NTRA GRADUATION PROJECT COMPETITION

Ongoing (Academic year 2025/2026)

Project title	Ailixir: AI-Powered Platform for De Novo Drug Discovery & Molecular Dynamics
Project Track	Artificial Intelligence / Digital Health
University	Mansoura University
Department/Faculty	Computer Science & Information Sciences
Industrial partner (if any)	

PROF. .....

FACULTY/INSTITUDE DEAN

[SIGNATURE ORGANIZATION]

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A. Project Information

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Project Track	Artificial Intelligence / Digital Health
University	Mansoura University
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Industrial partner (if any)	

B. Supervisor Information

Supervisor Name	
Title	
Work Address	
Mobile	
E-mail	
Brief summary of expertise	

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C. Project Members Information

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* Please note that the first name will be referred to as the main **contact person** for the whole group in addition to the Project Supervisor.

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REVIEW THE FOLLOWING POINTS BEFORE SUBMITTING THE PROPOSALS:

- **Proposals will be evaluated based on:**

  (1) its impact on society/industry specially telecommunication sector,

  (2) clarity and validity of objectives,

  (3) originality,

  (4) writing and presentation quality,

  (5) completing ALL the required fields

- **Review the language of the proposal.**

  It is important that the document is correct from grammatical and vocabulary points of view. Low quality language is one of the major reasons for rejecting proposals.

- **Avoid plagiarism.**

  Never "copy and paste" from a website or a paper. Read from multiple sources and write your own proposal with your original language.

- **References citation.**

  If you used ideas or a sentence from any resource link a website, a paper, or a book, this must be included in the references section. Proposals that doesn't include the correct references are rejected.

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A. PROJECT DESCRIPTION

Applicants shall provide a brief description of their project. This description should include the following:

1. OVERVIEW

(i) Problem definition, (ii) approach and tools/techniques, and (iii) overview of system modules.
Use block diagrams and figures to describe your ideas. Be as clear as possible about the ideas in order to show the reviewer the value of your idea.

(i) Problem definition:

Traditional drug discovery is a time-consuming, expensive, and high-risk process, taking over 10 years and costing billions of dollars with a high failure rate. Researchers face challenges in exploring the vast chemical space (estimated at ~10^60 possible compounds) to find novel drug candidates for critical diseases like Cancer.

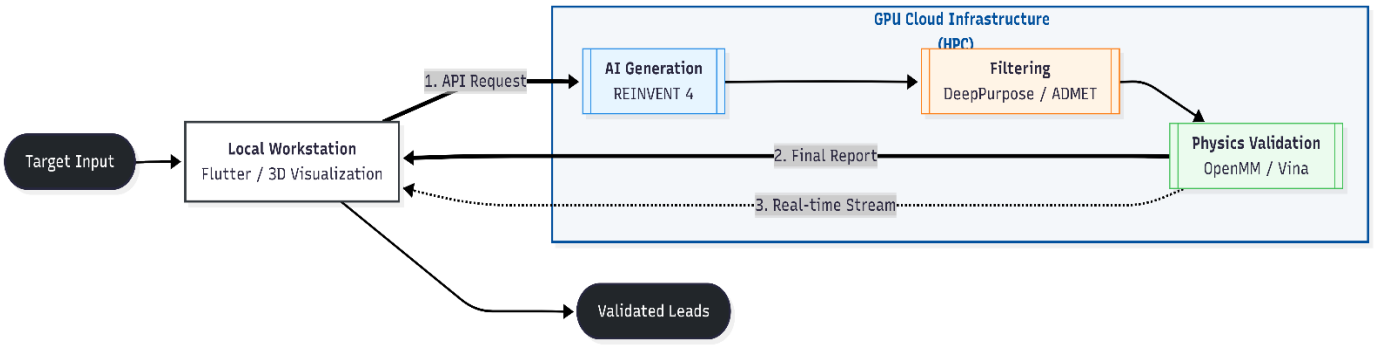
(ii) Approach and tools/techniques:

Ailixir is an end-to-end cloud-based platform that leverages Generative AI and High-Performance Computing (HPC) to accelerate this process.

- **Generative AI: Using REINVENT4 (Reinforcement Learning) to generate novel chemical structures from scratch based on target protein sequences.**
- **Predictive AI: Using DeepPurpose for binding affinity prediction and Chemprop for toxicity/safety filtering.**
- **Physics-Based Validation: Utilizing OpenMM engine facilitated by the "Make-it-Rain" cloud-computing framework for Molecular Dynamics (MD) stability tests, alongside AutoDock Vina for 3D docking simulations. This ensures high-throughput, reproducible, and scientifically validated simulations within a cloud-native environment.**

(iii) Overview of system modules:

The system consists of a User Dashboard (Frontend), an Orchestration Backend (handling API requests), and an AI/Simulation Engine running on GPU-accelerated cloud infrastructure. The pipeline flows from Target Input to AI Generation to Toxicity Filtering to 3D Docking to MD Simulation to Final Reporting.



2. IMPACT

Why do you consider this project? What is its impact on community/market/end user/… specially telecommunication sector?

- **On Society: Ailixir accelerates the finding of cures for critical diseases (e.g., Lung Cancer), potentially saving lives and making medication more affordable by reducing R&D costs.**
- **On Telecommunication Sector & IT: The project demonstrates an advanced use case for High-Performance Computing (HPC) and Big Data transmission, directly aligning with the National AI Strategy and the Digital Egypt vision.**
- **Data Sovereignty: By providing a locally-hosted AI platform, Ailixir ensures National Data Sovereignty, allowing Egyptian research institutions to process sensitive genomic and chemical data within a secure local infrastructure instead of relying on expensive and restricted foreign platforms.**
- **Edge & Cloud Synergy: The system utilizes Edge Computing concepts by performing initial predictive filtering and visualization on local workstations to reduce latency, while offloading heavy Molecular Dynamics (MD) trajectories to the GPU-cloud. This showcases the essential role of 5G and high-capacity fiber networks in handling real-time streaming of massive scientific datasets (Terabytes of data).**
- **Scientific Community: It democratizes access to advanced drug design tools, allowing researchers with limited computational resources to run complex simulations via the cloud.**
- **This project represents a non-traditional but high-impact application of telecommunication infrastructure, showcasing how next-generation networks can support national scientific and biomedical innovation.**

3. NOVELTY AND FEATURES

Explain (i) novelty (ii) features, and (iii) related products, if any.
Originality doesn't always mean coming up with completely new ideas. Building on previously developed project and adding new modules that increase their value is considered novelty. Doing a previous idea with lower cost or a better performance is considered novelty.

(i) novelty:

- **Advanced Molecular Engineering: Unlike traditional "Virtual Screening," Ailixir implements Scaffold Hopping and De Novo Design. This allows the AI to move beyond known chemical classes to discover entirely new molecular cores.**
- **Multi-objective Property Optimization: The core innovation lies in our Multi-objective Reinforcement Learning approach. The system doesn't just generate "active" molecules; it simultaneously optimizes for a "Pareto Front" of multiple properties: High Binding Affinity, Low Toxicity (ADMET), and High Synthetic Accessibility. This ensures that the generated leads are not only effective but also safe and chemically feasible to manufacture.**
- **Novelty Verification Strategy: To guarantee uniqueness, we implement a multi-stage validation pipeline cross-referencing global databases (PubChem/ChEMBL). For commercial scaling, the platform integrates with CAS SciFinder-n to verify the absence of CAS Registry Numbers, ensuring the candidates are patentable "First-in-Class" molecules.**
- **Novelty Screening: High-scoring candidates undergo similarity searches using tools like SwissSimilarity and SureChEMBL to check for existing patents, ensuring a high degree of originality in the discovered leads.**

(ii) Features:

- **End-to-End Automation: From protein sequence to validated drug candidate report in one click.**
- **Safety-First Approach: Integrated ADMET and Toxicity filtering to ensure generated drugs are safe.**
- **Scaffold Decoration & Hopping : Ability to fix a specific chemical core and automatically generate thousands of analogs (R-group optimization) to maximize binding affinity for specific targets.**
- **3D Visualization: Interactive browser-based viewing of Protein-Ligand interactions.**
- **Scalability: Built on a modular architecture allowing integration of new AI models.**

(iii) Related products: Commercial tools like Schrödinger are extremely expensive, complex, and require high-end workstations. Open-source academic codes are fragmented, hard to use, and lack a unified workflow. Ailixir bridges this gap by providing a professional, cloud-native, and scaffold-aware interface for powerful open-source tools, making advanced drug design accessible to researchers on any device.

4. DELIVERABLES

What is the project final outcome (HW device, SW package, simulation ...)?
It is important to clearly identify the final outcomes supported by evidence and results.

1.Ailixir Cross-Platform Application:

- **Ailixir Desktop Workstation (Primary):** A powerful, high-performance desktop application developed using **Flutter**. It is optimized for visualization, orchestration, and monitoring of heavy computational tasks executed on cloud infrastructure, detailed **3D molecular visualization**, and real-time data analysis. The application provides a professional dashboard for managing the entire drug discovery pipeline on Windows, macOS, and Linux.
- **Mobile Companion App (Optional/Secondary):** A cross-platform mobile version for remote monitoring of simulation progress and viewing final validation reports on the go.

2.AI Models:

Fine-tuned Generative and Predictive models for drug discovery.

3.Simulation Pipeline:

Automated scripts for Docking (Vina) and Molecular Dynamics (OpenMM).

4.Validated Case Study:

To ensure the absolute novelty of generated leads, Ailixir performs automated cross-referencing against **PubChem and ChEMBL**. Furthermore, the platform architecture is **ready for integration with professional databases like CAS SciFinder-n** to perform final patent clearance and CAS Registry verification before moving to the clinical stage."

5.Technical Documentation:

Source code and user manual.

5. BUSINESS PLAN AND MARKET ANALYSIS

Market research is essential to be included, whether national or multinational, showing the level of competition, business opportunities, and the niche added value. Do you foresee any potential market for your project? Do you expect any demand on the final product?

- **Market Need: The global AI in Drug Discovery market is projected to reach billions by 2030. Pharmaceutical companies and research universities are desperate for tools to cut research time.**
- **Target Audience: Academic Researchers, Biotech Startups, and Pharmaceutical R&D departments.**
- **Business Model: A SaaS (Software as a Service) model where users pay a subscription or "Pay-per-Compute" fees to access high-end GPU resources for their simulations without buying expensive hardware.**
- **Competitive Advantage: Ailixir offers a localized, cost-effective alternative to global giants, optimized for the specific needs of academic research and small biotech firms.**

6. ROLE OF THE INDUSTRIAL PARTNER (IF ANY)

What is the type of support to be provided by the industrial partner (technical, financial, access…)?

Partner Entity: Faculty of Pharmacy (Expert Consultancy & Scientific Validation).

Type of Support: Technical, Biological Validation, and Domain Expertise.

Detailed Contributions:

Biological Target Definition: The partner provided critical insights into selecting specificweb protein as a primary target, defining the specific binding sites (Kinase Domain) that our AI should prioritize.

Scaffold-Based Guidance: Expert feedback on the "Synthetic Feasibility" of AI-generated molecules. This ensures that the compounds designed by Ailixir aren't just theoretically high-scoring, but are actually possible to synthesize in a chemical lab.

Pharmacological Standards (ADMET): Setting the strict criteria for drug-likeness (Lipinski's Rule of Five) and safety profiles (Toxicity filters) to ensure the candidates meet pharmaceutical industry standards.

User Experience (UX) for Researchers: Guiding the development of the Desktop Workstation features to ensure the workflow matches the real-world needs of medicinal chemists and lab researchers.

Future Validation Access: Providing a roadmap for potential In-Vitro (wet-lab) testing to validate the top candidates generated by our platform in the next phase of development.

"The partner also suggests access to specialized professional databases and literature (e.g., CAS SciFinder-n) to cross-verify the novelty of the generated De Novo leads against existing patent landscapes."

7. Project EXPENSES

List the main equipment, tools, modules, components, software, … that were used to implement the project.

Item	Type (Hardware/ Software/ Other)	Specifications (brief description)	Cost (LE.)
1	Hardware	Workstation Upgrade: High-speed RAM (32GB+) and NVMe SSDs to handle large MD trajectory files locally.	45,000
2	Software/Cloud	Google Colab Pro+ / Cloud GPU Credits (Simulation)	15,000
3	Hosting & Deployment	Domain name, SSL, and backend hosting for secure API services and cloud orchestration.	2,000
4	Data Storage	Secure Cloud Storage for massive Datasets (PDB, ChEMBL, and generated MD files).	3,000
5	Software Tools	Professional UI/UX Assets, Flutter deployment tools, and Software Licenses & Scientific Visualization Tools.	10,000
6	Research	Research Dissemination & Scientific Validation.	15,000
7	Novelty Screening	Access to public chemical databases (PubChem, ChEMBL, SureChEMBL APIs)	0
8			
9			
10			
Total Project Cost		**90000**	

REFERENCES
Cite to the references those related to your idea

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