System Requirements Specification (SRS) for Ailixir

1. Functional Requirements (F.R.)

These requirements define the core functionalities the system must perform for the user.

User and Access Management

ID	Functional Requirement	Description	Source (Use Case)
F.R. 1.1	**Secure Registration & Login**	The system must allow researchers to securely register and log in using email and a password.	Login, Register
F.R. 1.2	**Profile Management**	The system must allow users to modify their personal details and change their password.	Manage Profile
F.R. 1.3	**Admin Dashboard**	The system must provide a dedicated interface for the **Admin** role to manage user accounts and view system statistics.	Manage Users & Stats

F.R. 2: Core AI Functionalities (AI Pipeline)

ID	Functional Requirement	Description	Core Stage
F.R. 2.1	**Compound Input**	The system must accept compounds in **SMILES** and **.sdf** formats, providing an interface to convert them to the internal processing format (e.g., **.sdfqt** if needed).	Generation
F.R. 2.2	**Efficacy Prediction**	The system must provide a tool to predict the efficacy of a compound against a specified disease target.	Prediction
F.R. 2.3	**Safety Filtering (ADMET)**	The system must evaluate the **ADMET** properties of a compound to assess its safety, absorption, and toxicity.	Filtering
F.R. 2.4	**Drug Repurposing**	The system must suggest potential therapeutic uses for a known compound.	Drug Repurposing

F.R. 3: Simulation and Visualization

ID	Functional Requirement	Description	Source (Use Case)
F.R. 3.1	**Protein Target Input**	*The system must accept the Protein via **PDB ID** or file upload in **.pdb** format, and the service must include a **preparation/conversion** step to convert the protein to the **.pdbqt** format before starting the simulation.	Run Docking Simulation
F.R. 3.2	**Docking Execution** **(Binding)**	The system must perform molecular docking simulation between the input compound and the target protein.	Run Docking Simulation
F.R. 3.3	**3D Visualization**	The system must display the compound and its binding site with the protein in an interactive **3D viewer**.	View 3D Visualization

F.R. 4: Job System and Community

ID	Functional Requirement	Description	Source (Use Case)
F.R. 4.1	**Job Status Tracking**	The system must provide an interface to track the status of submitted AI tasks (Pending, Running, Completed, Failed).	View History & Results
F.R. 4.2	**Result Export**	The system must allow result export in standard files (**CSV** or **PDF**), which contains the tested poses and conformations of the compound.	Export Report
F.R. 4.3	**Chat with AI**	The system allow chatting with agent about chemistry ,drugs and disease.	Chat with AI
F.R. 4.4	**News**	User can be UpToDate for new news ,share and save it.	View news

2. Non-Functional Requirements (N.F.R.)

These requirements specify the quality attributes and constraints of the system.

N.F. 1: Performance

ID	Non-Functional Requirement	Measurement
N.F.R. 1.1	**API Responsiveness**	*# The response time for non-AI operations must be less than **500 milliseconds**.
N.F.R. 1.2	**Simple AI Latency**	*# Results for simple AI predictions must be provided in under **60 seconds e.g.Admit.**
N.F.R. 1.3	**Docking Completion Time**	*# Users must be notified of the Docking simulation result within a maximum of **15 minutes** for standard compounds.
N.F.R. 1.4	**System Throughput**	*#The system must be able to handle **30 concurrent AI jobs** without significant degradation.

N.F. 2: Security

ID	Non-Functional Requirement	Description
N.F.R. 2.1	**Data Encryption**	All sensitive data transmission must occur over **HTTPS/SSL**, and passwords must be stored using **strong hashing**.
N.F.R. 2.2	**Access Control**	The system must strictly enforce that users can only view or delete the jobs and data they created (**Ownership**).
N.F.R. 2.3	**API Key Protection**	API keys for external services must never be exposed to the client-side (Frontend).

N.F. 3: Usability

ID	Non-Functional Requirement	Description
N.F.R. 3.1	**User Feedback**	The application must provide **continuous and clear feedback** (e.g., progress bars) for long-running AI tasks.
N.F.R. 3.2	**Design Consistency**	The UI must be consistent, intuitive, and optimized for mobile devices.

N.F. 4: Scalability and Maintainability

ID	Non-Functional Requirement	Description
N.F.R. 4.1	**Modular Design**	The code must be structured using OOP principles like **SRP** and **Separation of Concerns** to allow independent updates of AI services.
N.F.R. 4.2	**Deployment Strategy**	The services must be containerized (using **Docker**) to facilitate easy horizontal scaling and deployment.
N.F.R. 4.3	**Code Documentation**	The internal codebase must be thoroughly documented using standardized methods (e.g., Docstrings).