

Prediction Procedure:

The screenshot shows the RDTTox web application interface. On the left, the 'RDTTox - Controls' sidebar contains an upload section with a 'Browse files' button, a 'Show uploaded dataset preview' checkbox (checked), and a 'Run prediction' button. On the right, the main area is titled 'RDTTox' and contains instructions about uploading an Excel file and a corresponding upload button. Three red dashed circles with numbers 1, 2, and 3 are placed over the 'Browse files' button, the 'Show uploaded dataset preview' checkbox, and the 'Run prediction' button respectively. Red arrows point from these circles to text annotations: 'Give input here' for step 1, 'Check the preview of the uploaded data from here' for step 2, and 'Then run to get the output' for step 3.

1 Give input here

2 Check the preview of the uploaded data from here

3 Then run to get the output

The screenshot displays the 'OECD TG 407 & 422 Results' section. It features a table with three columns: 'NAME', 'Predicted Class', and 'AD Status'. The table contains eight rows of data. Below the table, there is a 'Download results as Excel' button, which is highlighted with a red dashed rectangle. A red arrow points from this button to the text 'Download the results from here'.

NAME	Predicted Class	AD Status
3407-42-9	Less Toxic	Inside AD
6786-83-0	More Toxic	Inside AD
5137-55-3	More Toxic	Inside AD
9002-92-0	More Toxic	Outside AD
41272-40-6	More Toxic	Inside AD
108-82-7	Less Toxic	Inside AD
39711-79-0	Less Toxic	Inside AD

Download results as Excel

Download the results from here

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