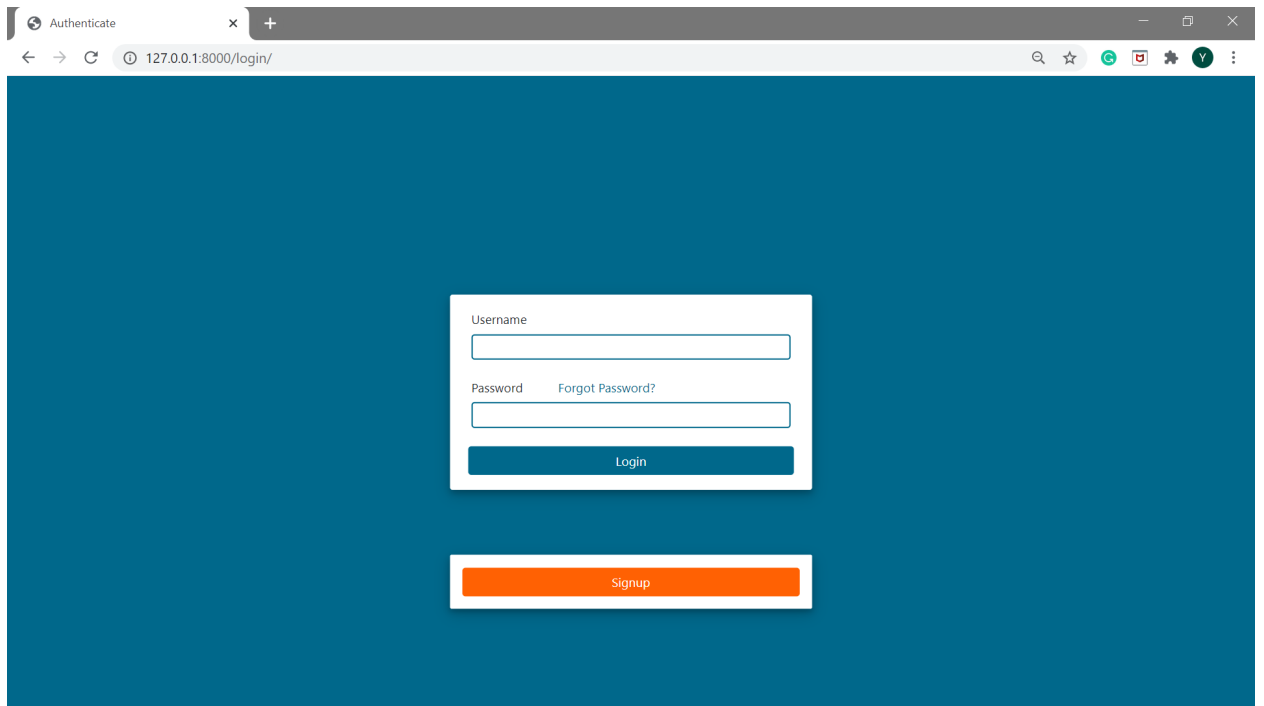


# 1. LOGIN

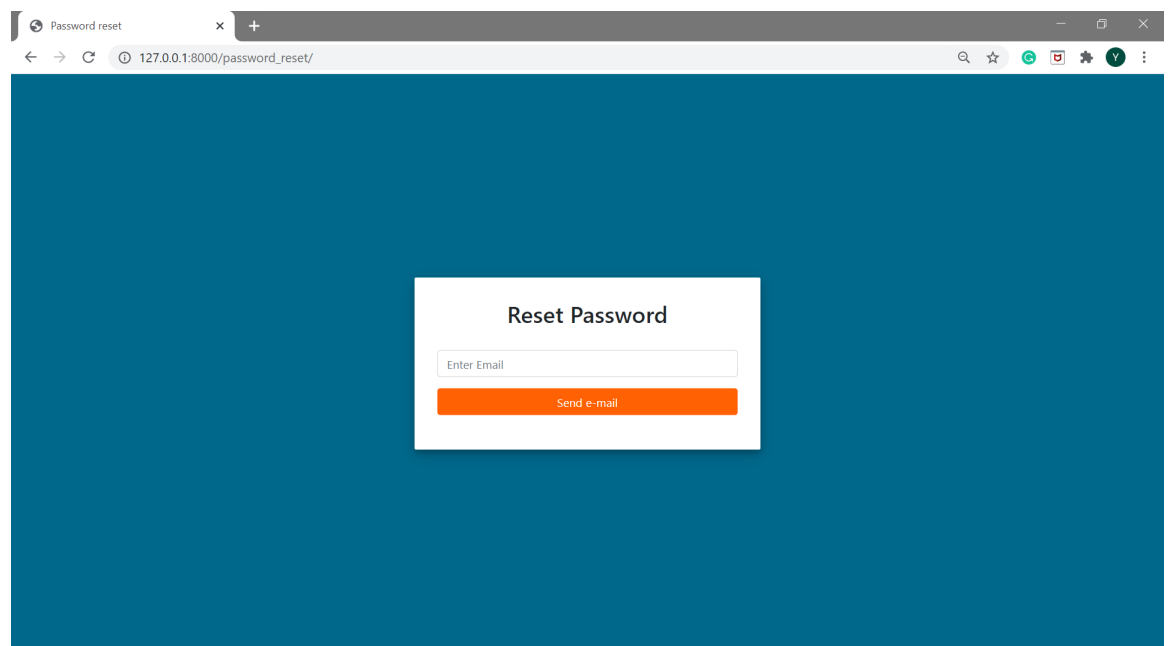


## A. Login

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

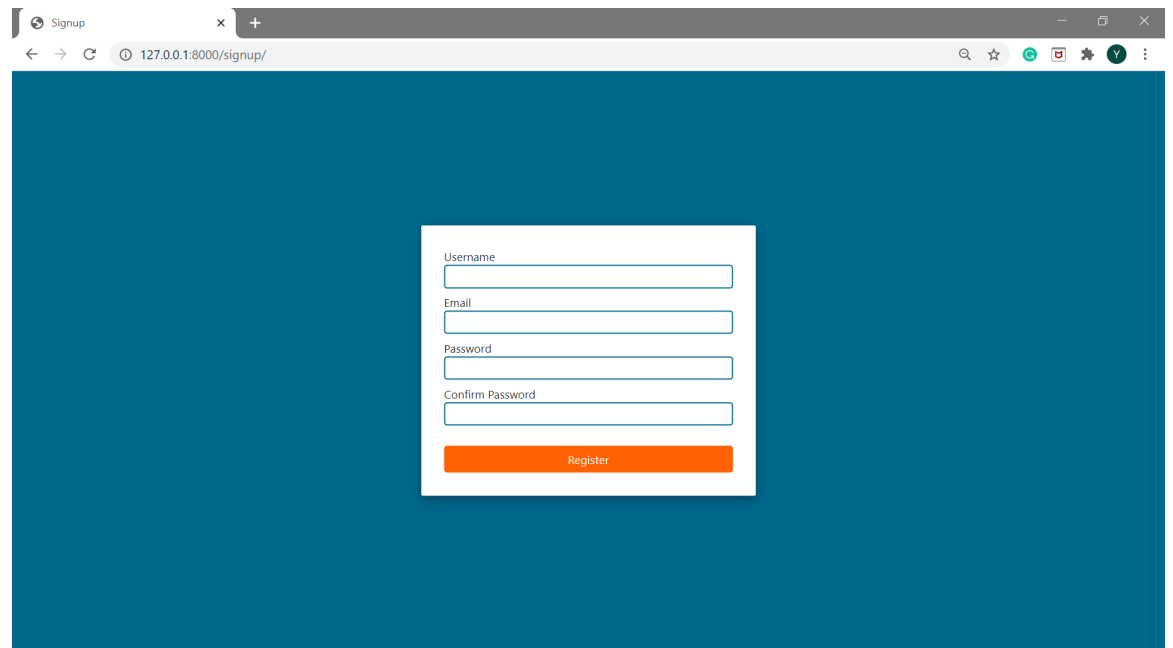
**\*\* Forget Password \*\***

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



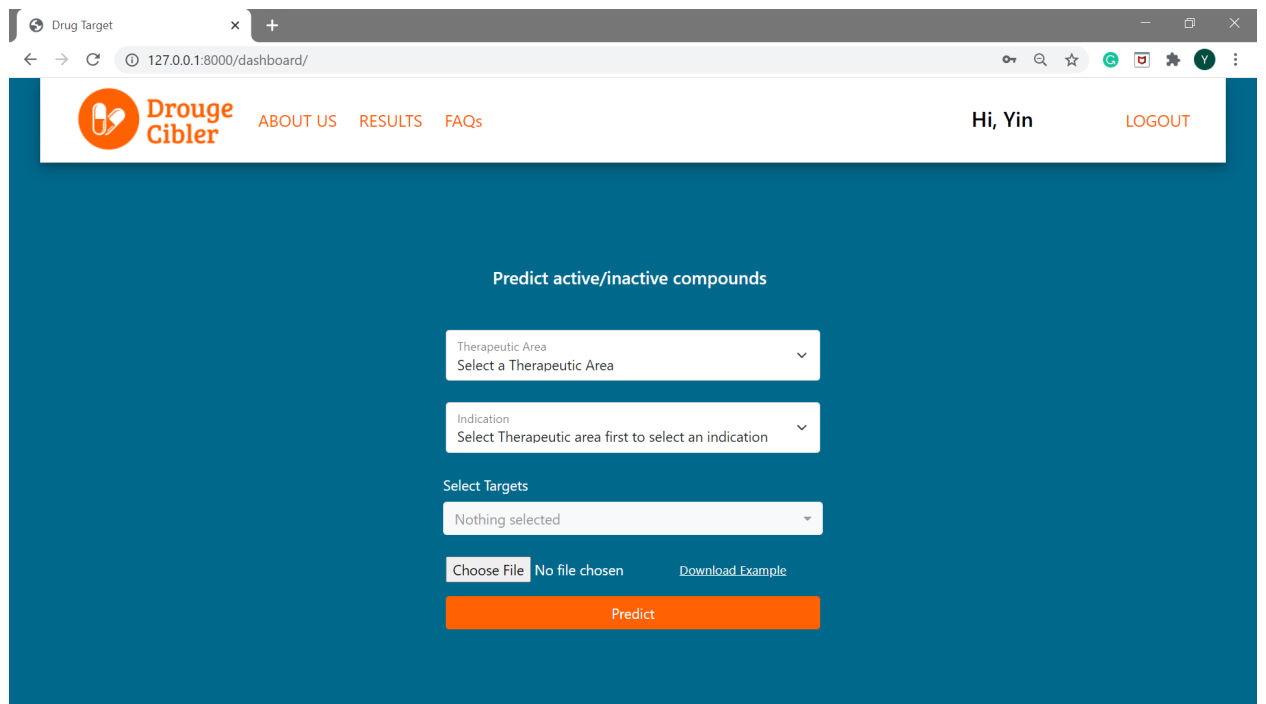
## B. Sign Up

Register an account by your email address.



A screenshot of a web browser showing a 'Sign Up' page. The browser's address bar displays '127.0.0.1:8000/signup/'. The page has a solid blue background. In the center, there is a white rectangular form with the following fields: 'Username', 'Email', 'Password', and 'Confirm Password'. Each field is represented by a white input box with a thin blue border. Below these fields is an orange button labeled 'Register'.

## II. Drouge Cibler



A screenshot of the 'Drug Target' dashboard for 'Drouge Cibler'. The browser's address bar shows '127.0.0.1:8000/dashboard/'. The dashboard has a white header bar with the 'Drouge Cibler' logo on the left, navigation links 'ABOUT US', 'RESULTS', and 'FAQs' in the center, and a user greeting 'Hi, Yin' with a 'LOGOUT' link on the right. The main content area has a blue background. At the top of this area is the heading 'Predict active/inactive compounds'. Below this are three dropdown menus: 'Therapeutic Area' (with the placeholder 'Select a Therapeutic Area'), 'Indication' (with the placeholder 'Select Therapeutic area first to select an indication'), and 'Select Targets' (with the placeholder 'Nothing selected'). Below the dropdowns are two links: 'Choose File' and 'Download Example', followed by a text status 'No file chosen'. At the bottom of the form is an orange button labeled 'Predict'.

### 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.

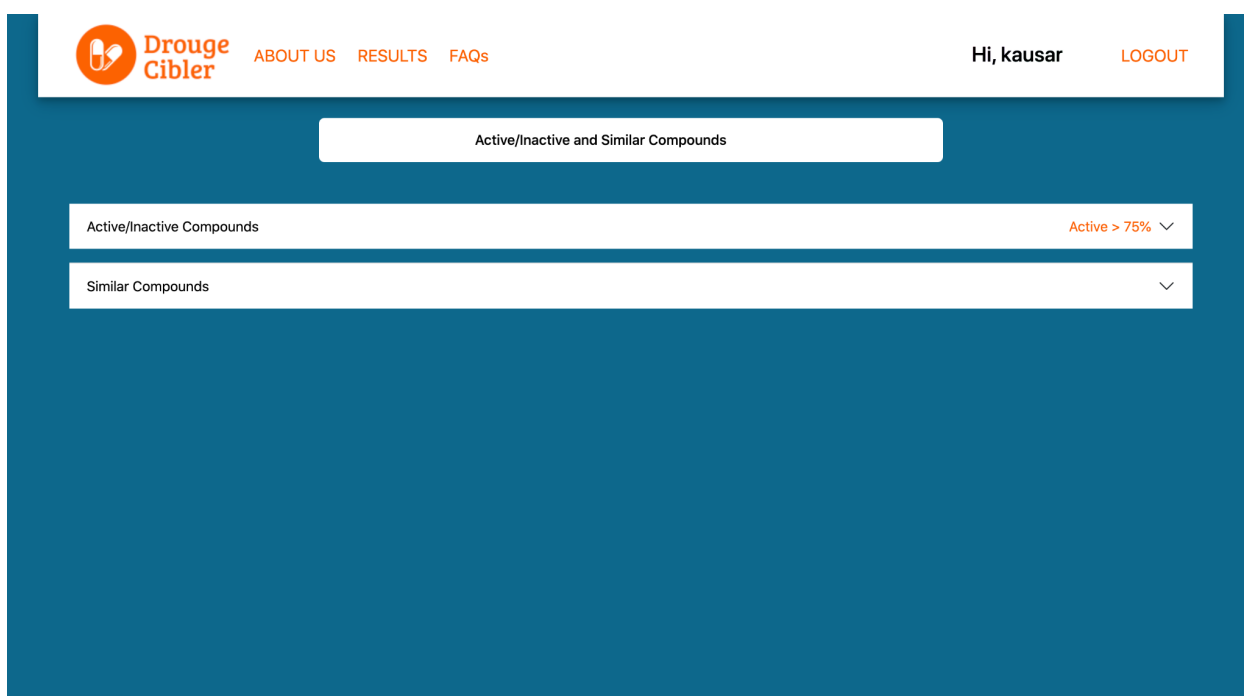
## D. Choose File

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.

Drouge  
Cibler

[ABOUT US](#)

[RESULTS](#)

[FAQs](#)

Hi, kausar

LOGOUT

Active/Inactive and Similar Compounds

Active/Inactive Compounds


Active > 75% ^

Compounds	EGFR	IGF1R	MIA-PaCa
<chem>COc1cc(N2CCN(C)CC2)ccc1Nc1nc2c(n1)-c1c(nn(C)c1-c1cccc1C)CC2</chem>	30.5%	95.0%	34.0%
<chem>CCc1ncnc(-c2ccc(Cl)c(C(=O)N(C)C)c2)c1C#Cc1ccc(N)nc1</chem>	14.5%	7.5%	31.5%
<chem>COc1cc(O)cc(/C=C/c2ccc(OC)c(N)c2)c1.Cl</chem>	0.5%	9.5%	92.94%
<chem>CC(=O)N(c1cccc1)c1cc2c(cc1Nc1cccc1)C(=O)NC2=O</chem>	0.0%	1.0%	16.0%
<chem>C=CC(=O)Nc1cccc(N2C(=O)N(c3ccc(-c4cccc4)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1</chem>	98.5%	21.5%	38.0%

Similar Compounds

v

## B. Similarity Compounds

Drouge  
Cibler

[ABOUT US](#)

[RESULTS](#)

[FAQs](#)

Hi, kausar

[LOGOUT](#)

Active/Inactive and Similar Compounds

Active/Inactive Compounds

Active > 75% ▾

Similar Compounds

⬆

Compounds Similar to COc1cc(N2CCN(C)CC2)ccc1Nc1nc2c(n1)-c1c(nn(C)c1-c1cccc1C)CC2

⬆


Compounds Similar to COc1cc(O)cc(/C=C/c2ccc(OC)c(N)c2)c1.Cl

⬆

Compounds Similar to C=CC(=O)Nc1cccc(N2C(=O)N(c3ccc(-c4cccc4)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1

⬆

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


ABOUT US RESULTS FAQs
Hi, kausar LOGOUT

Active/Inactive and Similar Compounds

Active/Inactive Compounds Active > 75% ▾

Similar Compounds ⬆

Compounds Similar to COc1cc(N2CCN(C)CC2)ccc1Nc1ncc2c(n1)-c1c(nn(C)c1-c1ccccc1C)CC2 ⬆

Compound: COc1cc(N2CCN(C)CC2)ccc1Nc1ncc2c(n1)-c1c(nn(C)c1-c1ccccc1C)CC2

Similarity: 0.92


Query Compound

Result Compound

Similarity Map

## IV. FAQs

Find answers for frequently asked questions in FAQs.


ABOUT US RESULTS FAQs
Hi, Yin LOGOUT

FAQ's

- What are the targets that are shown in the section?**  
 There are four targets EGFR, IGF1R, MIA-PaCa, mTOR which are used to identify the probability for a compound's active/inactive nature.
- Can multiple targets be selected at the same time?**  
 Yes, they can be selected.
- What is the reason for using two different types of classification for obtaining the results?**  
 To get accurate results and for comparison purposes, we have used two ways of classification.
- Why is it taking so long to get the results?**  
 Normally for a small list of compounds, it takes around 1 minute to generate results as the model is running in the background. In case you have uploaded as input a file that has many compounds, it might be delayed to produce the results.
- Can the results be produced for large amounts of data?**  
 Yes, you can enter your email address where the results would be received after the model is done running in the background.
- What is the correct format for uploading the input file?**  
 A list of only the compounds as a csv format. You can find an example input file next to the choose file button.
- What if I do not want to enter my email address?**

## 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.

## 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

[Linked in](#)



AYUSH DADHICH

[Linked in](#)



KAUSAR PERVEEN

[Linked in](#)



YIN YANG

[Linked in](#)