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Introduction to Next-Generation Drug Development

Ms. Neha Tyagi[a*], Ishika[b]

[a]M. Pharmacy (Research Scholar), Geeta Institute of Pharmacy, Geeta University, Panipat, India, nehatyagi9306@gmail.com
[b]M.Pharmacy, Institute of Pharmaceutical Sciences, Kurukshetra University, Kurukshetra, Ishikaantil63@gmai.com

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A B S T R A C T

The process of finding new drugs is intricate and multidimensional, propelled by scientific advancements and cutting-edge technologies. In the fifteen years after Smith and O'Donnell, the Method of New Drug Development and Discovery . Second Edition (2005), the fields of drug discovery and development have seen tremendous changes. Developments within comprehension of biology in humans and illness have discovered new territory for substances to aim for, and this development of Knowledge has been quickened by the creation of innovative research instruments. Additionally, new platforms to effectively sort.Advances in understanding of human biology and disease have uncovered fresh territory for drugs to target, and this progression of knowledge has been accelerated by the invention of new investigational tools. Further, new platforms to efficiently sift through the drug candidates have made it easier to find that needle in the haystack, the drug that will treat a disease safely and effectively. What's more, the processes of drug discovery and drug development, once separated in independent silos of sorts, have become increasingly integrated. No longer is the drug candidate handed off from drug inventor to drug developer like runners in a track relay meet. These changes in the drug discovery and development processes have reverberated throughout the biotech world, significantly impacting the scientific methodology employed for drug discovery initiatives as well as the institutional platforms underlying biomedical research.

I. Introduction

The process of finding a chemically therapeutic medication to treat and manage a condition is known as drug discovery. In order to create a medication to prevent or mitigate the effects of a sickness, researchers typically find novel medications by obtaining new insights into the illness process. Finding possible medications, synthesizing them, characterizing them, screening them, and evaluating their therapeutic efficacy are all steps in the drug development process. A chemical will move on to medication development after clinical trials if it shows promising results in these studies. The significant resources needed for both clinical trials and research and development make drug discovery and development expensive. From the time a novel medicinal molecule is discovered until it is commercially available for patient therapy, it usually takes 13 to 15 years. Research & development costs for each successful medication are estimated to be between $800 million and $1.5 billion. This figure includes the costs spent as a result of many failures. Only one of the 4,000–10,500 compounds that undergo research and development is approved. The intricacy of the research and development process accounts for the failure of numerous compounds and the length of time required to deliver a single medication to patients. A wealth of resources, the best logical and scientific minds, cutting-edge lab equipment, and thorough project management are all necessary for success. Good fortune and perseverance are also necessary. In the end, the process of finding new drugs . For billions of patients, there is still hope, faith, and relief [1,2].

Different phases in the development of drugs

1. Identification of drug targets.
2. Validation of targets.
3. Lead optimization and lead compound identification.
4. Characterization of the product
5. Development and formulation.
6. Preclinical investigations.
7. The new drug application under investigation.
8. Research studies.
9. Drug marketing and approval

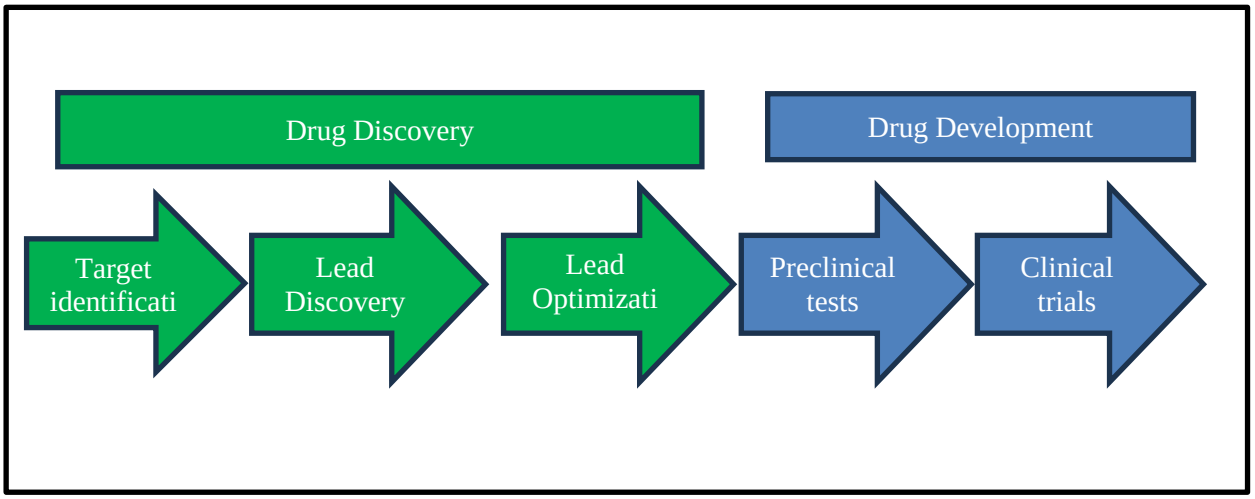


Fig 1: The drug development process.

Identification of the target : The initial stage of the drug development process is target identification. It can be characterised as both the disease's phenotype and the potential cause of a certain condition. The naturally occurring cellular or molecular structure implicated in the disease's pathophysiology could be this target [4].

Methods for identifying targets [5].

1. Bioinformatics based on data mining.
2. Genetic correlation.
3. Profile of expression.
4. Phenotypic and pathway analysis.
5. Screening for functions.

Validation of the target: Another stage in the drug discovery process is target validation. Since there isn't a clinical trial option at this point, we go through a validation process. In order to go through the validation procedure, the target must be obtained from target discovery. There are two main processes to target validation. The first is to conduct the experiment to confirm the reproducibility by employing several methods, such as research on current medications, biochemical expression cloning, affinity chromatography, microarray DNA, and suppression. Additionally, the second step requires us to chemically introduce the variant to the ligand target environment, genomics using chemical methods against the protein-encoding genome [6].

Lead chemical identification and lead optimisation : We must identify the lead molecule that exhibits drug-like properties in the lead identification process. In contrast, lead optimisation requires that the lead compound be optimised in relation to the target receptor in order for it to proceed to the drug development stage [6].

Characterisation of the product : If the medication molecule exhibits the highest level of therapeutic efficacy during product characterisation, then It needs to be described in terms of the size, shape, strength, weakness, toxicity, and biological activity. Pharmacokinetic and pharmacodynamic research in its early phases is beneficial to describe the medicinal compound's mode of action [7].

Formulation and development: At this point, the physiochemical characteristics of active Pharmaceutical chemicals are chosen to create a stable and ideal dose form for a given delivery method.

Preclinical research: Preclinical research primarily consists of in vitro, in vivo, and animal population trials. These studies provide information on dosage and toxicity levels. Researchers evaluate the results of the pre-clinical trials and determine whether the medication may be tested on humans [8].

This pre-clinical research involves a variety of experiment types, like as :

1. studies on single-dose toxicity.
2. Dose studies that are repeated.
3. Research on safety pharmacology.
4. Research on genotoxicity.
5. Research on carcinogenicity

Pre-clinical trials involve a number of steps, including :

1. The medication target must be determined.
2. Create a bioassay.

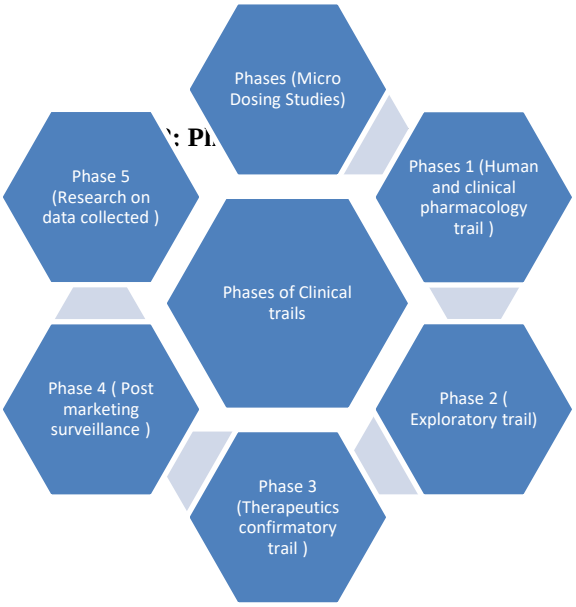
3. The medicine must be screened using the assay method.
4. We must determine dangerous and effective dosages.
5. Lastly, we must submit an application for an investigational new drug (IND) approval [9].

The Procedure for Investigational New Drugs (IND)

An application to begin human clinical trials is submitted to the FDA. If pre-clinical research revealed the medication to be both safe and effective. The FDA will receive the IND application from a sponsor [9]. Additionally, the FDA will have a pre-IND meeting to go over a number of topics, including

1. The pre-clinical trial design.
2. The clinical trial's planned protocol.
3. The investigational drug's composition, production, and management.
4. Clinical experiments
5. Clinical investigations

Clinical trials : Clinical trials are the systematic investigation of a novel medication or an experimental drug in healthy human volunteers to produce data to assess a new medicine's safety, effectiveness, and toxicity in order to identify a novel chemical. Phase 0, Phase 1, Phase 2, Phase 3, Phase 4 and Phase 5 are some of the classifications for clinical trials as illustrated in Figure 3, and each of these clinical phases will be covered in the sections that follow [10, 11].



The effectiveness of the phases table

Table 1: Clinical Trial Phases [13]

Stages	The main objective	Dosage	Patient observation	The quantity of participants	Remarks
Preclinical	Information on pharmacokinetics, toxicity, and non-human efficacy	Unlimited	Investigator	Animals in vivo and in vitro	….
Phase 0	Pharmacokinetic and Pharmacodynamic	tiny sub-therapeutic	Clinical investigator	10 individuals	Often skip from this phase
Phase I	Drug testing for dosage range on healthy volunteers	Frequently subtherapeutic but with increasing dosage	Clinical investigator	20–100 individuals	establishes whether the medication is effective and safe.
Phase II	Medication testing on patients to evaluate safety and effectiveness	Dosage for treatment	Clinical investigator	100–300 individuals	evaluates the medication's potential for effectiveness
Phase III	Drug testing on	Dosage for	Personal	A thousand to	determines the

	patients to evaluate safety and effectiveness	treatment	physician and clinical researcher	two thousand people	medication's therapeutic effect
Phase IV	Post-marketing surveillance: observing drug use in public	Dosage for treatment	Personal doctor	Anyone seeking medical attention from their doctor	Observe the long-term consequences of drugs
Phase V	Translational studies	Absence of dosage	Not a single	Every report was utilised.	Date-collected research

Drug development in antiquity :

According to certain research, Palaeolithic people were aware of the use of poisonous bitter herbs or psychoactive plants for self-medication [14]. The human race settled from nomadic life about 10,000 years ago and began cultivating plants for food, initiating the agricultural evolution that led to both infectious disease plagues and civilisation [15,16]. Since there was no medical system in the past, the main source of medicine for the Plants, which were generally found by accident, were used to treat illnesses. A few of the "drugs" found to have no therapeutic value, like tea and alcohol, while some are dangerous and addictive, like opium and cannabis [17]. Cultures and religions had a significant influence on the practices of using plants as medicines, which were passed down or inscribed on caves [18, 19].

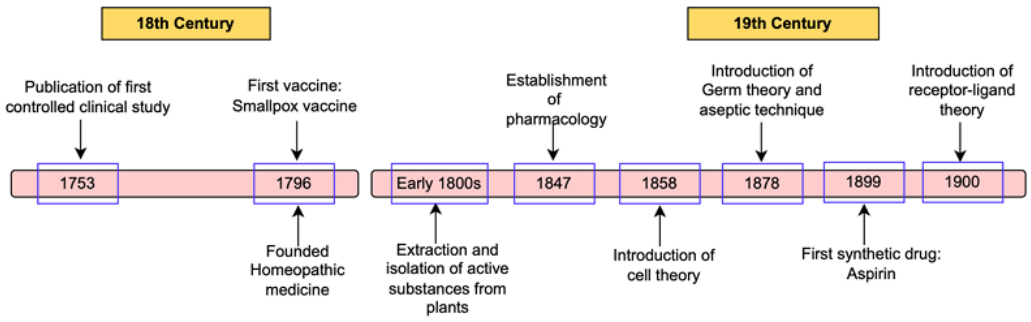
18th-century drug discovery

Clinical trials and preventative medicine were first used in the 18th century when James Lind presented his research on scurvy prevention using his first controlled clinical investigation in 1753 that established the idea of scientific drug efficacy assessment [16,17]. The first vaccination was created in 1796 when English doctor Edward Jenner used cowpox to vaccinate individuals to prevent smallpox, which ultimately resulted in the eradication of vaccinate individuals to prevent smallpox, which ultimately resulted in the disease's elimination in 1979 [17]. Samuel Hahnemann established homoeopathic medicine that same year [17].

19th-century drug discovery

The development of chemistry in the 19th century made it possible to separate and isolate active Herbal plant compounds are advancing small molecule medicine development figure 4.

Highlights of drug discovery research from the 18th century to the 19th century.



Important medicinal ingredients like morphine, atropine, quinine, and alkaloids were first identified and harvested from the plants in the early 19th century [17]. The best medication for severe pain is still morphine. Meanwhile, the advancement of synthetic chemistry resulted in the creation of aspirin, the popular medication made from The plant's salicylic acid is still one of the most popular medications in the world. In 1899, aspirin was introduced to the market as an analgesic, and it was successful in reducing pain and reduction of inflammation. Aspirin's antiplatelet action led to its repurposing in 1982 aspirin's roles in cardiovascular disease and other conditions are still being investigated [20,17]. The 19th century also saw advancements in biomedicine. In 1847, Rudolf Buchheim established a brand-new field called pharmacology, to comprehend organism physiology and apply it to medicine [16]. Rudolf Virchow, a German pathologist, developed cell theory eleven years after the field of pharmacology was established, strengthening our understanding of biology, cell pathology, and medicine [21,16].

Chemist Loius Pasteur made the discoveries of stereochemistry and isomers in He put up the germ theory in 1878, which was crucial to the creation of sterilisation and vaccination, often known as aseptic procedure in medicine [22]. Paul Ehrlich's introduction of receptor-

ligand theory, which accelerated the development of chemotherapy, was another significant accomplishment of the late 19th century [23]. Additionally, this sparked interest in target-directed drug discovery and the ligand-receptor strategy, which are still used today.

Since the 20th century, drug discovery

Separation of medicinal compounds from non-plant sources The production of drugs that were not derived from plants began. Heparin extracted from dog livers and insulin extracted from dog pancreas were utilised to treat severe diabetes and blood clots, respectively, around the beginning of the 20th century. While streptomycin and tetracyclines were extracted from soil bacteria, antibiotics like penicillin, ciclosporin, and tacrolimus were isolated from the fungus [24].

Alexander Fleming's 1928 discovery of penicillin, the first antibacterial medication, has saved many lives. Subsequently, the successful deciphering of the structure of penicillin yielded numerous other antibiotics that are related to structure, like ampicillin. One of the most widely used antibiotics in use today is penicillin [17, 18, 25]. Acetanilide was found to be able to reduce fever in the 1880s, however it was also discovered to be hematotoxic. Phenacetin was synthesised after acetanilide was discovered in 1913 and was employed in the early decades of the 20th century as an antipyretic [26]. When phenacetin's metabolites were examined about 1948, it was discovered that they produced poisonous anilide. However, it was discovered that one of its metabolites was a reactive substance named like paracetamol or acetaminophen, which was introduced in 1953 and quickly became a popular antipyretic [26, 17]. Even now, one of the most used medications is paracetamol [17]. The first successful human-to-human blood transfusion during surgery in 1906 marked the beginning of cell therapy. The first bone marrow transplant to treat aplastic anaemia was carried out in 1939, which also marked the beginning of research on bone transplant therapy [27].

Another achievement of cell therapy was the first bone transplant between an unrelated donor and recipient after several decades of work [27]. The first stem cell was created in 1981 using murine embryos, and the effectiveness of stem cells in cell therapy has been thoroughly researched up to this point [28].

Drug discovery through computation :

Prior to the 1950s, drug compounds were found by randomly screening a several manufactured or natural substances. Together with the development of chemical synthesis and the idea of how drugs work, In the 1950s, rational drug design began to be used in drug discovery studies [29]. Around the 1960s, the quantitative structure-activity relationship (QSAR) was introduced [30, 31].

In the meantime, drug discovery in medicinal chemistry is still advancing. Early in the 1980s, the article "The Next Industrial Revolution: Computational aided drug design (CADD) researchers were intrigued by the article "Designing Drugs by Computer at Merck" in Fortune magazine [32]. Large libraries of tiny compounds may be produced for high-throughput screening thanks to combinatorial chemistry, which was originally developed in the 1990s [32]. Many of the chemicals in the screening libraries were not found to be promising medications, however combinatorial libraries are more useful when a small library concentrates on certain scaffolds and the combination of hit-to-lead optimisation techniques in drug development [32].

A few medications had been successfully approved by CADD, including captopril for Saquinavir for HIV (1995), ritonavir, dorzolamide for glaucoma (1995), and hypertension (1981) and Aliskiren for hypertension (2007), zanamivir for influenza (1999), and indinavir for HIV (1996) [33–35].

Limitations/ Restrictions of conventional drug development methods:

Fig : 3 Limitations/ Restrictions of conventional drug development methods:

Role of AI in drug development:

Artificial Intelligence (AI) refers to computer-based systems that imitate human intelligence such as learning, reasoning, and decision-making. In recent years, Al has shown remarkable progress in many areas, especially in drug discovery and drug delivery [36-38]. The use of Al in these fields helps in faster drug development, better prediction of drug behavior, and the design of more effective and safer medicines. In drug delivery, Al has become very important because it helps improve how drugs are transported to the target site in the body. Traditional methods are slow, costly, and complex, whereas Al can analyze large datasets quickly and suggest optimized solutions [39].

Evolution of Al in Drug Discovery

The use of Al in drug discovery started in the 1960s with the development of the DENDRAL program at Stanford University [40,41].AI has since been applied throughout different stages of drug discovery, covering target identification, lead optimization and drug discovery [41,42]. Initially, Al was used to predict pharmacological properties of compounds. With technological advancement, Al is now used in target identification, lead optimization, protein structure prediction, and drug design [43]. Tools like MolAICal help design drugs that can specifically target proteins in the body.

Role of Al in the Pharmaceutical Industry

Al plays an important role in solving various challenges in the pharmaceutical industry:

Al analyzes large biological datasets to identify disease-related targets. It predicts interactions between drug candidates and biological targets [44,45]. Machine learning helps in predicting pharmacokinetics and toxicity, reducing animal testing. Al supports personalized medicine by analyzing real-world patient data. Tools like IBM Watson help in faster diagnosis and efficient data analysis, enhance medical care and reducing cost [46]. AI improves pharmaceutical manufacturing and supports personalized drug production. Despite these advantages, challenges such as data privacy, ethical issues, and regulatory guidelines must be addressed.

1.6 Scope of Drug Delivery Systems

- Localized drug delivery
- Better patient compliance
- Overcoming biological barriers
- Personalized and responsive delivery systems
- Targeted drug delivery
- Controlled and sustained drug release
- Improved bioavailability Reduced toxicity and side effects
- Improved drug stability [47]

2.1 Role of Al in Formulation and Design

Earlier, formulation scientists mainly used statistical tools like response surface methodology. These methods often fail when formulations become complex. Modern Al techniques such as neural networks and genetic algorithms solve these issues by handling complex data and learning patterns. The practical applications of artificial intelligence in pharmaceutical manufacturing, including drug research and development (R&D), drug repurposing enhancement of pharmaceutical productivity, and clinical trails. These application minimize the requirement for human labor and significantly accelerate the drug development process [48]. Al supports almost

every stage of the pharmaceutical product life cycle including drug discovery, formulation development, quality testing, marketing, and post-marketing surveillance. Al reduces human effort, saves time, and improves accuracy, efficacy [49].

2.2 Machine Learning for Excipient and Dosage Form Prediction

Machine Learning (ML) is a major part of Al. One important ML technique is Artificial Neural Networks (ANNs), which mimic the working of the human brain. ANNs consist of neurons arranged in layers. They take input data, process it, and produce output [50].

Learning types:

Supervised Learning (SL): Uses known input-output data and is widely used in formulation development. SL, the network is trained using guidance provided during the learning process ,where it is supplied with corresponding input – output data pairs. SL is considered the very most popular and valuable network for formulation purposes [50,51].

Unsupervised Learning: Finds patterns in data without predefined outputs. Supervised learning is most useful for predicting excipients and dosage forms [51].

Al in Pre formulation Research

Pre formulation studies involve understanding a drug's physicochemical properties such as solubility, stability, and compatibility with excipients [52]. Traditional methods are costly and slow. Al helps by:

- Predicting solubility, stability, permeability, and particle size.
- Identifying formulation problems early.
- Reducing experimental workload and development time [53]

Extensive database generating pre formulation studies can be processed using particularly ML, DL, AI technology, computational modelling, to forecasting a variety of properties such as solubility, particle size distribution, stability and permeability. During the initial stage of product formulation, when experimental data may be limited and this predictive capability is particularly beneficial [53].

Sustainable and green chemistry in drug development:

Environmental issues in pharmaceutical industry:

Environmental sustainability has become a central part of pharmaceutical business management, with respect to cleaner production, sustainable use of manufacturing materials, sustainability of the global supply chains, and human resources [54].

In recent decades pharmaceutical residues in the environment have raised concern because of their reported adverse effects on wildlife [55-57].

Studies have reported substantial pharmaceutical pollution in surface waters worldwide [58,59].

Most pharmaceutical residues in the environment originate from human excretion of pharmaceuticals and their metabolites to the sewage systems[60].

The highest environmental concentrations are typically measured in densely populated areas, or in developing countries with limited sanitation [61,59] .

To account for the environmental risks of medicines use, some countries have adapted environmental classification systems that rely on risk-based evaluation of active pharmaceutical ingredients (APIs), in accordance with the regulatory environmental risk assessment (ERA) guidance [62].

In the EU, the ERA of new APIs has been a mandatory part of marketing authorization (MA) since 2005 (2001/83/EC Article 8(3)(ca)). Although publicly available ERA data are very limited, the MA holder can voluntarily provide it to the classification system, initially established as a part of the Swedish electronic product information system (Fass.se), and later adopted in Norway (Felleskatalogen.no) and Finland (Pharmacafennica.fi). This risk-based assessment accounts for both drug consumption and measured ecotoxicological hazard by comparing the predicted environmental concentration to the predicted no-effect concentration. The utility of ERA-based classification is, however, much debated because of a lack of comprehensive ecotoxicological data and the discrepancies within it [63,64].

Moreover, pharmaceutical manufacturing can also be a major source of pharmaceutical pollution in areas where environmental legislation that affects permitting of pharmaceutical plants is lax. With the concentration of pharmaceutical raw material manufacture in low-income countries, the lack of regulatory enforcement has resulted in alarmingly high levels of pharmaceutical pollution, especially in Asia [65].

Besides environmental exposure by pharmaceutical residues, the environmental impacts of medicines also arise from drug production (e.g., energy and clean water consumption), distribution (including transportation and storage), and end-of-life (unused, discarded medicines).

Principle of green chemistry :

The 12 principles of green chemistry were first introduced by Paul Anastas and John Warner in 1998. These principles focus on minimizing or entirely eliminating the use of toxic solvents in chemical processes, as well as preventing the generation of waste from these processes. The 12 principles of green chemistry are illustrated in Fig. 2.

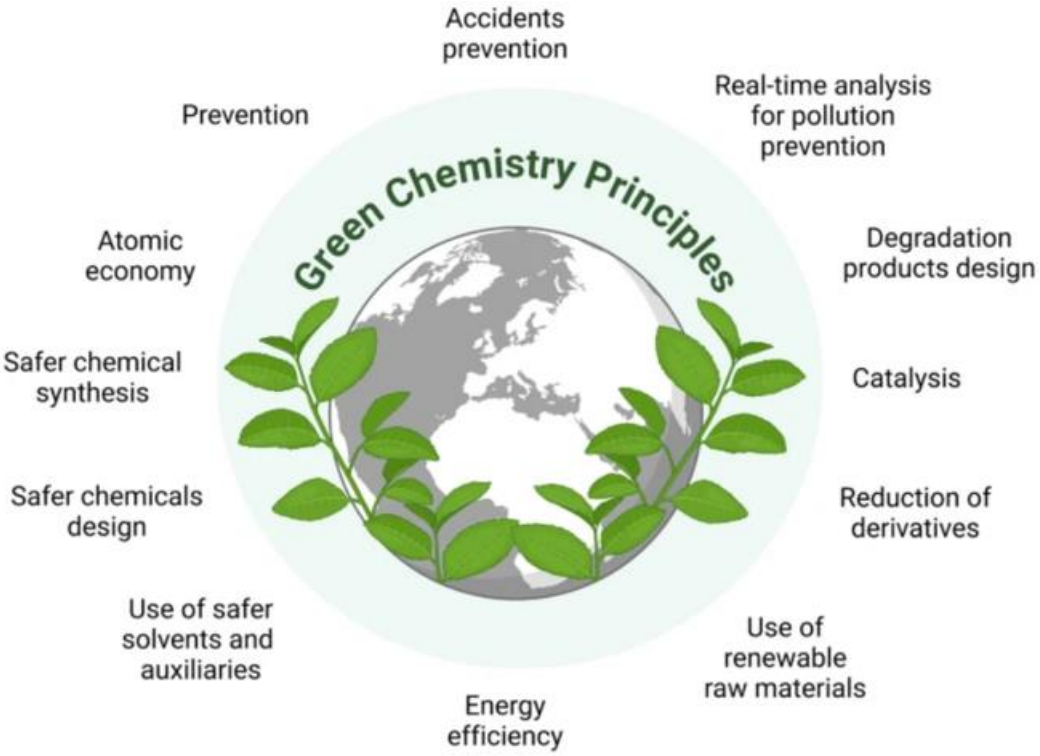


Table 1 The 12 principles of green chemistry [66,67]

SNO.	Conceptual	A Brief Description
1.	Avoidance	To save the environment, we should cease producing waste.
2.	The economy of atoms	Reactions should be engineered to generate fewer byproducts and waste.
3.	safer synthesis of chemicals	Reduce the use of dangerous chemicals to protect people and the environment.
4.	Designing safer chemicals	Chemicals should be effective yet less harmful.
5.	Using safer solvents	Carefully select solvents to minimise pollution and make them less hazardous.
6.	Efficiency of energy	Reduce energy consumption by employing more efficient procedures and techniques.
7.	Raw materials that are renewable	Make use of naturally occurring or reusable materials.
8.	Decrease in derivatives	Reduce waste and chemical usage by avoiding additional steps in reactions.
9.	The process of catalysis	To speed up reactions and lessen dangerous substances, use catalysts.
10.	Design with deterioration in mind	After use, chemicals should decompose into safe compounds.
11.	Analysis in real time	Continually monitor reactions to avoid dangerous drugs.
12.	Preventing accidents	To prevent mishaps, use safe products and techniques.

Future Prospective: Although early-stage drug discovery has been significantly impacted by existing AI

technologies, their full translational potential is still in the early stages. Overcoming current constraints through the creation of more integrated, reliable, and clinically aware AI systems will define the next ten years. Collaborative frameworks that protect privacy, multi-modal data fusion, and the development of dynamic avatars for patients High-quality datasets are required.

Improved model transparency, Clear regulatory guidelines for Al - based tools. Al accelerates discovery of natural product-based drugs and Techniques like NLP, GANs, and transformers analyse complex data. Challenges include limited data and structural complexity. Hybrid Al and rule-based methods are needed [68]

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