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Artificial Intelligence and Machine Learning (AI/ML) Models for Predicting Drug-Induced Kidney Injury (DIKI) in Small Molecules

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Abstract

The predDIKI package predicts the probability of drug-induced kidney injury (DIKI) using key physicochemical properties and off-targets. This document explains how to install the package and use its Shiny application for easy DIKI risk prediction and classification.

Installation Instructions

Step 1: Install Required Packages

To use `predDIKI`, you first need to install the necessary R packages. The following R code will check and install any missing dependencies:

```r
# List of required packages
packages <- c(
        'openxlsx', 'ggplot2', 'reshape2', 'ggforce',
        'glmnet', 'caret', 'nnet', 'e1071',
        'ggrepel', 'shiny', 'testthat'
)

# Function to check and install missing packages
install_if_missing <- function(pkg) {
    if (!require(pkg, character.only = TRUE)) {
        install.packages(pkg, dependencies = TRUE)
        library(pkg, character.only = TRUE)
    }
}

# Install required packages
lapply(packages, install_if_missing)
```

Step 2: Install predDIKI Package

Once the required packages are installed, you can install the **predDIKI** package from a local file. Replace `'/path/to/predDIKI_0.1-0.tar.gz'` with the actual path to the package file:

```r
install.packages('/path/to/predDIKI_0.1-0.tar.gz', repos = NULL, type = 'source')
```

Step 3: Run the Shiny App

```r
library(predDIKI)
predDIKI_app()
```

How to Use the Shiny Application

Step 1: Download the Input Template

- On the front page of the Shiny app (shown in **Figure 1**), click the "Download Template" button to get an Excel template.
- Fill in the required information about the physicochemical properties and off-targets for your test compounds.

Step 2: Upload Your Data

- Use the "Browse" button on the Shiny app to upload your completed Excel file.

Step 3: Run the Prediction

- After uploading the file, click the "Run predDIKI" button. The app will generate probability scores predicting nephrotoxicity for the test compounds.

Step 4: View and Download Results

- The results, including a violin plot comparing the nephrotoxicity probabilities for reference and test compounds, will be displayed (see **Figure 2**).

- Both the plot and the result table can be downloaded for further use.

Offline Use and Internal Deployment

Since the installation file and all source code are provided, `predDIKI` can be run entirely on your local machine without needing to upload data to a public server. If you want to deploy the application on an internal server, you can easily do so using free open-source technologies like ShinyProxy.

Figures
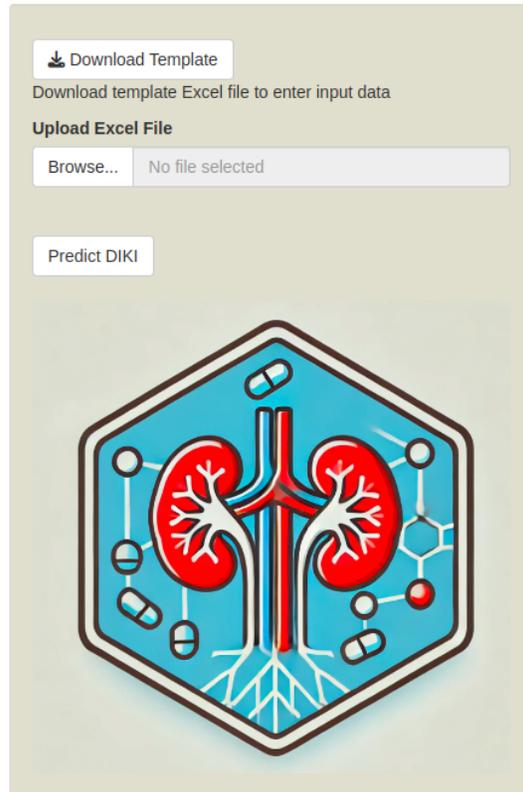
Figure 1: Front page of 'predDIKI' Shiny application.
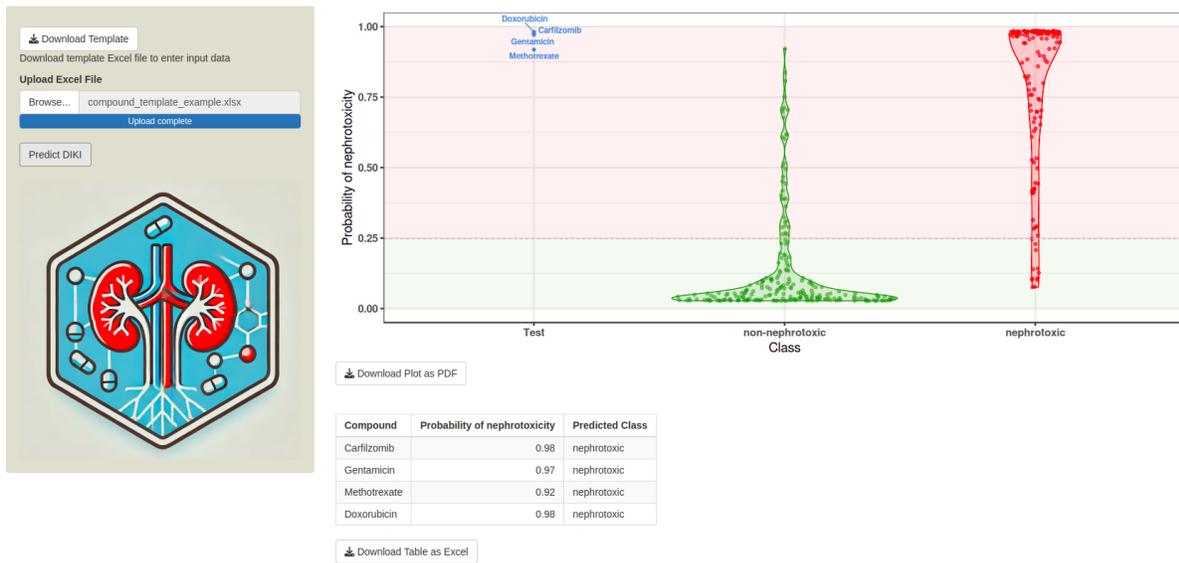
Figure 2: Example output from the 'predDIKI' Shiny application.