

S10: *MDM2pred* Usage

MDM2pred is an online (open source) web application developed using the K Neighbors machine learning developed in the present study. The application is developed in Python programming language and utilizes the *Streamlit* library (<https://github.com/streamlit/streamlit>) for its web components.

The application accepts a SMILES string (single mode) or a list of SMILES in a CSV file (batch mode), it processes the SMILES of any chemical compound as input and provides the predicted pIC50/IC50 values against MDM2 as the output along with a 2D diagram and the IUPAC name of the input (only in the single mode). *MDM2pred* is accessible from <http://ynlab.mu.edu.tr/tr/mdm2pred-6997>. The basic aspects and usage of the application are explained in Figure S1.

Figure S1 illustrates the access and usage of the *MDM2pred* application. The interface is shown in a browser window with the URL <http://ynlab.mu.edu.tr/tr/mdm2pred-6997>. The application is titled "MDM2pred" and is developed by Naeem Abdul Ghaffar, Aysegül Yılmaz, and Hülya Sözlü Koşman. The interface includes a 3D molecular model of MDM2, a description of the application, instructions for using the application, an input field for SMILES, a result section showing the predicted IC50, pIC50, 2D diagram, and IUPAC name, and a performance matrix of the K Neighbors model.

Labels a through f point to the following features:

- a: Link to *MDM2pred*'s main page application.
- b: General information and description about the application.
- c: Instructions for using the application.
- d: Input SMILES entry section.
- e: Result of the application, namely, the IC50, pIC50, 2D diagram of the compound, and its IUPAC name.
- f: Performance matrix of the K Neighbors model.

Figure S1. Access and usage of the *MDM2pred* application. (a) link to *MDM2pred*'s main page application; (b) general information and description about the application; (c) instructions for using the application; (d) input SMILES entry section; (e) result of the application, namely, the IC50, pIC50, 2D diagram of the compound, and its IUPAC name; (f) performance matrix of the K Neighbors model.

The source files of the application and codes to reproduce its results are available at: <https://github.com/naeemmrz/MDM2pred>