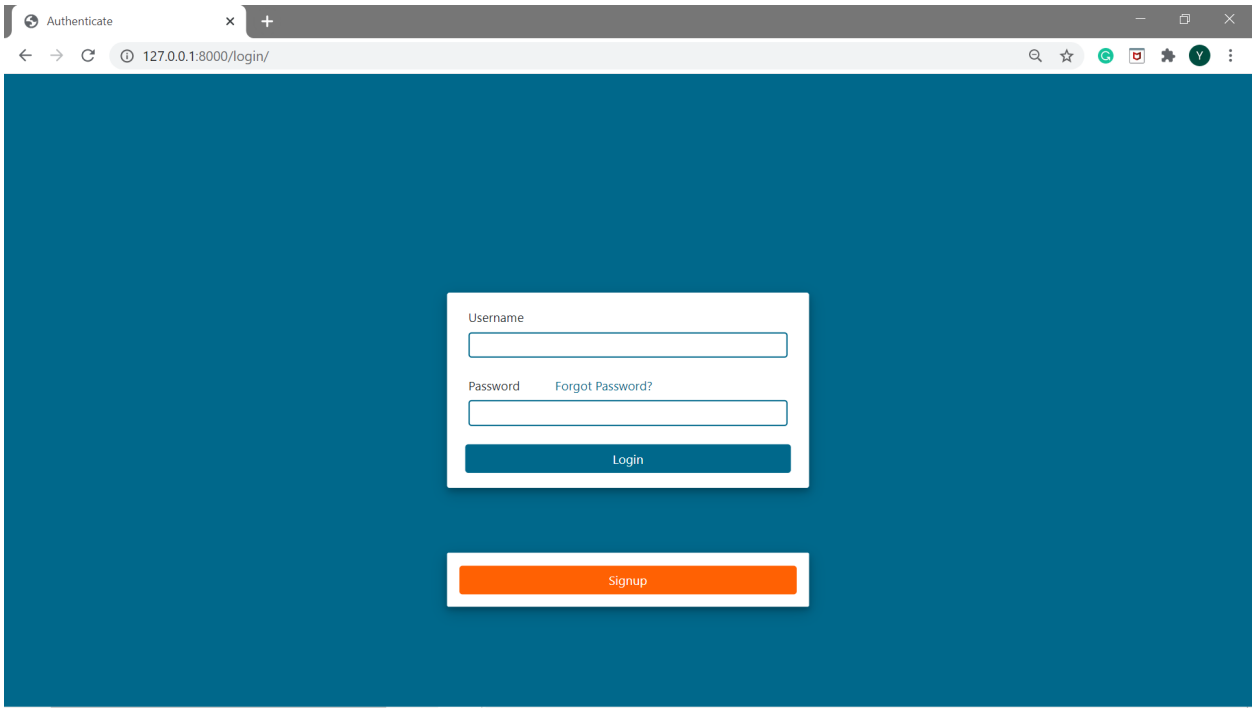
1. LOGIN

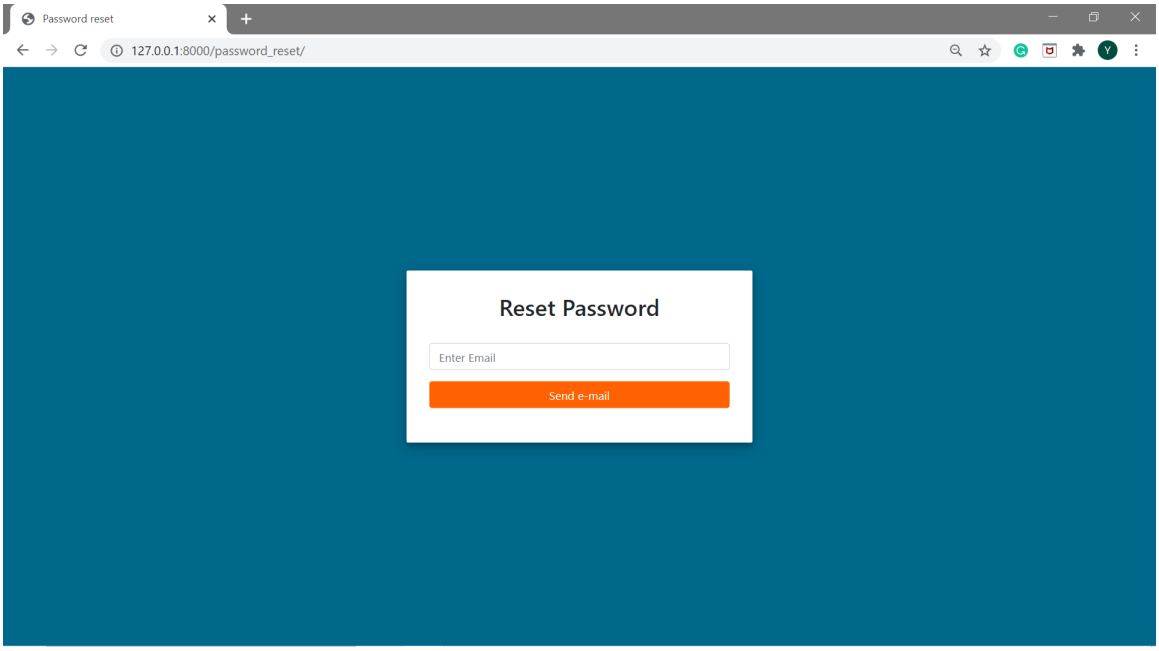


A. Login

If you already registered an account, login the website by your email address and password.

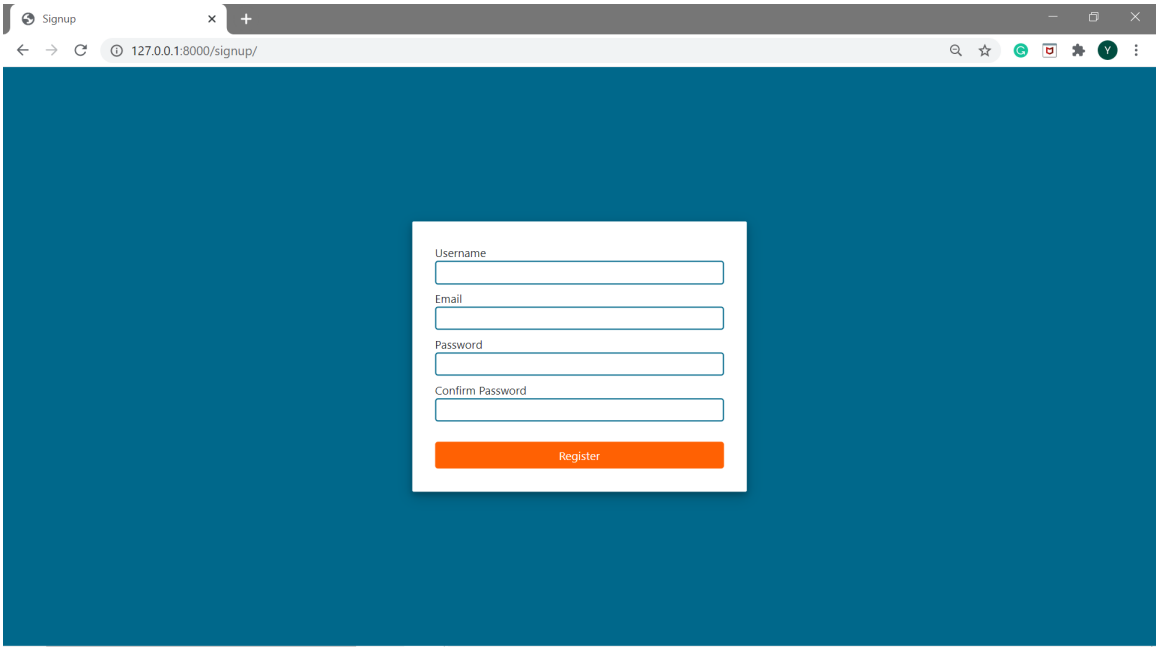
**** Forget Password ****

Click on the 'Forget Password?' and enter your registered email address to reset the password.

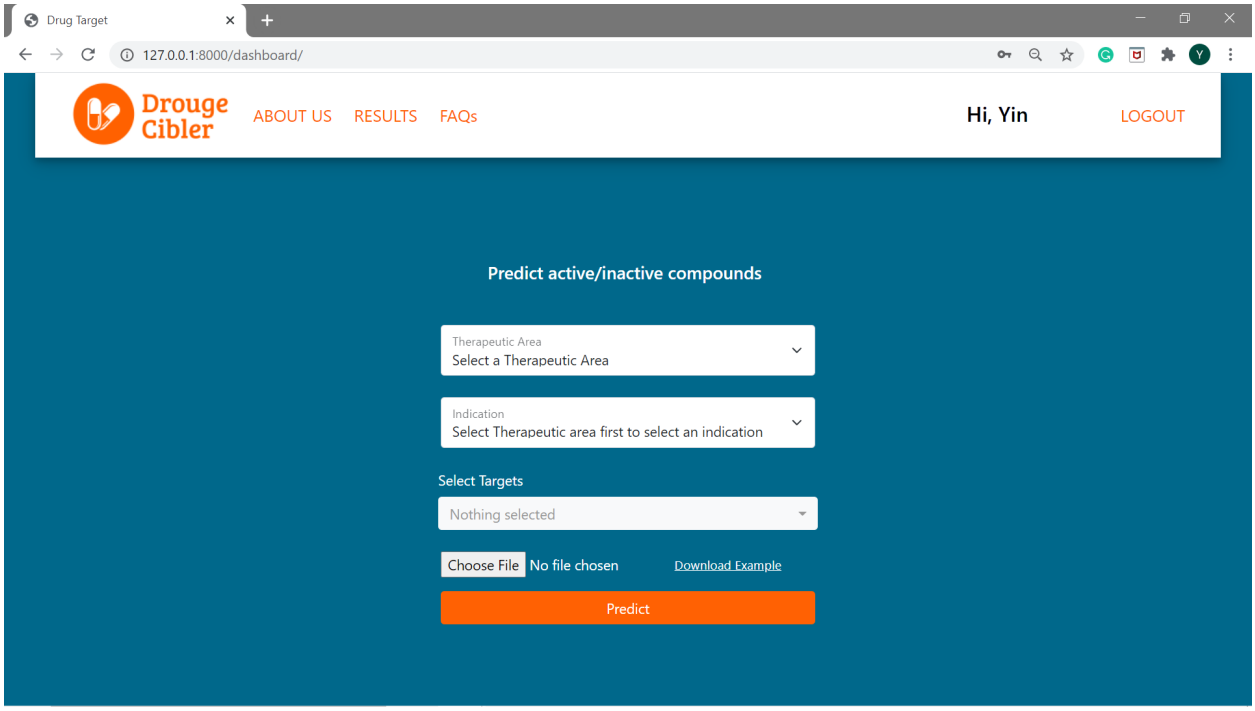


B. Sign Up

Register an account by your email address.



II. Drouge Cibler



A. Therapeutic Area

Select a therapeutic area for the disease of interest from the drop down list.

B. Indication

Select an indication of the therapeutic area from the drop down list for the disease of interest.

C. Targets

Select one or multiple targets of interest for compounds' bioactivity prediction.

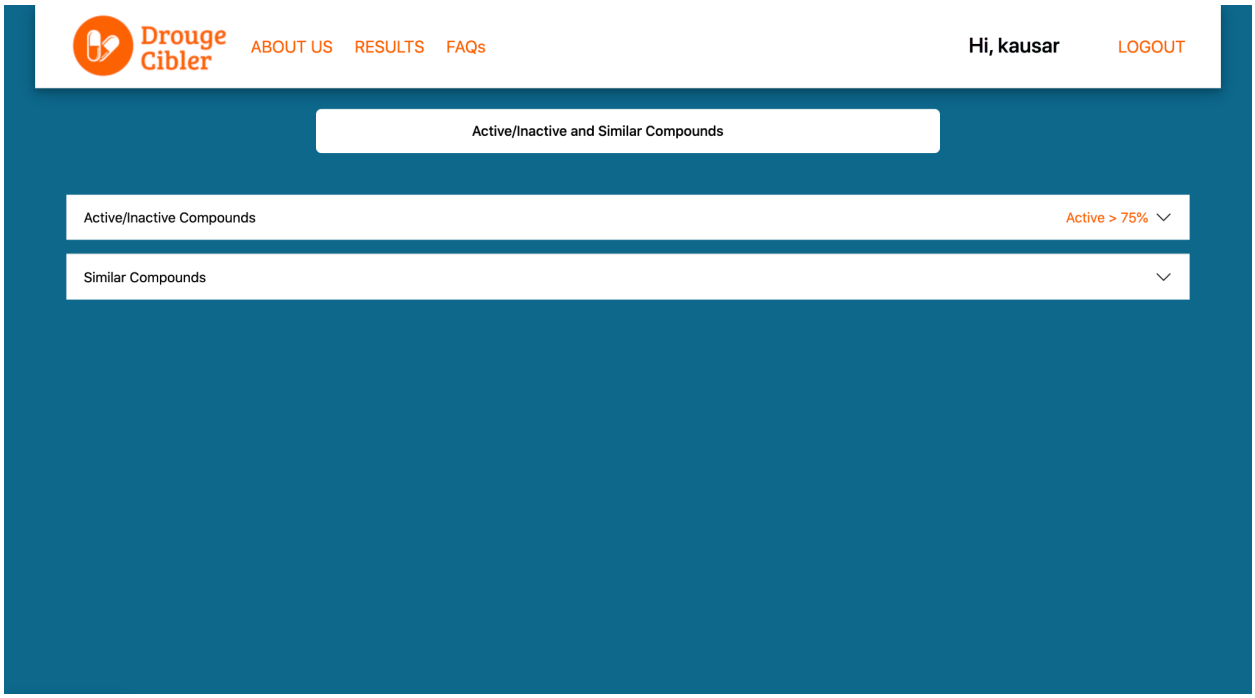
D. Choose File

Upload your csv file with SMILE notations in a column named 'canonical_smiles'.

E. Predict

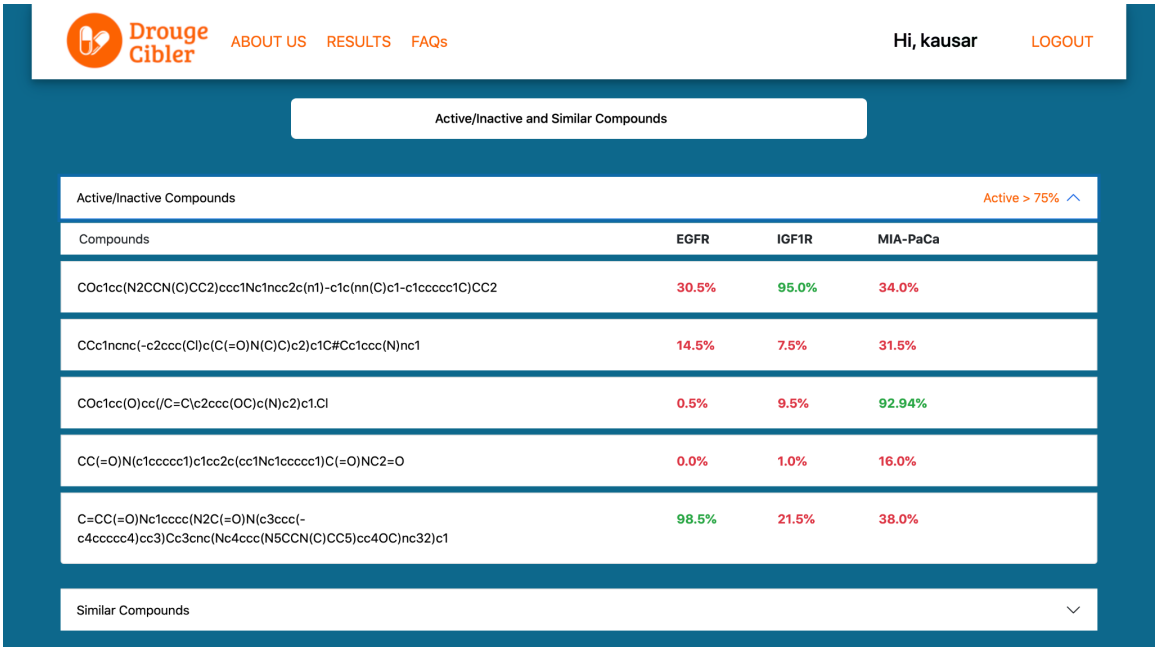
Click on the 'Predict' for bioactivity prediction.

III. RESULTS

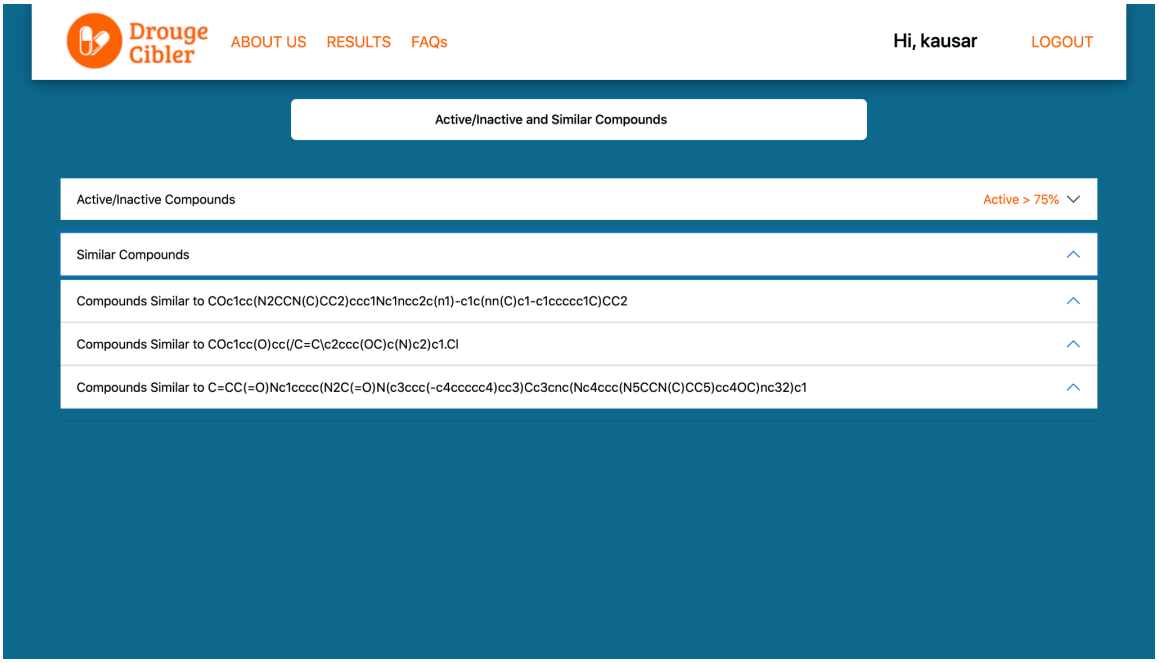


A. Active/Inactive Compounds

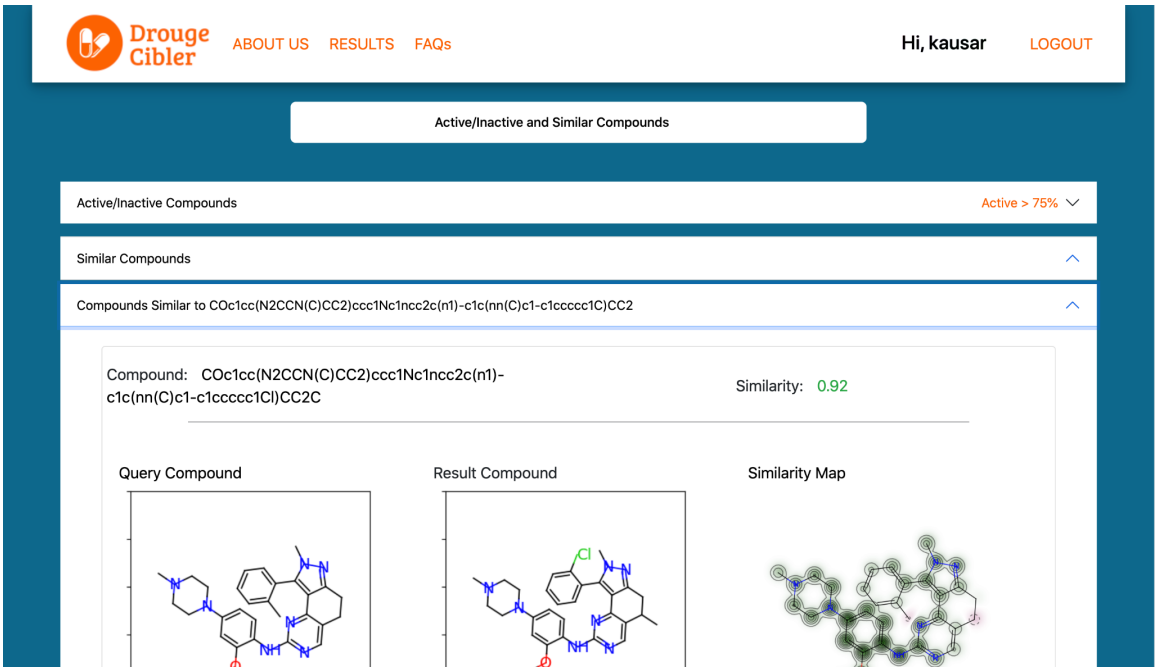
The probability of the test compound that is active to each selected target will be shown as a table below. By default, we consider the compound with higher than 75% probability as an active compound for the target.



B. Similarity Compounds

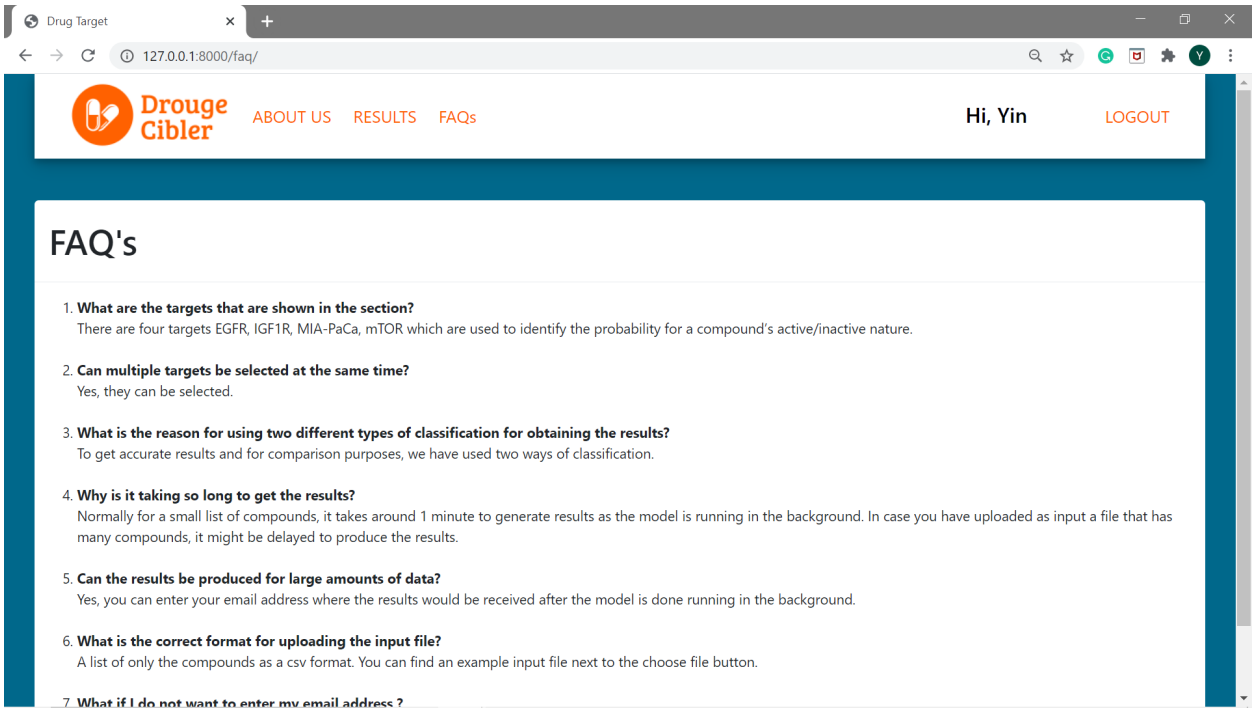


In this part, the active compounds in the backend database with >90% chemical structure similarity to each test compound will be listed.



IV. FAQs

Find answers for frequently asked questions in FAQs.



V. About us

Know more about this project and meet the team.

Click on the bar code below each member can link to his/her linkedin profile.

Drouge Cibler HOME ABOUT US RESULTS FAQs USER MANUAL Hi, kausar LOGOUT

About the Project

In order to ensure rapid drug development, this project is useful in identifying the potential drug compounds which can be classified as active/inactive for given four targets after knowing their probability. A higher probability above 80 indicates an active compound where as a lower probability below 20 indicates an inactive compound.

Approach

The results are predicted with the help of two models running in the background :

- **Binary Label Classification (Model1)** works by evaluating the probability through a single model for each target so there are four different models for four different targets.
- **Multi Label Classification (Model2)** works by evaluating the probability through a single model for all given targets i.e there is one model for all four targets.

Meet the team

ANURAG GUNTI

LinkedIn

AYUSH DADHICH

LinkedIn

KAUSAR PERVEEN

LinkedIn

YIN YANG

LinkedIn