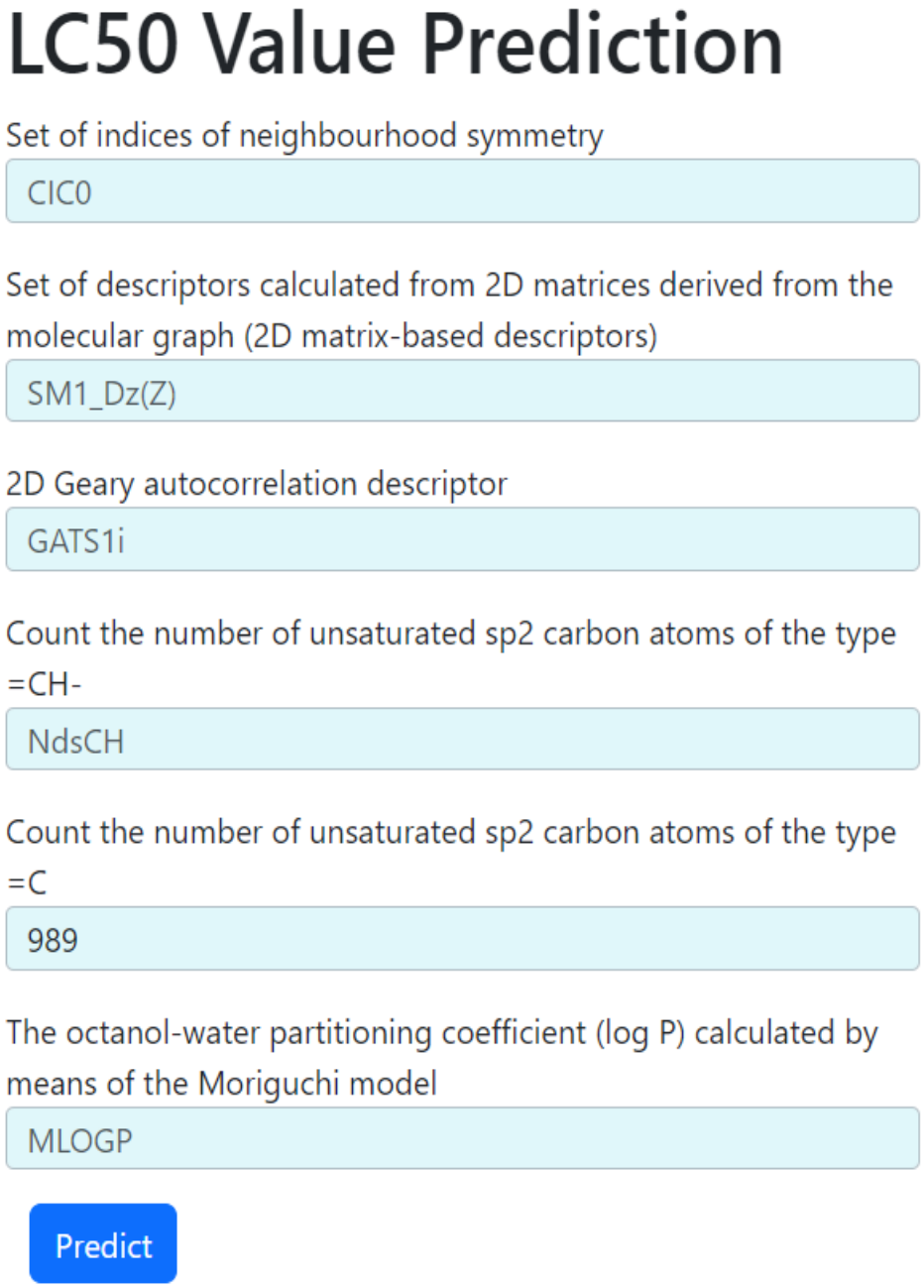
LC50 VALUE PREDICTOR

Wireframe Documentation

Homepage

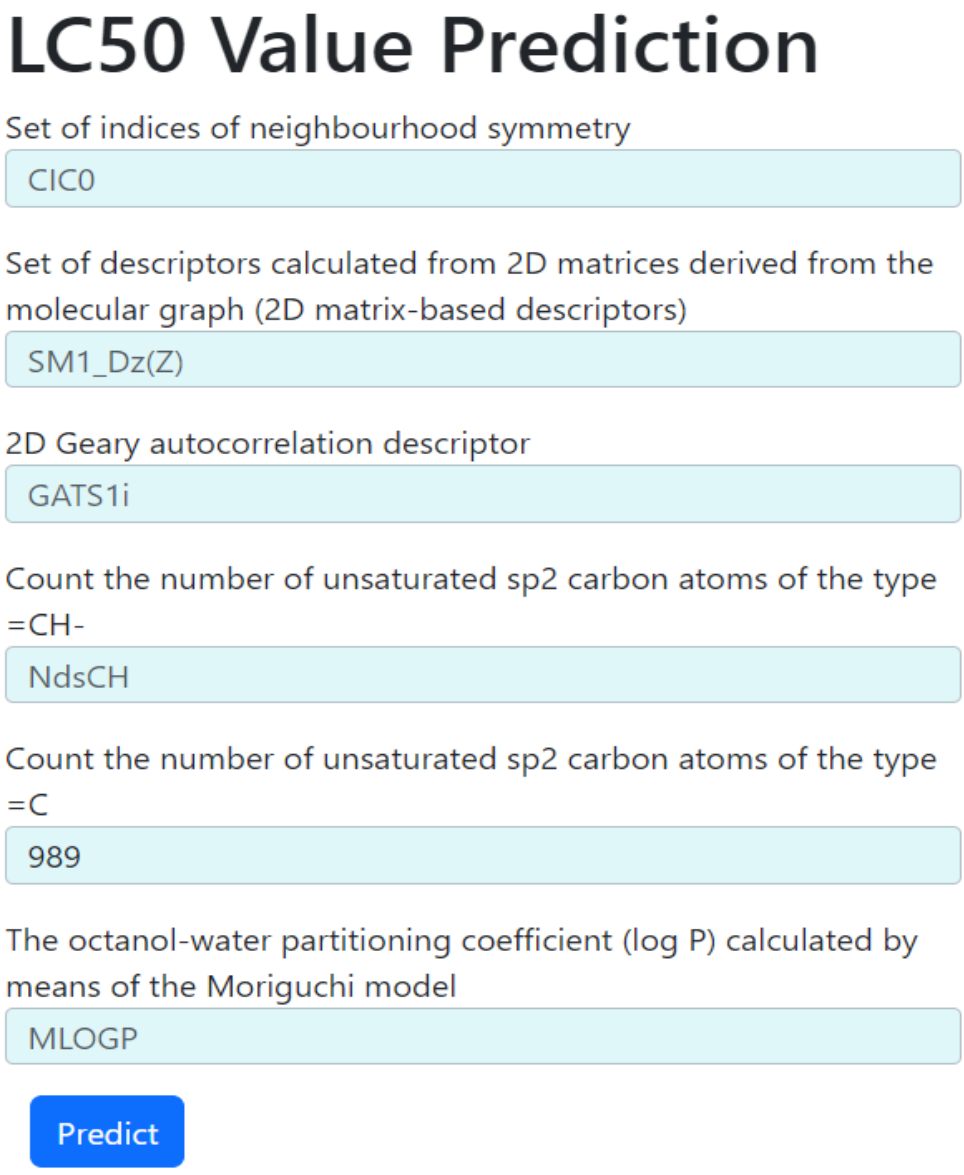
LC50 value predictor's Homepage into Two Sections:

1. Homepage that will ask for User Inputs for 6 mandatory chemical input values , to be entered into 6 entry widgets.



2. The Predict Button below the 6 entry widgets which on clicking takes the user to the Predict Page with Expected Value response on top of the page or an Internal Server Error message if invalid input has been entered.

Based on User's inputs, the LC50 value predictor calculates and predicts an Expected LC50 toxicity value. A sample view of Homepage showing results is below:



Predict Page

LC50 Value Prediction

Set of indices of neighbourhood symmetry

12

Set of descriptors calculated from 2D matrices derived from the molecular graph (2D matrix-based descriptors)

50

2D Geary autocorrelation descriptor

56

Count the number of unsaturated sp2 carbon atoms of the type =CH-

4

Count the number of unsaturated sp2 carbon atoms of the type =C

4

The octanol-water partitioning coefficient (log P) calculated by means of the Moriguchi model

8

Predict

The LC50 value is [4.809375]

Expected LC50 value displayed on top after entering 6 chemical descriptors and clicking Predict.

The application goes to a predict page where output response is predicted.