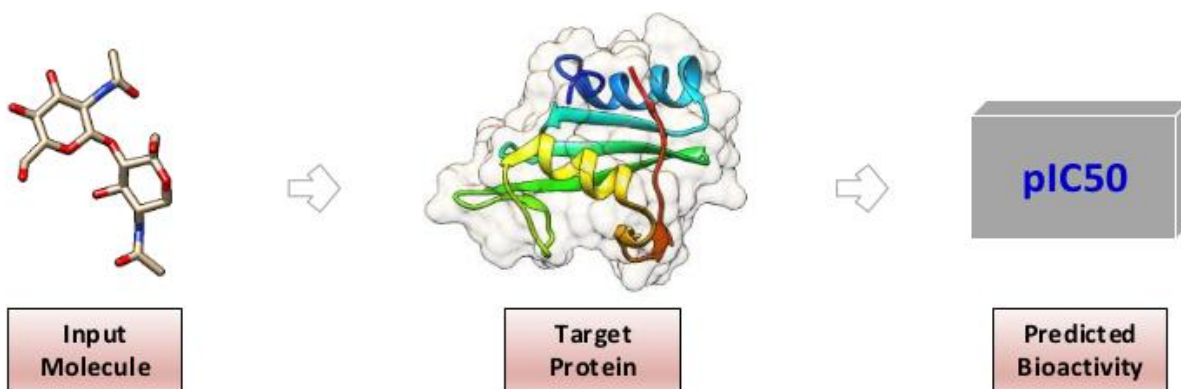


USER MANUAL OF BIOPREDICT

BIOPREDICT *Bioactivity Prediction App*



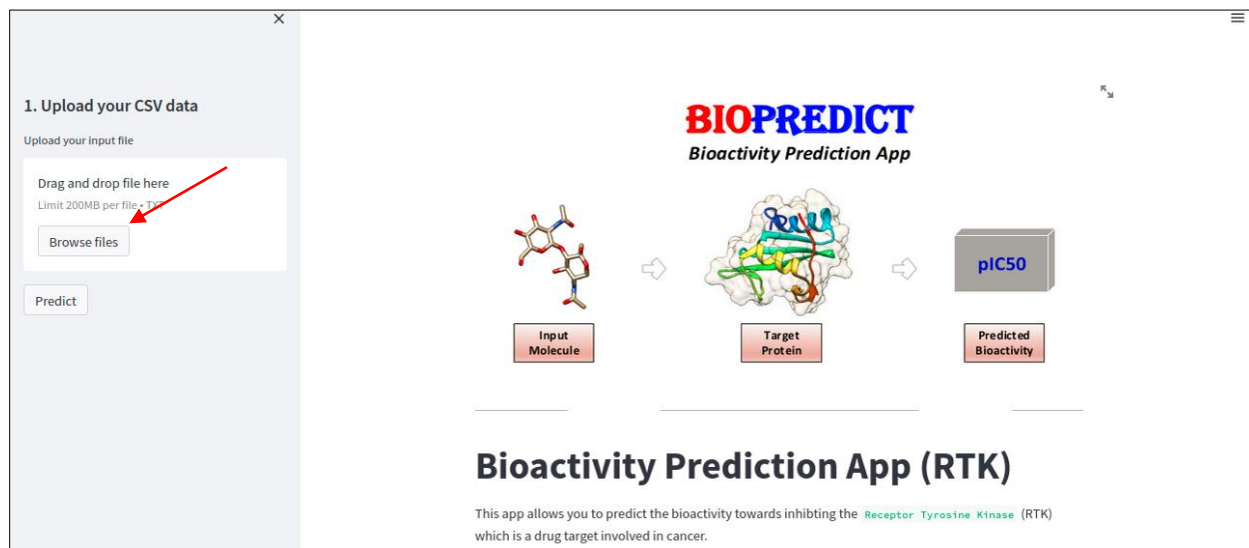
Launch the app by typing the following command

streamlit run app.py

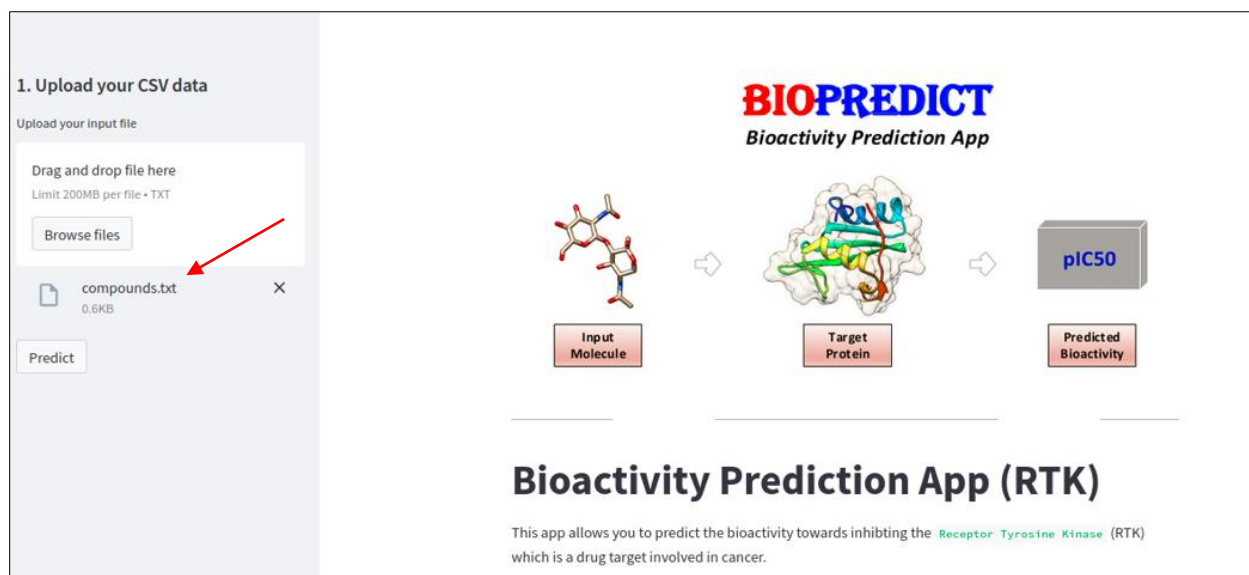
If you do not have prior streamlit installed, install it, by following command:

Pip install streamlit

The app will be opened in the default browser.



Click on browse button to browse the input file from the local disk.



The file is uploaded as shown with the arrow.

Click on predict button to start running prediction of input compounds

Bioactivity Prediction App

Bioactivity Prediction App (RTK)

This app allows you to predict the bioactivity towards inhibiting the **Receptor Tyrosine Kinase (RTK)** which is a drug target involved in cancer.

Acknowledgements

- The app is modified and originally built in **Python + Streamlit** by [Chanin Nantasenamat]
- The app is modified and used in **Python + Streamlit** by [Rashid Hussain]

Upload input data in the sidebar to start!

The following information/windows will be shown while running the app in tabular form. The app is running as shown with the red arrows, and can be stop by clicking on stop button.

Original input data

	0	1
0	<chem>Cc1cc(C(=O)N2CCN(C)CC2)[nH]c1/C=C/C1(=O)Nc2ncnc(Nc3ccc(F)c(Cl)c3)c21</chem>	CHEMBL305246
1	<chem>O=C(C5c1ncnc2c1sc1nc(N3CCOC(C)C3)c3c(c12)CCCC3)Nc1ccco1</chem>	CHEMBL1774326
2	<chem>CN(C)CCCN(C(=O)/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1</chem>	CHEMBL334801
3	<chem>O=C1C(=O)N(Cc2cccc2)c2ccc(S(=O)(=O)N3CCCC3)cc21</chem>	CHEMBL3099522
4	<chem>Cl(C1=C2Sc3cccc3N2CC1)=C1/CC([n+])2c1sc1ccccc12</chem>	CHEMBL518593
5	<chem>Oc1cc(O)cc(Oc2c(O)cc(Oc3c(O)cc(O)cc3O)cc2O)c1</chem>	CHEMBL2391422
6	<chem>O=C(O)/C(O)=C/C(=O)c1cccc(OC2ccc(Cl)cc2)c1</chem>	CHEMBL492771
7	<chem>COc1ccc([C@@H]2CC([O-]c3c(O)cc(O)cc3O2)cc1O</chem>	CHEMBL399121
8	<chem>O=C(Nc1ccc([N+](=O)[O-])cc1Cl)c1cc(Cl)ccc1O</chem>	CHEMBL1448
9	<chem>O=C(O)/C(O)=C/C(=O)c1cccc1OCc1ccccc1</chem>	CHEMBL499444

Calculating descriptors...

