<u>Opendd v1 usage direction</u>

1. Run the 'opendd_1.py' file from a suitable python IDE (e.g. spyder) in a custom conda environment. The below gui window should appear.


2. (i) Download the example database of human coagulation factor X from chembl as csv format: https://www.ebi.ac.uk/chembl/g/#browse/activities/filter/target_chembl_id%3ACHEMBL244%20AND%20standard_type%3A(%22Ki%22)
(ii) Extract the downloaded file and save it as 'opendd_1/chembl_drug_prediction/input_data/ FX_targets_Ki_all_values.csv'. Then remove the rows other than '=' in 'Standard Relation' column and save the file as 'opendd_1/chembl_drug_prediction/input_data/ FX_targets_Ki_only_equal_values.csv'. This file will be used as the source file to construct the descriptor dataset.
(iii) Click on 'Browse csv' option on the GUI and select the 'opendd_1/chembl_drug_prediction/input_data/ FX_targets_Ki_only_equal_values.csv'.
(iv) After couple of hours, the descriptor dataset will be available at 'opendd_1/chembl_drug_prediction/input_data/ target_descriptors.csv'. At the same time, the

image dataset will be available at 'opendd_1/chembl_drug_prediction/input_data/target_images'.

If the datasets are already synthesized and available, directly go to step 3.
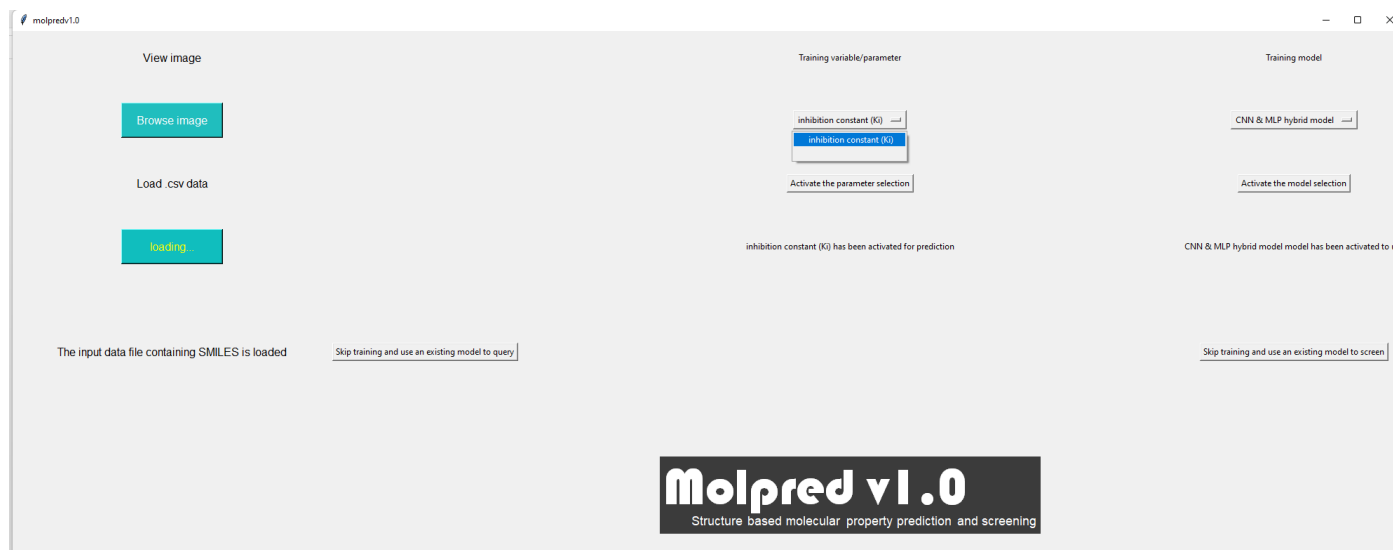
3. Select the training parameter (inhibition constant (Ki)) as below and click on the 'Activate the parameter selection'.
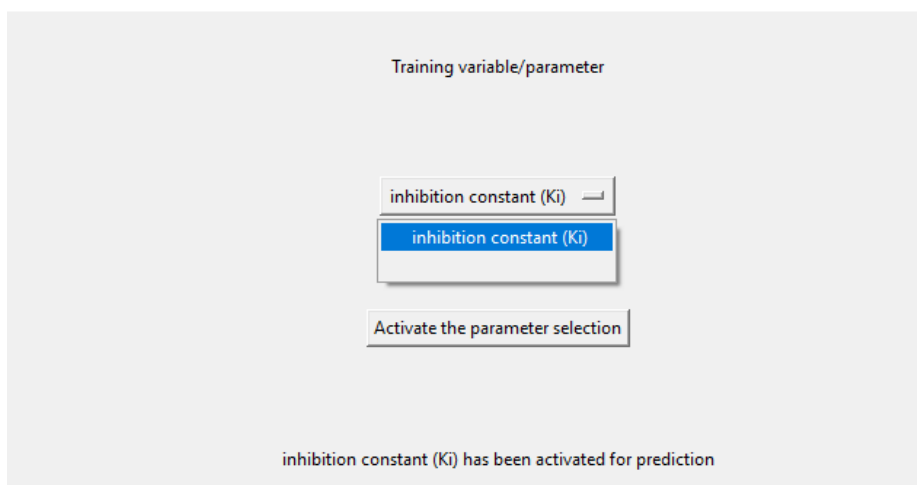
4. Select the training model ('CNN & MLP hybrid model') from the drop down option as shown below. Then activate the model selection button.
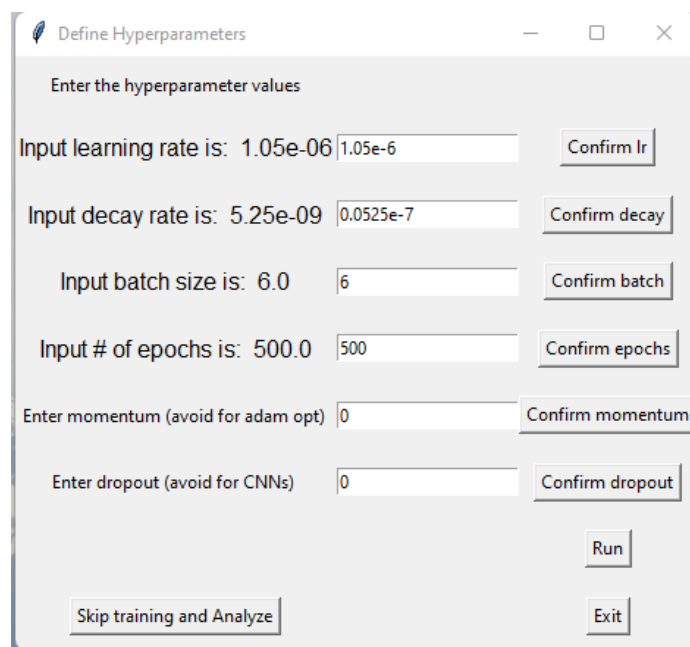
5. Once the model has been activated, input the network hyperparameters for executing the training. The confirm buttons as shown below are optional. These are just to check that the parameters are taken as inputs. Then click 'Run' button and start the training.

6. After the training is completed, the below window appears. The results are available as .png plots at this location 'opendd_1/chembl_drug_prediction/output_results'.