

PM-BioPred: User Tutorial

Web-server for predicting compound bioactivity against Plant, Bacterial, Fungal, and Viral proteins

1. Access the Web Server

Open your browser and visit: <https://pmbiopred.streamlit.app/>

You will see the homepage with navigation options (Home, Prediction, Developers, Contact Us):



Figure 1: Homepage

This page introduces the tool and gives basic information about its purpose and use.

2. Navigate to the Prediction Page

Click **Prediction** from the left sidebar.

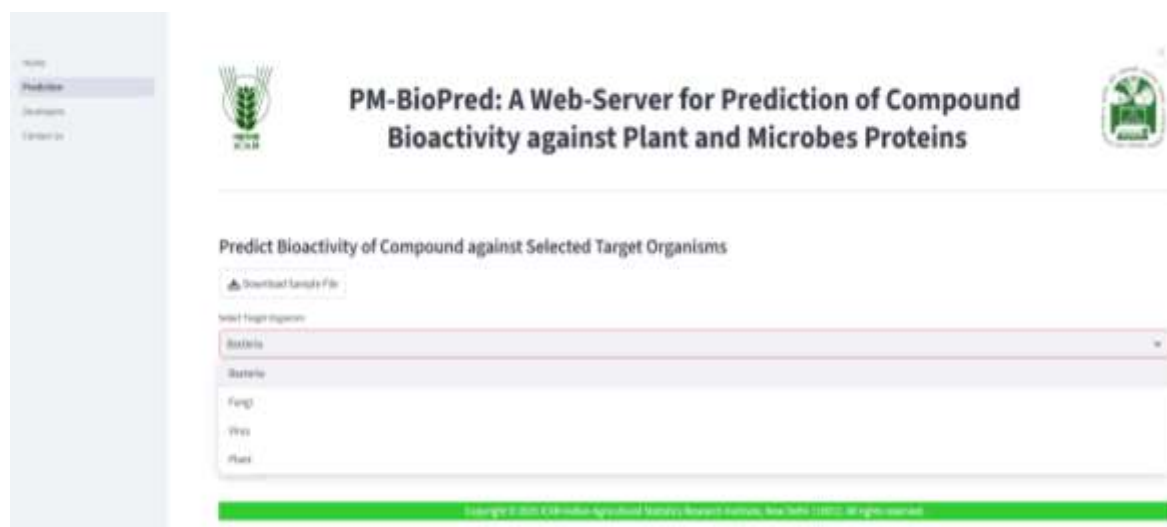


Figure 2: Navigation to Prediction Page

This opens the prediction interface where you can submit your compounds.

3. Choose Target Organism

In the dropdown menu “**Select Target Organism**”, choose the type of biological target:

Option	Meaning
Bacteria	Predict antibacterial compound activity
Fungi	Predict antifungal compound activity
Virus	Predict antiviral compound activity
Plant	Predict plant-protein modulator activity

Note: Models are trained separately for each organism group for improved accuracy.

4. Prepare Your Input File

PM-BioPred accepts a **CSV file** with two required columns:

molecule_id	SMILES
CHEMBL132431	CN(Cc1...
CHEMBL275309	Nc1nc...

Example:

	A	B	C	D	E	F	G	H	I	J	K
1	molecule_id	SMILES									
2	CHEMBL132431	CN(Cc1cnc2nc(N)nc(N)c2n1)c1ccc(C(=O)NC(CCC(=O)O)C(=O)O)c2ccccc12									
3	CHEMBL132142	Nc1nc(N)c2cc(CNc3ccc(C(=O)NC(CCC(=O)O)C(=O)O)c4ccccc34)cnc2n1									
4	CHEMBL275309	Nc1nc(N)c2cc(CNc3ccc(C(=O)NC(CCC(=O)O)C(=O)O)cc3)cnc2n1									
5	CHEMBL1977479	CC(=O)Nc1ccc(C(C(F)(F)F)(C(F)(F)F)C(F)(F)F)cc1									
6	CHEMBL1979770	CN(C(=O)c1cccc(S(C)(=O)=O)c1)c1c(N)n(Cc2ccccc2)c(=O)[nH]c1=O									
7	CHEMBL2005366	O=c1cc(CSc2ccc(C(F)(F)F)cn2)nc2ccc(Br)cn12									
8											
9											
10											
11											

Figure 3: Sample CSV

Guidelines

- **molecule_id** can be any identifier (e.g., ChEMBL ID, internal code, compound name)
- **SMILES** must be valid chemical SMILES notation
- File must be in **CSV format**
- Maximum file size: **200MB**

Click “**Download Sample File**” on the page to get the correct template.

5. Upload Your File

Click **Drag and Drop file here** or **Browse files** and upload your CSV.

After uploading, the filename will appear on the page.

6. Run Prediction

Press the **Predict** button.

PM-BioPred will process your compounds using ML models and display the results.

7. Interpreting Results

The output table includes:

Column	Meaning
Molecule ID	ID provided by user
SMILES	Input SMILES string
Probability (Active)	Likelihood compound is bioactive
Probability (Inactive)	Likelihood compound is inactive
Prediction	Active or Inactive label

Example output:

Home
Predictive
Download
Contact Us

Predict Bioactivity of Compound against Selected Target Organisms

Download Sample File

Select Target Organism

Bacteria

Upload CSV with columns: Compound ID, SMILES

Drag and drop file here
Limit: 100MB per file x 10

example.csv 1KB (0)

Predict

ID	Windows ID	SMILES	Probability, Gram	Probability, NonGram	Probability
0	1-149998,133331	C1=CC=C(C=C1)C(=O)N1C=CC(=O)N1C=CC(=O)N1C=CC(=O)N1	0.99	0.00	Yes
1	1-149998,133340	Nc1cc(NC(=O)Nc2cc(C)cc(C)cc2)cc(C)cc1	0.94	0.05	Yes
2	1-149998,171689	Nc1ccc(NC(=O)Nc2cc(C)cc(C)cc2)cc1	0.98	0.02	Yes
3	1-149998,167470	CC1=CC=C(C=C1)C(=O)N1C=CC(=O)N1	0.98	0.01	Yes
4	1-149998,1707712	C1=CC=C(C=C1)C(=O)N1C=CC(=O)N1C=CC(=O)N1	0.99	0.01	Yes
5	1-149998,1300340	O=C1C=CC(=O)N1C=CC(=O)N1	0.99	0.01	Yes

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Figure 4: Result Table

Interpretation Example

Molecule	Active Prob	Inactive Prob	Prediction
CHEMBL132431	0.616	0.384	Active

Molecule	Active Prob	Inactive Prob	Prediction
CHEMBL2005366	0.19	0.81	Inactive

Higher probability = higher confidence in prediction.

Exporting Results

Click **Download** (built-in browser table download) to save results.

8. Next Steps

You can now take **Active-predicted compounds** forward for:

- ✓ Molecular docking
- ✓ MD simulations
- ✓ Laboratory testing
- ✓ Lead optimization