

Solution Challenge



Team Details

1. Team name: (**AlphaMed-IQ**)
2. Team leader name: Saurabh Sati
3. Problem Statement: Accelerating Drug Discovery with Generative AI

 **Revolutionizing Drug Discovery with AI** **Two Integrated Pipelines:**

- **Drug Discovery Pipeline:** Uses **AlphaFold2**, **MolMIM**, **Oracle Model**, and **DiffDock** to predict, generate, and optimize small molecules for drug development.
- **Protein Design Pipeline:** Leverages **AlphaFold2**, **RFDiffusion**, **ProteinMPNN**, and **AlphaFold-Multimer** to design stable and functional protein binders.

 **Key Benefits:**

-  **Faster & Cost-Effective** – Reduces drug discovery timelines from **years to months**
-  **AI-Powered Predictions** – Enhances accuracy in **molecular docking & sequence optimization**
-  **Gemini AI Integration** – Provides **real-time insights for researchers**
-  **User-Friendly Web Platform** – Built with **Streamlit & Figma UI** for seamless accessibility

 **Impact:**

- Accelerates **biotech and pharmaceutical research**
- Enables **automated, scalable, and AI-powered** drug design
- **Bridges the gap** between AI and biomedical breakthroughs 

Opportunities & Unique Value of Our AI-Driven Drug Discovery Platform 🚀

◆ How is it Different from Existing Solutions?

- ✓ **End-to-End AI Integration** – Combines **structure prediction, molecule generation, binding affinity evaluation, and docking refinement** in **one seamless pipeline**.
- ✓ **Duality of Innovation** – Unites **small-molecule drug discovery & protein binder design** in a **single AI-powered system**, unlike solutions that focus on only one.
- ✓ **Real-Time Research Assistance** – Gemini AI integration provides researchers with **instant insights, hypothesis generation, and workflow optimization**.

◆ How Does It Solve the Problem?

- ⌚ Accelerates drug discovery from **years to months**
- 💰 Reduces **experimental costs** through AI-driven molecule screening
- 🎯 Enhances precision in selecting promising candidates for trials

◆ Unique Selling Proposition (USP)

- ⭐ **AI-Driven Dual Approach** – Revolutionizes both **drug discovery & protein engineering**, unlocking more biomedical breakthroughs
- ⭐ **Streamlit-Based Web App** – User-friendly, interactive, and accessible to researchers worldwide
- ⭐ **Faster, Smarter, Cost-Effective** – Combining two powerful pipelines, it optimizes drug development while minimizing lab experiments

Key Features of Our AI-Powered Drug Discovery & Protein Design Platform

◆ **AI-Driven Drug Discovery**

-  **AlphaFold2** – Predicts 3D protein structures
-  **MolMIM** – Generates diverse small molecules
-  **Oracle Model** – Evaluates drug-likeness & binding affinity
-  **DiffDock** – Optimizes molecular docking & interactions

◆ **AI-Powered Protein Design**

-  **RFDiffusion** – Optimizes protein conformations
-  **ProteinMPNN** – Designs stable protein sequences
-  **AlphaFold-Multimer** – Validates protein-protein interactions

◆ **Gemini AI Integration**

-  **Real-time research assistant** for insights & hypothesis generation
-  **Automated workflow optimization**

◆ **Web-Based & Scalable**

-  **Streamlit-powered UI** – Interactive & user-friendly
-  **Cloud-based deployment** – Accessible anytime, anywhere
-  **API integration** for advanced research

Process Flow Diagram for AI-Driven Drug Discovery & Protein Design

Step 1: Protein Structure Prediction

- ◆ **User Input** → Upload target protein sequence
- ◆ **AlphaFold2** → Predicts 3D structure

Step 2: AI-Driven Small Molecule Drug Discovery

- ◆ **MolMIM** → Generates diverse drug-like molecules
- ◆ **Oracle Model** → Evaluates & ranks molecules based on binding affinity & ADMET properties
- ◆ **DiffDock** → Optimizes molecular docking poses

Step 3: AI-Powered Protein Binder Design

- ◆ **RFDiffusion** → Optimizes protein conformation
- ◆ **ProteinMPNN** → Designs amino acid sequences for stability
- ◆ **AlphaFold-Multimer** → Validates interactions between designed proteins

Step 4: Research & Optimization

- ◆ **Gemini AI** → Assists researchers with insights, hypothesis generation, and workflow optimization

Step 5: Web Interface & Accessibility

- ◆ **Streamlit Web App** → Displays results, visualizations & predictions
- ◆ **API Integration** → Supports further research & development

 Architecture Diagram for AI-Powered Drug Discovery & Protein Design Solution System Components & Workflow:**1 Input Layer (User Interaction & Data Upload)**

- ◆ Protein Sequence Input (FASTA format)
- ◆ Small Molecule Input (Optional, for drug discovery)
- ◆ User selects AI models to run (Drug Discovery or Protein Binder Design)

2 AI Processing Layer (Back-End AI/ML Models) Drug Discovery Pipeline:

- AlphaFold2 – Predicts 3D protein structure
- MolMIM – Generates diverse small molecules
- Oracle Model – Scores molecules based on binding affinity & ADMET properties
- DiffDock – Predicts optimal binding poses

 Protein Design Pipeline:

- RFDiffusion – Generates optimized protein conformations
- ProteinMPNN – Designs amino acid sequences for stability
- AlphaFold-Multimer – Validates protein-protein interactions

 AI Assistant (Gemini Integration):

- Hypothesis generation & optimization suggestions
- Real-time insights on molecular interactions

3 Storage & Database Layer

- ◆ Database for storing user-uploaded sequences & molecules
- ◆ Cloud-based storage for AI-generated outputs (AWS S3, Firebase, or Local Storage)
- ◆ Molecular interaction logs & scoring history

4 Web Application & Visualization Layer (Front-End/UI)

- ✓ Streamlit-based UI for interactive results visualization
- ✓ 3D Protein-Molecule Docking Viewer
- ✓ Real-time AI insights via Gemini Chat Assistant
- ✓ Downloadable reports in CSV/PDF format

5 Deployment & Scalability

- ✓ Cloud Deployment (AWS/GCP/Render)
- ✓ Scalable API-based architecture for researchers & biotech companies

❖ Technologies Used in the Solution

◆ Development & Deployment

-  Google IDX (Cloud-based development)
-  FastAPI + Docker (Backend APIs)
-  Render (Scalable deployment)

◆ AI & ML Models

-  AlphaFold2  MolMIM + Oracle Model  DiffDock  RFDiffusion + ProteinMPNN  Gemini AI API

◆ Frontend & Visualization

-  Streamlit (Interactive UI for researchers)
-  PyMOL / ChimeraX (3D molecular visualization)
-  Plotly & Matplotlib (Data analytics)

◆ Storage & Data Processing

-  Google Firebase / PostgreSQL (Database)
-  AWS S3 / Google Cloud Storage (Molecular data storage)
-  RDKit + OpenMM (Computational chemistry & simulations)

◆ API Integrations

-  PubChem & ChEMBL API (Molecular data retrieval)



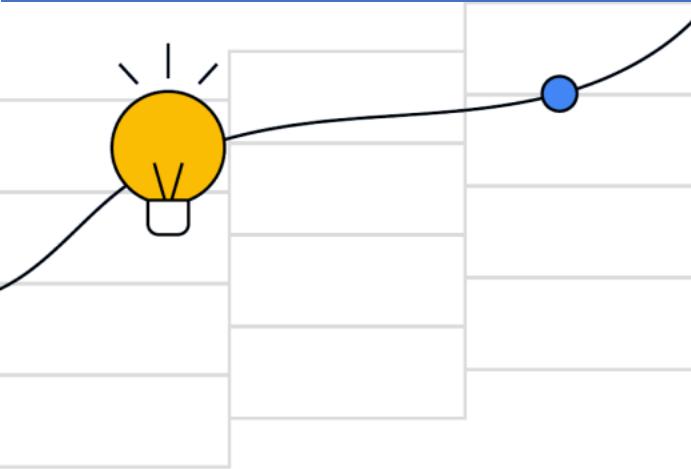
Snapshots of the MVP

 Future Development

- ◆ Advanced AI Integration – Improved **Gemini AI** insights & **Graph Neural Networks** for drug discovery
- ◆ Expanded Drug Discovery – AI-driven **toxicity prediction** & **multi-target drug design**
- ◆ Scalability & Usability – Cloud + On-premise deployment, **collaborative research tools**

|| Important Links ||

- 1.GitHub Public Repository :
- 2.Demo Video Link :
- 3.MVP Link :



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Thank you

