening (HCS) to the drug development process, with the ability to detect changes in single cells and differentiate from other types of cellular changes [45]	Automated HCS of drug compounds can dramatically alter the time and effort currently required for HCS of drug compounds [45]

3 Pre-clinical Testing

Preclinical testing is a vital stage in the process of developing drugs [46, 47] that involves initial laboratory screening and animal studies to evaluate the efficacy and safety of potential drugs [47]. The aim of animal testing is to predict treatment outcomes in humans and identify potential toxicities associated with a drug [47, 48]. However, preclinical testing is often plagued by failures, which can be attributed to various reasons, including:

1) mislabeling a potentially useful therapeutic agent as harmful [49], and 2) mislabeling a harmful drug as "safe" [49]. Issues like failures in animal studies resulting in animal deaths, thus leading to ethical and economic impacts on research [50]. An example is that preclinical toxicity studies may not always forecast lung injuries during clinical testing [51], like Janssen's proprietary compound JNJ-1 and fialuridine [51].

Artificial intelligence can benefit preclinical testing by improving and speeding up the identification of novel molecule-level targets such as genes or proteins [52, 53], with predictive analytics on toxicity, and PK/PD. Artificial intelligence can facilitate the arrangement of compounds for testing, resulting in time and cost savings [54]. From the screening of drugs to

the animal testing stage, AI could be a cost saver, including saving time from >25% to upto approximately 50% [54].

One pharmaceutical company, Insilico Medicine, had completed initial stages up to preclinical in just 30 months [54] for an AI-designed drug candidate (INS018-055) for idiopathic pulmonary fibrosis [54], a serious disease that leads to untreatable lung scarring [54].

Various AI-based tools and emerging technologies in preclinical testing are presented in Table 3 and Table 4, respectively.

Table 3: Artificial Intelligence Tools in the Field of Preclinical Testing

S.No	AI Tools	Functionalities	Applications
1.	eToxPred [55]	Evaluates potential drug candidates by utilising pretrained ML algorithms on molecular fingerprints [55]	Estimation of the toxicity of small organic compounds [55]
2.	TargeTox [56]	Capacity to produce data and integrate into an ML algorithm for the prediction of toxicity [56, 57]	Distinguishes potentially idiosyncratically toxic drugs from safe drugs [56, 57]
3.	PrOCTOR [58]	By considering the chemical properties of both molecule and drug target, it helps in toxicity prediction [58]	It is actively used in predicting the toxicity of anticancer and antidepressants [58]
4.	AnimalGAN [59]	An AI-based suite that involves learning from previous animal data to generate datasets for novel and untested chemicals [59]	Assessment of hepatotoxicity and nephrotoxicity [59]
5.	DeepLabCut [60]	It is an open-source pose estimation toolbox that provides animal tracking features needed for multi-animal scenarios [60]	Widely utilised deep learning platform for animal behavioural analysis [60]

Table 4: Patented/Filed Applications Using AI in Preclinical Testing

S.No	Applicant	Patent/Application No.	Patent	Potential Applicability
1.	Transcell Oncologics Private Ltd	US20230420079 [61]	A real-time platform or human MicroPhysiological Systems (hMPS) unit, and a digital platform with embedded AI to predict safety (pharmacology) risks from phenotypes,	Non-animal AI system called Digital Animal Free Testing (DAFT) System for predicting

S.No	Applicant	Patent/Application No.	Patent	Potential Applicability
			genotypes, and proteotype data sets acquired from test agents treated hMPS platform in a modular assay system [61]	efficacy and safety [61]
2.	Jackson Laboratory	US20230419498 [62]	An encoder-decoder segmentation neural network minimises human intervention by video tracking of animal behaviour using a neural network architecture. It involves minimal training and gives highly precise results [62]	The use of a neural network tracker can be used in various other experimental animals through transfer learning, thus a solution that can be generalised for bio-behavioural research [62]

4 Ethical Concerns

The usage of AI in the drug development process has enormous benefits, but multiple ethical concerns associated with its use needs to be addressed [63, 64]. The common ethical issues [64] include bias, security of sensitive data, privacy, misinformation, hallucinations of data, transparency in algorithms, and several others [64]. A careful consideration of ethical issues taken into account with AI-assisted drug development methods can pave the way towards better research and development of drugs with maximum benefits to patients' lives.

5 Conclusion

The combination of AI in the drug development process [65] is progressively changing the drug development landscape by replacing conventional methods with AI-driven methods of drug development [65]. A higher number of novel drugs are being developed at a fast pace by using AI-assisted methods. The industry's efforts to evaluate the various applications of AI show that it is eager to realise AI's full potential in order to carry out more productive and economical medication development. Regulators have published reflection papers and strategic action plans on AI, but there is still a dearth of precise and comprehensive regulatory guidance, including defining appropriate ethical and legal frameworks on the application of AI in the drug discovery and development process [66].

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Not Applicable

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