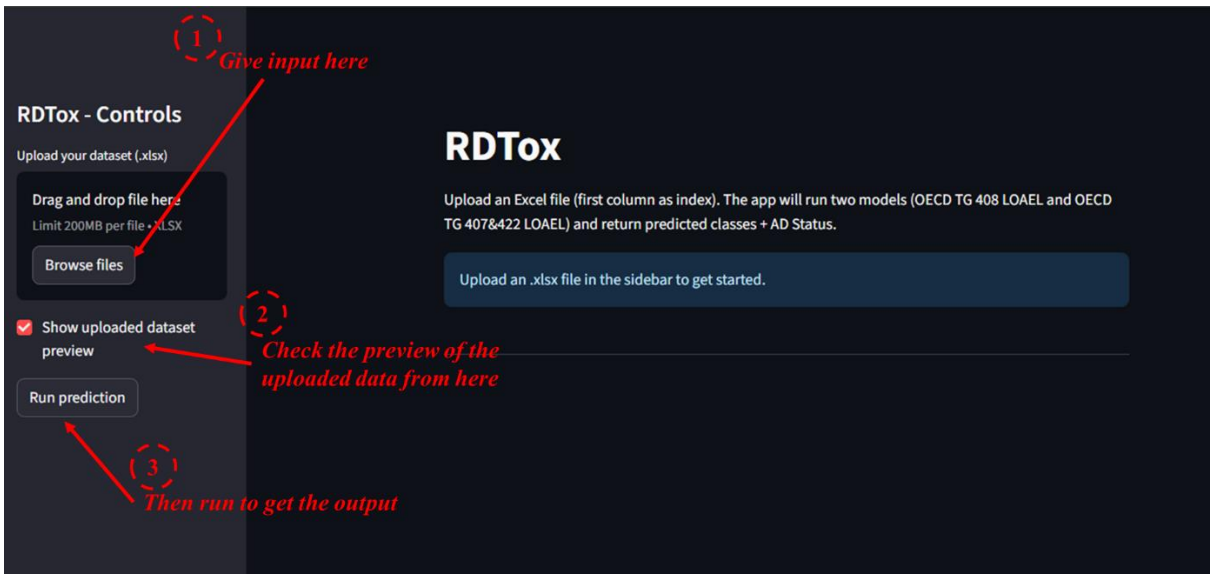
Prediction Procedure:



Input File Format:

The input file must be in .xlsx format. The first column should contain IDs, while the subsequent columns should include descriptors. It is not necessary to arrange the descriptors in any specific order; however, all specified descriptors must be included in a single input file. The required descriptors are shown below:

	A	B	C	D	E	F	G	H
1	B08[C-C]	B09[C-C]	nAA	F02[C-C]	B09[C-O]	nCb-	MaxssNH	MaxdsN
2	B04[C-N]	B09[C-N]	Eta_betaP	X4sol	C-024	C-026	Fsp3	C-003
3	B05[C-N]	MaxaaCH	Eta_beta	MaxaasC	B06[C-O]	SsCl	B05[N-O]	H-047
4	B06[C-C]	B01[C-O]	B03[C-O]	RDCHI	RCI	MCD	Eta_beta_	Eta_F_A
5	B03[C-N]	B08[C-O]	nBnz	B04[C-C]	F02[C-N]	B04[C-S]	Ui	N%
6	B07[C-C]	nIR	B04[N-O]	F05[C-N]	MaxsOH	B02[C-N]	SssNH	H%
7	B01[C-N]	B05[C-C]	B02[C-O]	NNRS	X2v	B02[N-N]	B04[C-Cl]	B03[N-O]
8	B07[C-N]	Uc	Rperim	BLTD48	MW	B10[C-N]	MaxssO	F05[C-Cl]
9	B06[C-N]	MaxaaN	MaxsCl	ESOL	NaasC	MaxsssN	F01[N-N]	minaaN
10	B08[C-N]	B10[C-C]	Eta_B	B05[C-O]	N-069	B04[C-O]	B03[C-S]	B01[C-S]
11								B10[C-O]
12								

Developed by

(Application developed by Souvik Pore, souvikpore123@gmail.com)

For further queries, please contact

Prof. Kunal Roy

Drug Theoretics and Cheminformatics (DTC) Laboratory

Department of Pharmaceutical Technology

Jadavpur University, Kolkata 700032, India

Email: kunal.roy@jadavpuruniversity.in