Drug Discovery AI - Project Documentation

# 1. Project Overview

The Drug Discovery AI project is designed to assist researchers and scientists in evaluating the drug-likeness and toxicity of molecular compounds using AI-based models. The system takes in compound details, processes the data using predictive models, and provides insightful visualizations and results. It aims to accelerate early-stage drug development by offering quick assessments of compound viability.

# 2. Installation & Setup

To run the project locally:  
1. Clone the repository or download and extract the zip file.  
2. Navigate to the project directory.  
3. Ensure Python 3.8+ is installed.  
4. Install dependencies using `pip install -r requirements.txt` or from the `pyproject.toml`.  
5. Run the app using `python app.py`.

# 3. File Structure

The main components of the project are organized as follows:  
- app.py: Main application file (likely Streamlit or Flask).  
- models/: Contains model logic like druglikeness and toxicity analysis.  
- utils/: Helper utilities for authentication and system operations.  
- data/: Contains datasets like logs and user details.  
- outputs/: Contains visual output files like charts and predictions.

# 4. How the App Works

Users input compound details via the app interface. These are processed by AI models located in the `models` directory. The models return predictions about drug-likeness and toxicity. Results are displayed using graphical outputs and stored in logs.

# 5. Model Details

The project uses cheminformatics models to evaluate:  
- Drug-likeness: Assesses the chemical features and structure.  
- Toxicity: Evaluates harmful effects based on molecular structure.

# 6. Usage Instructions

1. Launch the app with `python app.py`.  
2. Upload or enter molecule data.  
3. Click 'Analyze' to receive predictions.  
4. View outputs in graphical form and download results if needed.

# 7. Future Scope

- Integrate a larger training dataset to improve model accuracy.  
- Add support for 3D structure analysis.  
- Enable export to medical databases.  
- Implement user profile management and analytics dashboard.

# 8. Credits

Developed as part of a project focused on AI in drug discovery.  
Credits to open-source contributors and cheminformatics libraries used.