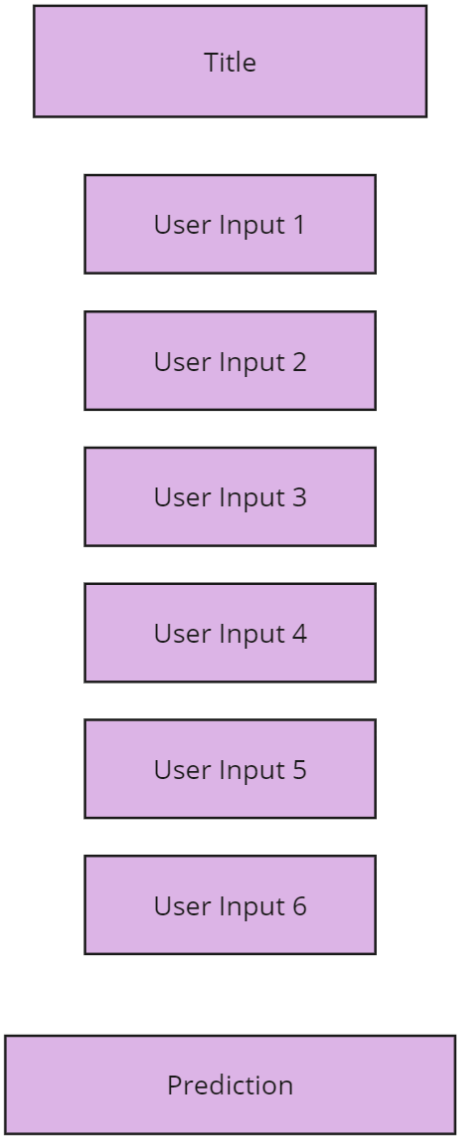
Prediction of LC50 value using Quantitative Structure Activity Relationship models

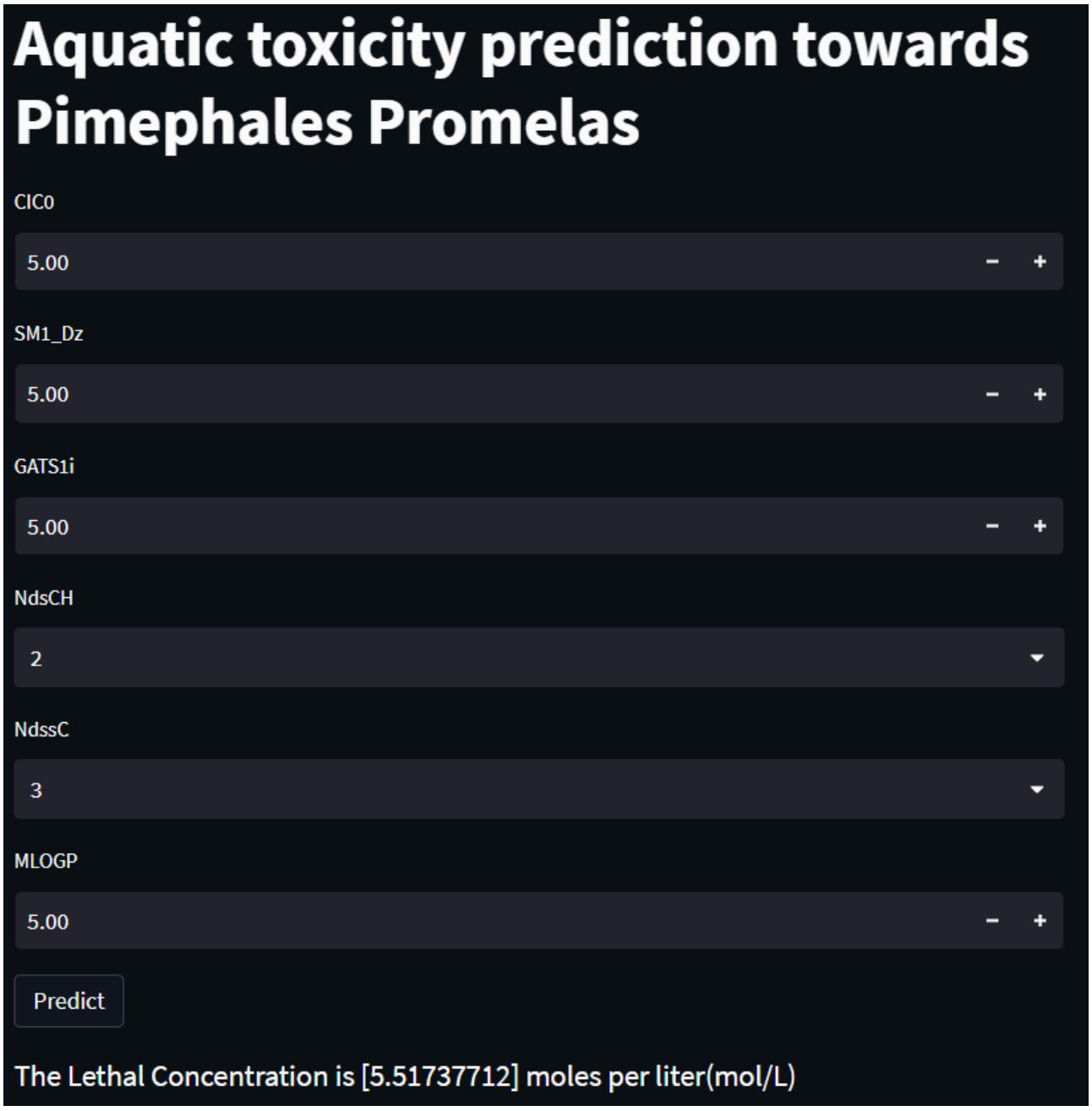
WIREFRAME DOCUMENTATION

Homepage

Designed UI



Implementation



The Streamlit app presented here is designed for predicting aquatic toxicity towards Pimephales Promelas based on a pre-trained machine learning model. The model, loaded from 'fish_model_5.sav', is complemented by a scalar ('fish_scale.sav') and a one-hot encoding function. The user interface allows for inputting various features related to aquatic toxicity, such as CIC0, SM1_Dz, GATS1i, NdsCH, NdssC, and MLOGP.

Upon entering the feature values, the user can initiate the prediction by clicking the "Predict" button. The input data is then processed by the model, and the predicted lethal concentration is displayed. The displayed result is in the unit of moles per liter (mol/L).

The code incorporates dropdown menus for categorical features (NdsCH and NdssC), enabling users to select values from predefined options. The default values for these dropdowns are set to 2 and 3, respectively. Additionally, numerical features such as CIC0, SM1_Dz, GATS1i, and MLOGP can be fine-tuned using number input fields, allowing users to specify values within a defined range.

The application follows a clean and user-friendly design, making it easy for users to interact with and obtain predictions. It leverages Streamlit's capabilities to create an intuitive web-based interface for toxicity prediction, facilitating the practical application of the underlying machine learning model.