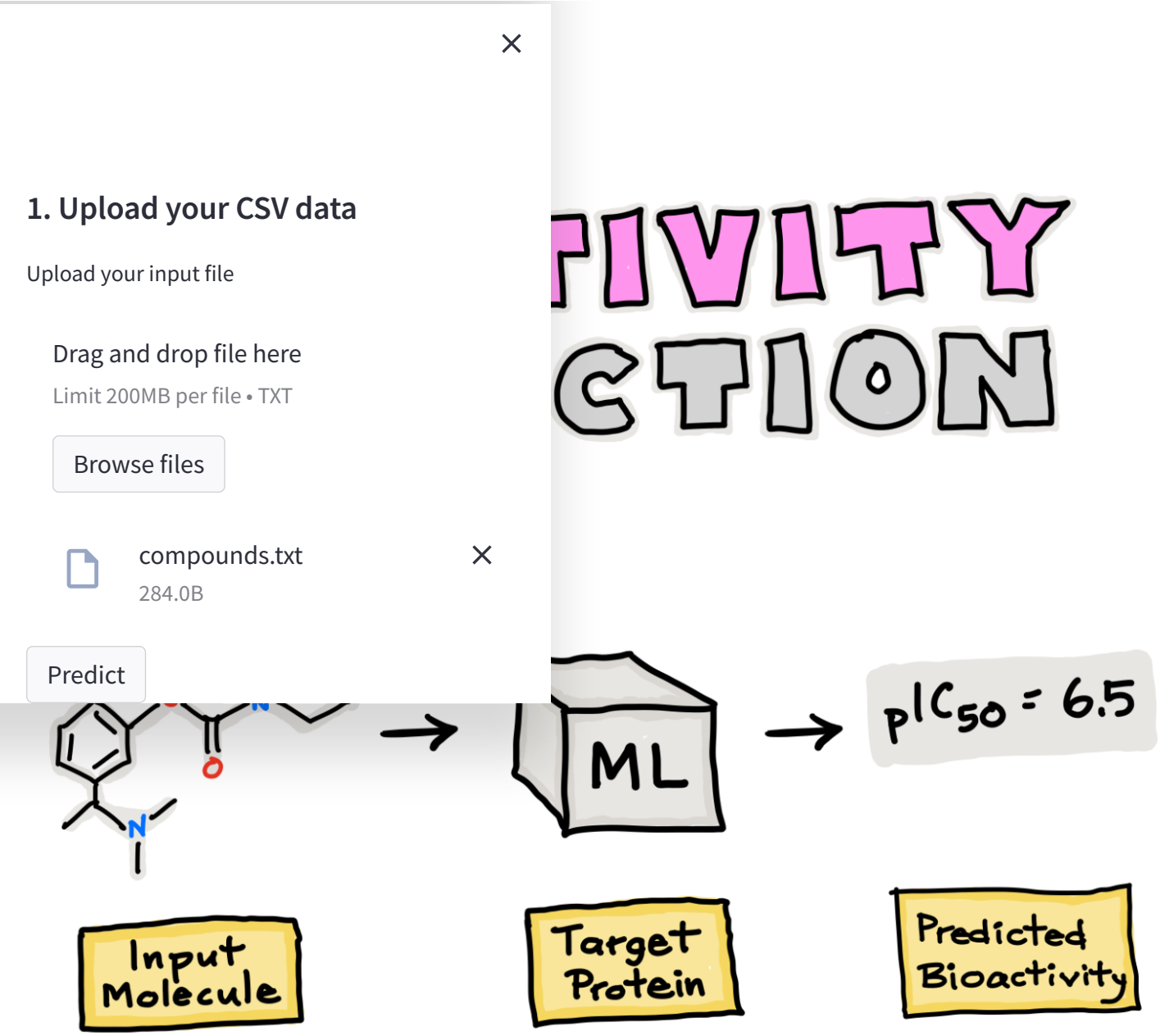

Bioactivity Prediction App (COVID19)

This app allows you to predict the bioactivity towards inhibting the `Replicase polyprotein` enzyme. `Replicase polyprotein` is a drug target for COVID19.

Acknowlegement

- The app is modified and originally built in `Python` + `Streamlit` by [Chanin Nantasenamat]

Original input data

	0	1
0	CCOc1nn(-c2cccc(OCc3ccccc3)c2)c(=O)o1	CHEMBL133897
1	O=C(N1CCCCC1)n1nc(-c2ccc(Cl)cc2)nc1SCC1CC1	CHEMBL336398
2	CN(C(=O)n1nc(-c2ccc(Cl)cc2)nc1SCC(F)(F)F)c1ccccc1	CHEMBL131588
3	O=C(N1CCCCC1)n1nc(-c2ccc(Cl)cc2)nc1SCC(F)(F)F	CHEMBL130628
4	CSc1nc(-c2ccc(OC(F)(F)F)cc2)nn1C(=O)N(C)C	CHEMBL130478

Calculated molecular descriptors

	Name	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc
0	CHEMBL130628	1	1	1	0	0	0	0	0	0	1	1	1	1	0	1	1
1	CHEMBL336398	1	1	1	0	0	0	0	0	0	1	1	1	1	0	1	1
2	CHEMBL133897	1	1	1	0	0	0	0	0	0	1	1	1	1	0	1	1
3	CHEMBL131588	1	1	0	0	0	0	0	0	0	1	1	1	1	0	1	1
4	CHEMBL130478	1	1	0	0	0	0	0	0	0	1	1	1	0	0	1	1

(5, 882)

Subset of descriptors from previously built models

	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc	Pubc
0	1	0	0	1	0	0	0	1	1	1	1	1	1	1	0	0	0	1	1
1	1	0	0	1	0	0	0	0	0	1	1	1	1	1	0	0	0	1	1
2	1	0	0	0	0	1	1	0	0	0	0	1	1	1	0	0	0	0	0
3	0	0	0	1	0	0	0	1	1	1	1	1	1	1	0	0	0	0	0
4	0	0	0	1	0	1	0	1	1	1	0	1	1	1	0	0	0	0	0

(5, 238)

(0, 256)

Prediction output

	molecule_name	pIC50
0	CHEMBL133897	5.9330
1	CHEMBL336398	5.9883
2	CHEMBL131588	5.0166
3	CHEMBL130628	5.1887
4	CHEMBL130478	5.1194

Download Predictions

Made with Streamlit