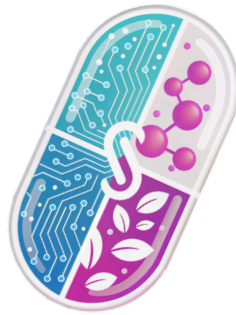




# Ailixir



**Mansoura University**

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**Bachelor of Science**

**in**

**Computer Science**

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# Introduction

Discovering a new drug is a notoriously complex, exhaustive, and high-risk process. It is a monumental gamble where average development times span 10 to 15 years, and the cost for a single approved medicine often exceeds \$2.6 billion [1]. Compounding this challenge, over 90% of drug candidates that enter human clinical trials are ultimately found to be unsafe or ineffective, resulting in catastrophic financial and human-capital losses [2]. Historically, identifying the active ingredients of traditional remedies was the primary method of discovery. More recently, this has been industrialized through high-throughput screening (HTS).

HTS is a process where large libraries of chemicals are tested for desirable effects within acceptable parameters of potency, metabolic stability, and selectivity. Selectivity is one of the more important factors, as it is a measurement of the effect the compound has on the selected target compared to its effect on other cells. A less selective drug may be toxic for consumption. After a compound that fulfills these requirements has been identified, clinical trials may be developed. However, it is unlikely for a perfect drug candidate to appear from early HTS runs. Even after a desirable "hit" compound has been found, medicinal chemists must use structure-activity relationships (SAR) to manually improve its properties.

As one can see, modern drug discovery, while more systematic, remains an expensive process that requires massive investments. Despite advances in technology and our growing understanding of biology, it remains a costly and lengthy endeavor with a low success rate. This inefficiency stems from its core reliance on physical trial-and-error screening, which is inherently slow, expensive, and limited in scale.

To overcome these fundamental bottlenecks, a paradigm shift is necessary. The industry and academia are increasingly turning to computational methods and Artificial Intelligence (AI). These *in silico* (computational) approaches replace the physical test tube with powerful algorithms. They allow for massive-scale virtual screening of chemical libraries numbering in the billions, predictive toxicology to spot non-viable candidates early, and molecular modeling to understand complex protein-ligand interactions at an atomic level. This grants researchers the crucial ability to "fail fast and fail cheap" by simulating outcomes digitally before committing to expensive and time-consuming lab work.

This project leverages these advanced computational techniques to propose a truly integrated, AI-driven ecosystem. Our system is not just another siloed tool; it is a holistic pipeline designed to automate and

accelerate the entire discovery workflow. We aim to build a platform that utilizes **Scaffold-based generation** to ensure chemical feasibility, filters for ADMET toxicity, and performs **automated high-speed molecular docking and MD simulations**. By architecting this system with an **integrated AI Research Agent** and an intuitive Cross-platform Desktop Application, we aim to democratize these tools, making them accessible to researchers and students worldwide.

## Problem Statement

The process of drug discovery is one of the most complex, expensive, and time-consuming challenges in modern science. Traditionally, developing a single new drug requires 10 to 15 years of continuous research and testing, with an average cost exceeding 2.6 billion USD. Despite this massive investment, over 90% of drug candidates fail during clinical trials, often after years of effort and financial loss. These limitations highlight an urgent need for a more efficient, intelligent, and accessible approach to discovering new medicines.

1. Slow and Inefficient Discovery Process

Researchers must manually test thousands of chemical compounds in laboratories to identify potential treatments for a specific disease. This process takes months or even years, and most compounds turn out to be ineffective or toxic. As a result, valuable time and resources are wasted on unpromising candidates.

2. Extremely High Research Costs

Laboratory experiments, chemical analyses, and safety tests are extremely expensive and require specialized equipment and large research teams. Because of this, small research institutions and universities cannot afford to conduct large-scale drug discovery projects, making this field dominated by major pharmaceutical companies.

3. Limited Accessibility and Analytical Tools

Not all researchers or students have access to the tools, data, or computational resources needed to analyze compounds or understand protein–ligand interactions. This creates a barrier for students and academics who wish to explore this field or develop AI-based research skills.

4. Lack of Educational and Interactive Platforms

Most existing AI-powered drug discovery platforms are either closed-source or too complex for beginners. There is no simple, professional-grade desktop environment that allows researchers and students to experiment, visualize, and understand how AI can accelerate drug discovery. This limits learning opportunities and innovation in the academic community.

5. Difficulty in Drug Repurposing

Many existing drugs have the potential to treat new diseases (as seen during the COVID-19 pandemic), but due to the absence of intelligent analytical tools, drug repurposing remains a slow and uncertain process, often based on luck or trial and error.

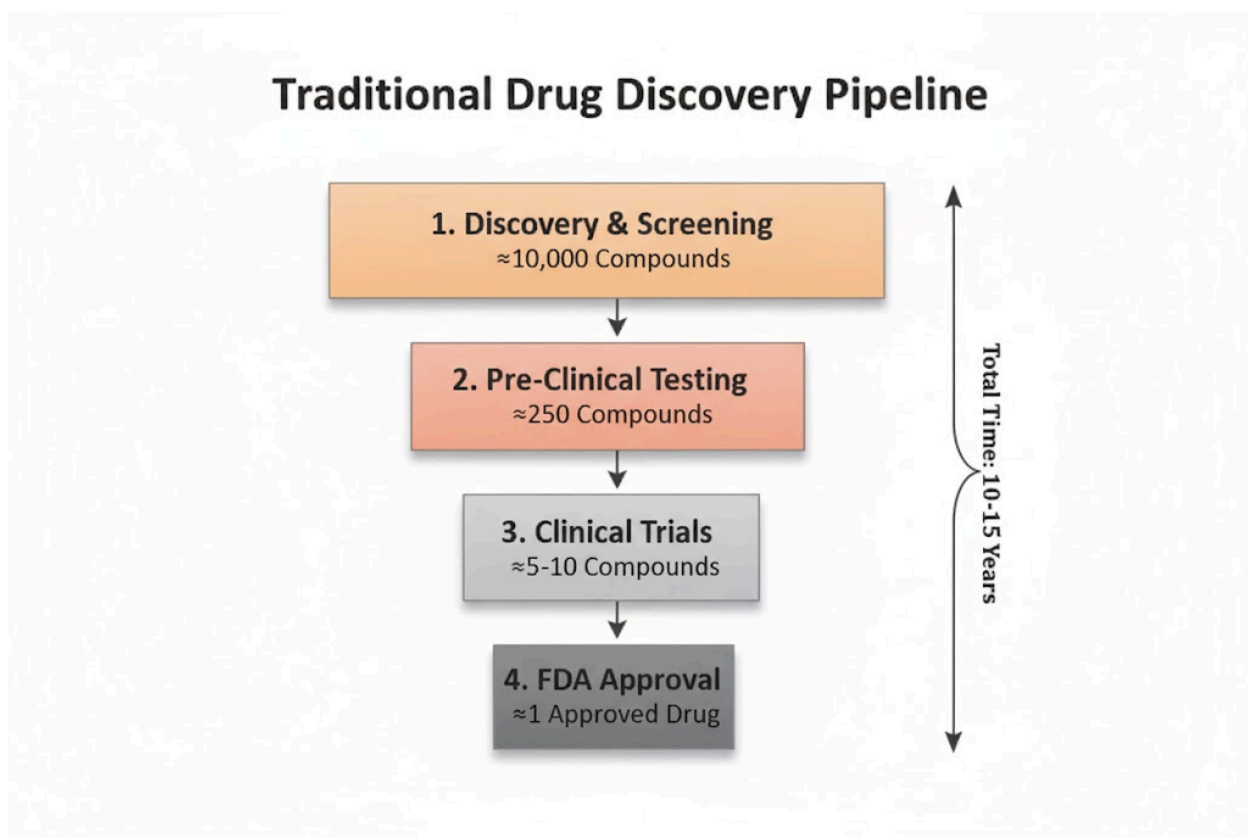
6. Computational Bottlenecks and Manual Labor. Current docking and simulation tools often require manual file preparation and hours of computational time (up to 6 hours for a single

high-quality run). This manual intervention creates a significant bottleneck, preventing high-throughput discovery and requiring deep technical expertise that many pharmacists and students lack.

## Motivation

The primary motivation for this project is born from a critical and undisputed failure in the pharmaceutical industry: the traditional drug discovery pipeline is fundamentally broken. The process, as it stands, is economically unsustainable and shockingly inefficient. Statistics paint a grim picture of this reality:

- Developing a single new drug is a monumental gamble, consuming **10 to 15 years** of research and an average of **\$2.6 billion** [1]. This decade-long process acts as an extreme funnel of attrition, where tens of thousands of initial compounds are screened just to find a handful worthy of testing.

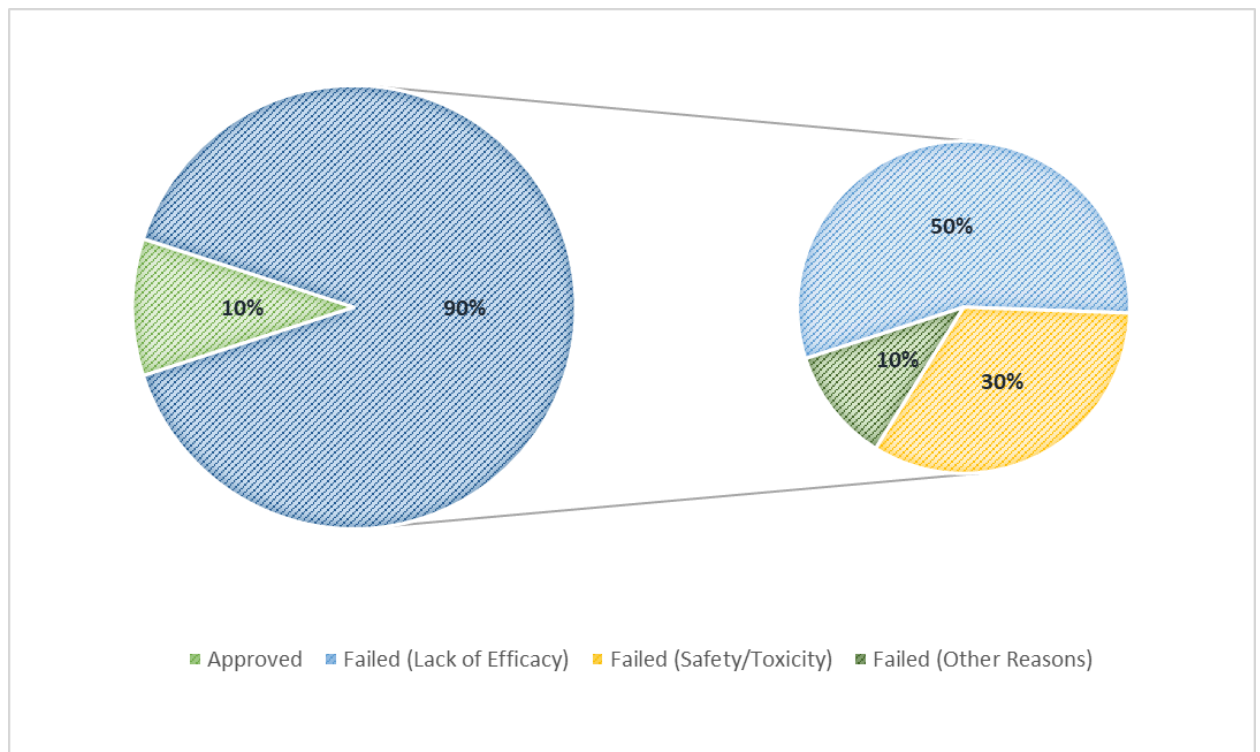


**Figure 1:** The Traditional Drug Discovery Funnel. This 10-15 year pipeline illustrates the process of attrition, where ~10,000 initial compounds are screened to yield only one

FDA-approved drug.

- Even after this massive investment of time and capital, the catastrophic failure rate reveals the core problem. Over **90% of all drug candidates** that enter human clinical trials fail.

This failure, however, is not random. It is predictable. A deeper analysis reveals why these drugs fail: the two largest drivers are **lack of efficacy** (the drug doesn't work, ~50%) and **unacceptable safety/toxicity** (the drug is harmful, ~30%) [2].



**Figure 2:** Root Causes of Clinical Trial Attrition. While over 90% of candidates fail (main pie), the breakdown (secondary pie) reveals the primary causes: lack of efficacy and safety/toxicity [2].

This is where our motivation lies.

These statistics are not just numbers; they are a clear map of the problem. They show that the industry wastes billions of dollars and years of effort advancing drugs that are destined to fail for reasons that can be predicted.

While Artificial Intelligence has emerged as a solution, existing tools (as reviewed in our Related Work section) remain fragmented. They often focus on one piece of the puzzle (like generation) while ignoring another (like safety). Furthermore, many are computationally prohibitive, closed-source, or too complex for non-experts, creating a significant barrier to entry.

This project is directly motivated by these gaps. We aim to build a holistic, end-to-end pipeline that directly attacks the two main causes of failure. Our system is designed to integrate:

1. **New Candidate Prediction** (to solve the efficacy problem).
2. **ADMET/Safety Filtering** (to solve the toxicity problem).

Furthermore, we are motivated to *democratize* this technology. By architecting our system as a user-friendly Cross-platform Desktop Application, we aim to break down the accessibility barrier, placing these powerful predictive tools directly into the hands of students, academics, and researchers.

In essence, we are motivated to transform a slow, fragmented, and broken process into a fast, integrated, and accessible one, guided by the data on why drugs fail.

## Objectives

The main objective of this project is to design and develop an AI-powered Cross-platform Desktop Application that automates and accelerates the process of drug discovery using deep learning and molecular simulation techniques.

To achieve this primary goal, the following specific objectives are defined:

1. **Predict New Compound Effectiveness:** Develop and integrate AI models capable of predicting the potential biological activity of new chemical compounds against specific disease targets.
2. **Enable Drug Repurposing:** Implement a feature that allows the AI to analyze an existing drug and predict other diseases it may effectively treat.
3. **Optimize Promising Lead Compounds:** Implement AI-based optimization models that suggest structural modifications to enhance the efficacy or reduce side effects of moderately active compounds.
4. **Implement Compound Similarity Search:** Develop a feature to find compounds similar to a given input, offering alternative options if the original is rare, costly, or unavailable.
5. **Integrate ADMET (Safety) Filtering:** Implement AI models to filter out unsafe or non-viable compounds before experimental testing by predicting their ADMET properties.
6. **Perform Automated Docking & MD Simulations:** Integrate tools to automate molecular docking and **Molecular Dynamics (MD) Simulations** to validate the stability of the drug-protein complex over time.
7. **Develop a User-Friendly Cross-platform Desktop Application:** Create an intuitive client-side

Cross-platform Desktop Application that allows users to submit requests and receive responses from the backend services.

8. **Provide 3D Visualization Services:** Implement a dedicated service to transform (SMILES) codes — a chemical notation system that represents molecular structures as ASCII strings—into 2D/3D structures and render protein-ligand interactions from docking results.
9. **High-Speed Workflow Automation:** Optimize the computational pipeline to reduce simulation time from **6 hours to under 10 minutes**, enabling rapid screening.
10. **AI Research Agent:** Develop an LLM-based analytical assistant that goes beyond simple conversation to provide deep scientific interpretation. The agent analyzes complex MD simulation and ADMET results to provide actionable insights, such as flagging specific risks like hepatotoxicity (liver toxicity) or low blood-brain barrier permeability, enabling researchers to "fail fast and fail cheap" before entering the lab.

## Literature Review – Related Work

### 1. BindDM: Reinforcement Learning-Based Molecular Optimization

- **Problem Addressed:** Most generative drug design models fail to optimize molecules for protein binding affinity directly. BindDM was proposed to overcome this limitation by integrating reinforcement learning with docking feedback as a reward function.
- **Methodology:** The model generates molecular candidates and evaluates them through iterative docking simulations. A reinforcement learning agent adjusts the molecular structures based on docking scores, guiding the generation toward higher affinity compounds.
- **Key Results:** BindDM achieved improved docking-based affinity metrics and enhanced diversity compared to standard VAEs and GANs. However, the method was computationally intensive and relied heavily on accurate docking approximations.
- **How This Project Differs:** Our project reduces computational dependency by using efficient post-generation filtering based on QED, SA, and similarity scoring, rather than incorporating docking in every training iteration. This improves scalability and allows faster large-scale molecular screening.

### 2. DrugGEN: Structure-Aware Molecular Generation



- **Problem Addressed:** Traditional generative models often ignore the protein’s structural information, producing molecules with uncertain binding relevance. DrugGEN aims to generate ligands that are aware of protein pocket structures.
- **Methodology:** It employs a graph-based deep learning framework where both the ligand and protein pocket are encoded as graphs. The model then learns to generate molecules conditioned on protein features to improve structural compatibility.
- **Key Results:** DrugGEN achieved high chemical validity (100%), strong internal diversity ( $>0.85$ ), and balanced novelty. Yet, it did not include synthetic accessibility or QED-based evaluation in its generation phase.
- **How This Project Differs:** Our model extends DrugGEN’s approach by incorporating comprehensive post-generation evaluation — including QED, SA, and Lipinski rule checks — to ensure both biological relevance and chemical feasibility before docking.

### 3. MolMIM: Molecular Mutation and Optimization Model

- **Problem Addressed:** Existing models often get trapped in limited chemical spaces, producing repetitive or known scaffolds. MolMIM introduces a mutation-based approach to explore new chemical regions.
- **Methodology:** It starts with known inhibitors and applies generative mutation operators guided by molecular property optimization (QED and binding affinity). The system iteratively mutates molecules until desired thresholds are reached.
- **Key Results:** MolMIM successfully generated optimized molecules with better QED and docking scores but showed lower novelty due to strong bias toward initial scaffolds.
- **How This Project Differs:** Unlike MolMIM, our workflow focuses on generating molecules from scratch, not by mutating existing ones. This allows for higher novelty and greater exploration of the chemical space while maintaining drug-likeness constraints.

### 4. LiGAN: Ligand Generation Using 3D Density Grids

- **Problem Addressed:** Most molecular generative models overlook the 3D spatial compatibility of the ligand with its binding site. LiGAN was designed to directly model spatial constraints through voxelized representations.
- **Methodology:** LiGAN uses a 3D convolutional neural network to predict ligand atom densities inside protein pockets, enabling the generation of physically realistic 3D structures.
- **Key Results:** The model achieved high structural compatibility but struggled with computational complexity and limited scalability. The grid-based representation also restricted chemical diversity.



- **How This Project Differs:** Our approach focuses on SMILES-level generation combined with post-processing chemical validation. This enables the generation of thousands of valid molecules with less computational cost and higher chemical diversity.

## 5. IDOLpro: Multi-Objective Drug Design Framework

- **Problem Addressed:** Balancing multiple drug design objectives — such as binding affinity, novelty, and druglikeness — is challenging for most single-objective models.
- **Methodology:** IDOLpro uses a reinforcement learning framework with a multi-objective reward function that simultaneously optimizes affinity, QED, and diversity scores.
- **Key Results:** The model demonstrated strong performance across several metrics but was limited by the need for precomputed docking data, which slows real-time molecule generation.
- **How This Project Differs:** Our project applies a multi-criteria selection system (QED > 0.5, SA < 4, similarity 0.3–0.7, Lipinski compliance) after molecule generation instead of during training. This post-filtering method increases flexibility and reduces computational overhead.

## Summary and How This Project Differs

Previous works like BindDM, DrugGEN, and LiGAN achieved impressive results in AI-driven molecule generation, but they often lacked integrated evaluation of drug-likeness, manufacturability, and binding relevance in a unified pipeline.

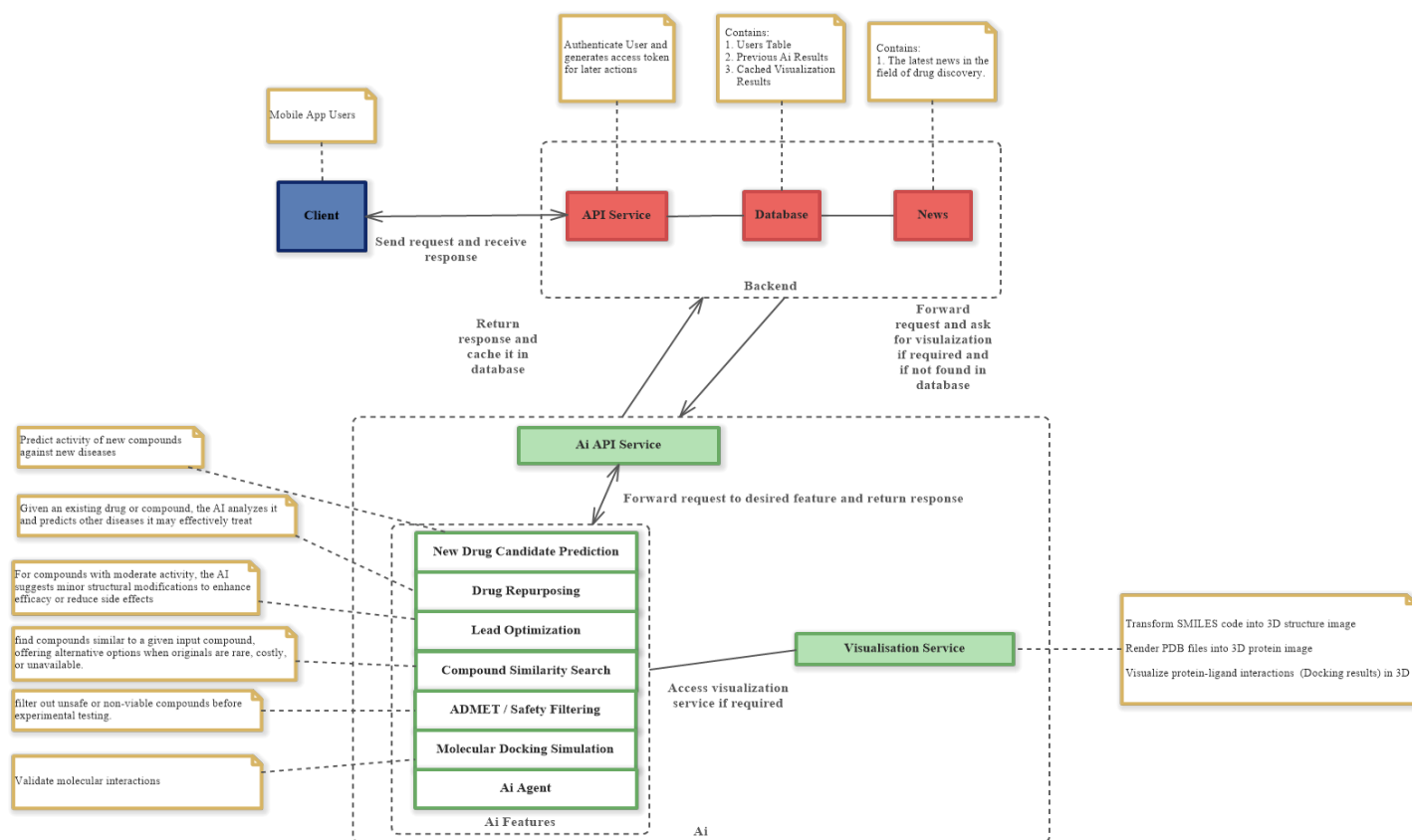
Our project bridges this gap through a hybrid design that couples deep generative modeling with systematic chemical and pharmacological filtering. Specifically:

- We emphasize post-generation chemical validation (QED, SA, Lipinski compliance) before docking.
- Our workflow allows scalable, target-specific molecule generation for AKT1 inhibitors without retraining.
- It ensures that generated molecules are not only chemically valid and novel, but also synthetically accessible and druglike, offering a more practical step toward experimental validation.
- We introduce **Workflow Automation**, reducing the docking setup and execution time by over 90% (from 6 hours to 10 minutes).
- We integrate an **AI Agent** to interpret complex MD simulation results, making high-end bioinformatics accessible to non-experts.

## Comparison of Related Work

Project Name	Primary Focus (Approach)	Drug-likeness Filtering (QED, SA, etc.)	Docking Integration	Key Limitation(s)
<b>BindDM [3]</b>	Generative Optimization (RL)	Limited (Focus on affinity)	During Training (As a reward)	Computationally heavy; very slow.
<b>DrugGEN [4]</b>	Generative (Structure-Aware Graph)	Not Included (in generation)	N/A (Generates for docking)	Lacks feasibility checks (SA/QED)
<b>MolMIM [5]</b>	Optimization (Mutation-based)	Yes (Guided by QED)	During Optimization	Low novelty (Biased to initial scaffolds)
<b>LiGAN [6]</b>	Generative (3D Density Grids)	Not Included	N/A (Generates 3D structures)	Computationally complex; low diversity
<b>IDOLpro [7]</b>	Generative Optimization (Multi-Objective RL)	Yes (As part of the reward)	During Training (Requires precomputation)	Slow; requires precomputed data
<b>Ailixir (Proposed)</b>	<b>Generative + Integrated Filtering Pipeline + AI Agent</b>	<b>Yes (Systematic Post-Generation )</b>	<b>Fully Automated + MD Simulation</b>	-

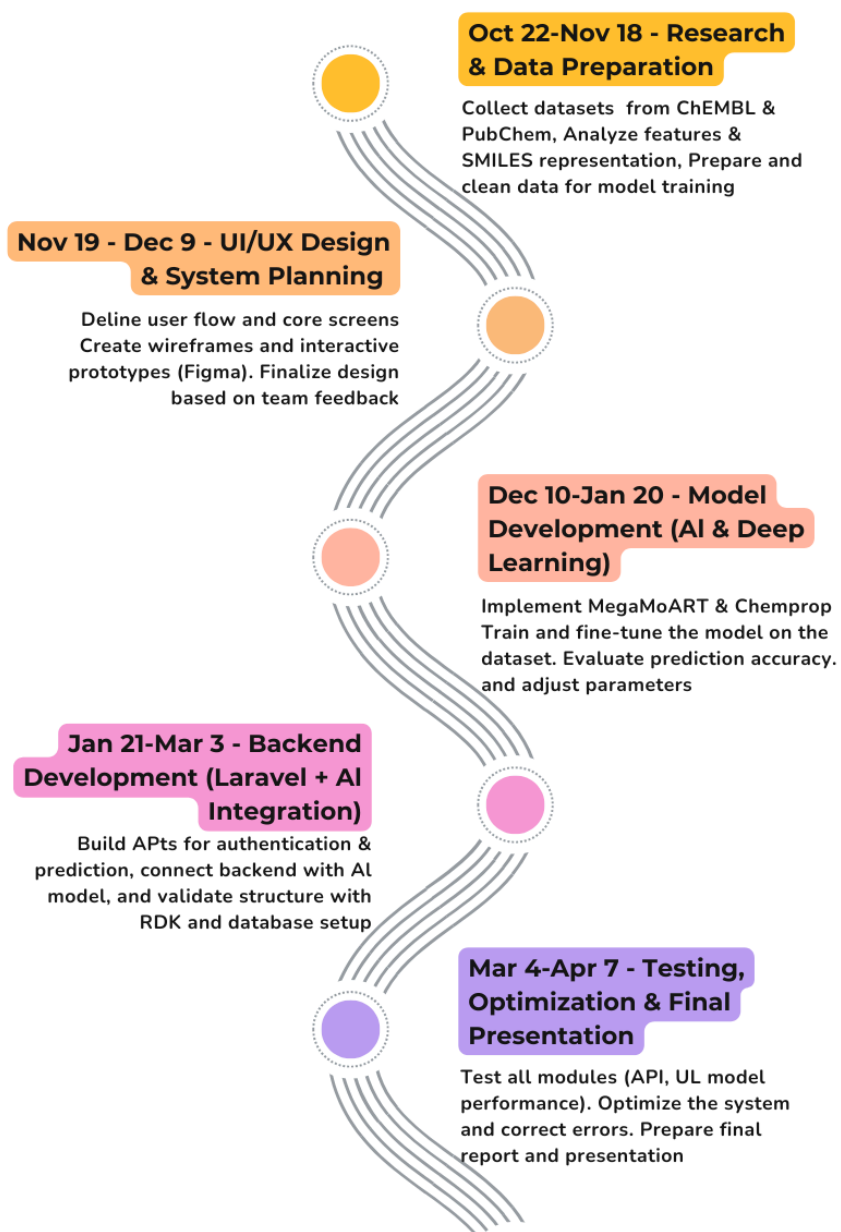
# System Architecture



**Figure 3:** System Architecture Workflow. This architecture illustrates the workflow of our AI-driven drug discovery system. The Client (Cross-platform Desktop Application) sends user requests to the API Service, which handles authentication, validation, and data routing. The API forwards requests to the AI Service, which contains specialized modules for tasks such as New Drug Candidate Prediction, Drug Repurposing, Lead Optimization, Compound Similarity Search, ADMET/Safety Filtering, and Molecular Docking Simulation. Each module performs a specific analysis to evaluate or improve potential drug compounds. When visualization is required, results are sent to the Visualization Service to generate graphical or 3D outputs. The final processed results, whether analytical, visual, or both, are returned to the Backend, stored in the Database (for caching and to reduce the work on the visualization service), and then sent back to the Client. The architecture features a specialized **Automation Layer** that handles high-throughput docking and MD simulations. Furthermore, a **Conversational AI Agent** sits between the API and the Client, allowing users to query simulation results and receive automated toxicity/efficacy reports using natural language.

## Timeline

# Timeline



## Sustainability and Environmental Impact (Green Chemistry)

Ailixir aligns with the goals of the **Environmental Forum** by promoting "Green Drug Discovery." Traditional pharmaceutical R&D generates massive chemical waste and consumes significant energy through failed laboratory experiments. By shifting the bulk of discovery to an **ultra-fast, automated virtual environment**, we:

- **Reduce Chemical Waste:** Minimizing "wet lab" trials by filtering 99% of candidates digitally.
- **Energy Efficiency:** Our optimized 10-minute automated pipeline consumes significantly less computational energy compared to traditional hours-long manual methods.
- **Eco-friendly Innovation:** Supporting sustainable research practices in Egyptian universities.

## Conclusion

The traditional drug discovery process is notoriously slow, costly, and inefficient, often taking more than a decade and billions of dollars to bring a single drug to market. Moreover, nearly 90% of candidate drugs fail during clinical trials, highlighting the urgent need for smarter, faster, and more reliable approaches.

Our proposed AI-powered drug discovery pipeline addresses this challenge by integrating artificial intelligence with computational chemistry. Through three key stages — generation, filtering, and simulation — the system can autonomously generate new chemical compounds, evaluate their validity and safety, and predict how effectively they interact with disease-related proteins.

By leveraging advanced AI models such as MegaMolBART, Chemprop, and molecular docking tools, our project aims to accelerate drug discovery, reduce research costs, and improve accuracy in identifying promising compounds. Beyond its scientific value, the system also supports innovation in healthcare and education, providing researchers with a powerful tool to explore new treatments more efficiently.

Through its unique focus on **automation, scaffold-based precision, and MD simulation**, Ailixir reduces the time-to-results from hours to minutes. This efficiency, combined with our **AI Research Agent**, makes the platform a cornerstone for sustainable and accessible pharmaceutical innovation.

Ultimately, this project represents a significant step forward toward a future where AI transforms pharmaceutical research, enabling the faster, more precise, and more accessible discovery of life-saving drugs.

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