**Manual for Fungicide Early Warning System**

**1. Overview**

The Fungicide Early Warning System is a GUI-based application designed to predict the biological responses (MDA and ROS) of organisms exposed to fungicides in aquatic or soil environments, and provide an early warning of potential risks. It uses machine learning models trained on relevant datasets to generate predictions based on user inputs.

**2. System Requirements**

Operating System: Windows, macOS, or Linux.

Software Dependencies:

Python 3.7 or higher.

Required Python libraries: tkinter, pandas, numpy, scikit-learn, openpyxl.

Training data files:

For aquatic environment: aquatic\_MDA\_train.xlsx and aquatic\_ROS\_train.xlsx.

For soil environment: soil\_MDA\_train.xlsx and soil\_ROS\_train.xlsx.

**3. Installation & Setup**

Download Files:

Download the application code (Fungicide\_warning.py) and the required training data files (see Section 2) from the GitHub repository.

Place all files in the same directory (folder) on your computer.

Install Dependencies:

Open a terminal/command prompt, navigate to the directory containing the files, and run:

# Install Python libraries

pip install pandas numpy scikit-learn openpyxl

# For Linux users (to install tkinter, required for GUI):

sudo apt-get install python3-tk

**4. Launching the Application**

Open a terminal/command prompt, navigate to the directory with Fungicide\_warning.py, and run:

python Fungicide\_warning.py

The application window titled "Early Warning System for Fungicides" will open.

**5. User Interface Layout**

The interface is divided into two main sections:

Left Panel (Data Input Area): For entering parameters (medium, compound, concentration, etc.).

Right Panel (Result Display Area): For showing prediction results (MDA, ROS, and risk warning).

**6. Step-by-Step Operation**

**6.1 Select the Environment Medium**

Choose between "Aquatic" or "Soil" using the radio buttons.

This selection automatically updates the available options for compounds, species, and tissues (specific to the chosen medium).

**6.2 Enter Input Parameters**

|  |  |
| --- | --- |
| Parameter | Description & Requirements |
| Compound | Select a fungicide from the dropdown menu (options depend on the selected medium). |
| Concentrations | Enter the concentration of the fungicide (in mg/kg or mg/L). Must be a numeric value (e.g., 0.5). |
| Exposure Time | Enter the exposure duration (in days). Must be a numeric value (e.g., 7). |
| Species | Select a target species from the dropdown menu (optional, but at least one of "Species" or "Tissue" must be selected). |
| Tissue | Select a target tissue from the dropdown menu (optional, but at least one of "Species" or "Tissue" must be selected). |

**6.3 Run the Prediction**

Click the "Model Prediction" button in the right panel.

If inputs are valid, the system will process the data using pre-trained models and display results.

**7. Interpreting Results**

The right panel shows three key outputs:

MDA Prediction:

Values: 0 (No Response), 1 (Inhibition), 2 (Stimulation).

Indicates the predicted MDA (Malondialdehyde) response of the organism.

ROS Prediction:

Values: 0 (No Response), 2 (Stimulation).

Indicates the predicted ROS (Reactive Oxygen Species) response of the organism.

Early Warning Result:

Potential Risk (displayed in red): Triggered if MDA is 1 or 2 and ROS is 2.

No Risk (displayed in green): All other cases.

**8. Troubleshooting**

"File Not Found" Error: Ensure the training data files (e.g., aquatic\_MDA\_train.xlsx) are in the same directory as Fungicide\_warning.py.

"Input Error" (Empty/Non-numeric Values): Ensure "Concentrations" and "Exposure Time" are filled with valid numbers (no text or symbols).

"Input Error" (No Species/Tissue Selected): At least one of "Species" or "Tissue" must be selected from their dropdown menus.

**9. Notes**

The models are trained on specific datasets; predictions are most reliable for inputs similar to the training data.

For updates or bug reports, refer to the GitHub repository where the application is hosted.