TOXBAI

User Manual

Ver 1.0

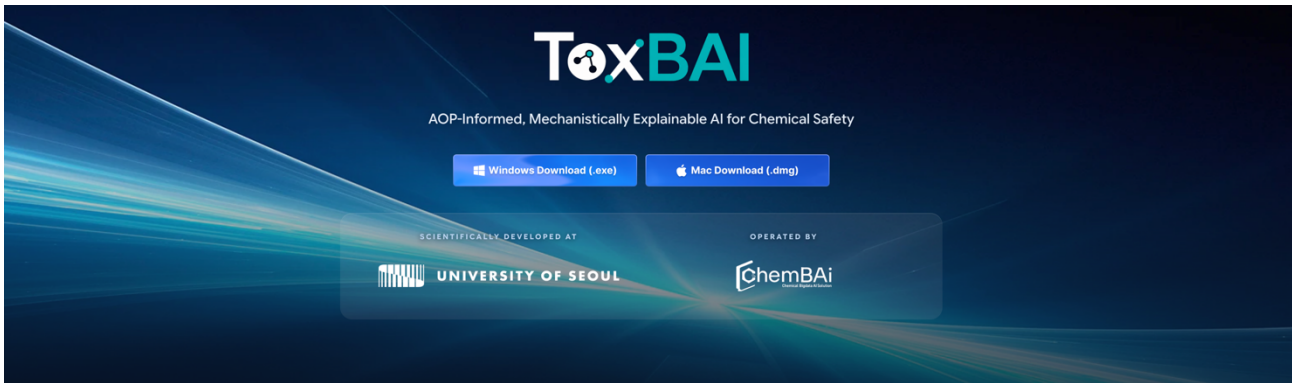
Developed by UNIVERSITY OF SEOUL

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Operated by ChemBAi

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1. Before You Begin

Please check the following before using the app.

1. Make sure your internet connection is working.
2. Have a Google account ready for sign-in.
3. Prepare the list of substances to enter, or an Excel file.

> In the current version, ToxBAI toolbox 1.0(Prediction) is the primary features. ToxBAI AOP-based AI and ToxBAI NGRA 1.0 appear as disabled coming-soon placeholders and will be released later. Molecular Properties and Find Analogs are no longer shown on screen.

2. Overall Workflow

File download site: www.toxbai.com

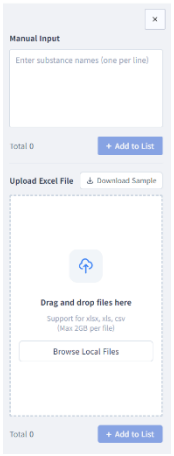
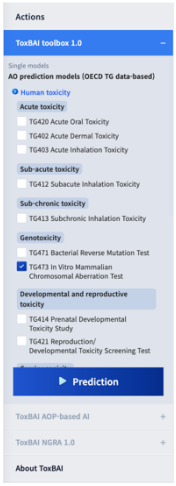
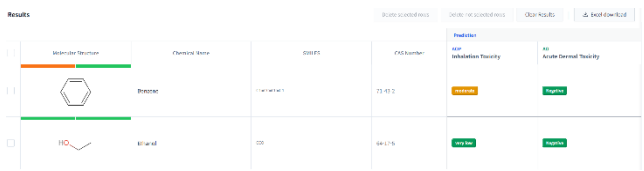
Use TOXBAI in the following order.

1	Launch the app
2	Sign in with Google
3	Enter initial user information and accept the terms
4	Enter substances
5	Validate the input
6	Select a prediction model
7	Run prediction
8	Review results
9	Review detailed results

10 Download to Excel or clear results

3. Screen Layout

The TOXBAI screen is divided into three main areas.

Area	Function	Screen Layout
1. Substance Input panel	Area for entering substances directly or uploading an Excel file	
2. Actions panel	Area for selecting a prediction model and running it	
3. Main screen	Area for reviewing the entered substance list and prediction results	

4. Launching the App and Signing In

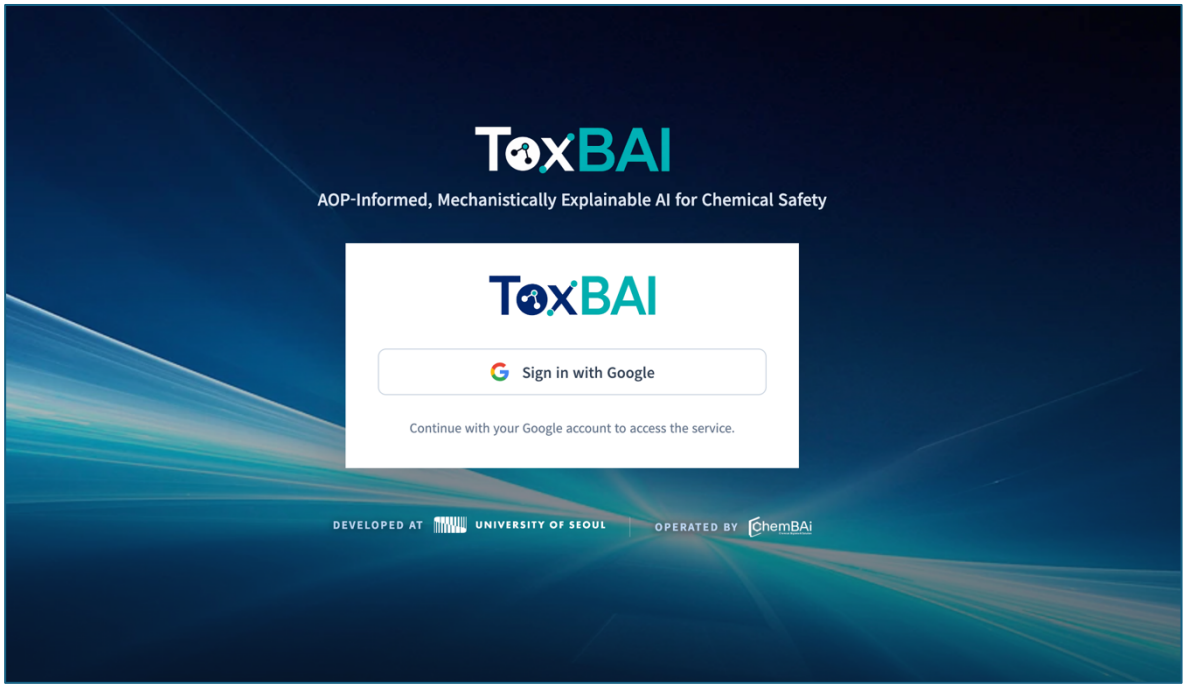
4-1. Launching the App

When you launch the app, it first checks whether the service is available.

- If everything is normal, the app moves to the next screen.
- If there is no network connection, a connection notice may appear.

*If you are using a version whose service has ended, use may be restricted.

4-2. Sign in with Google

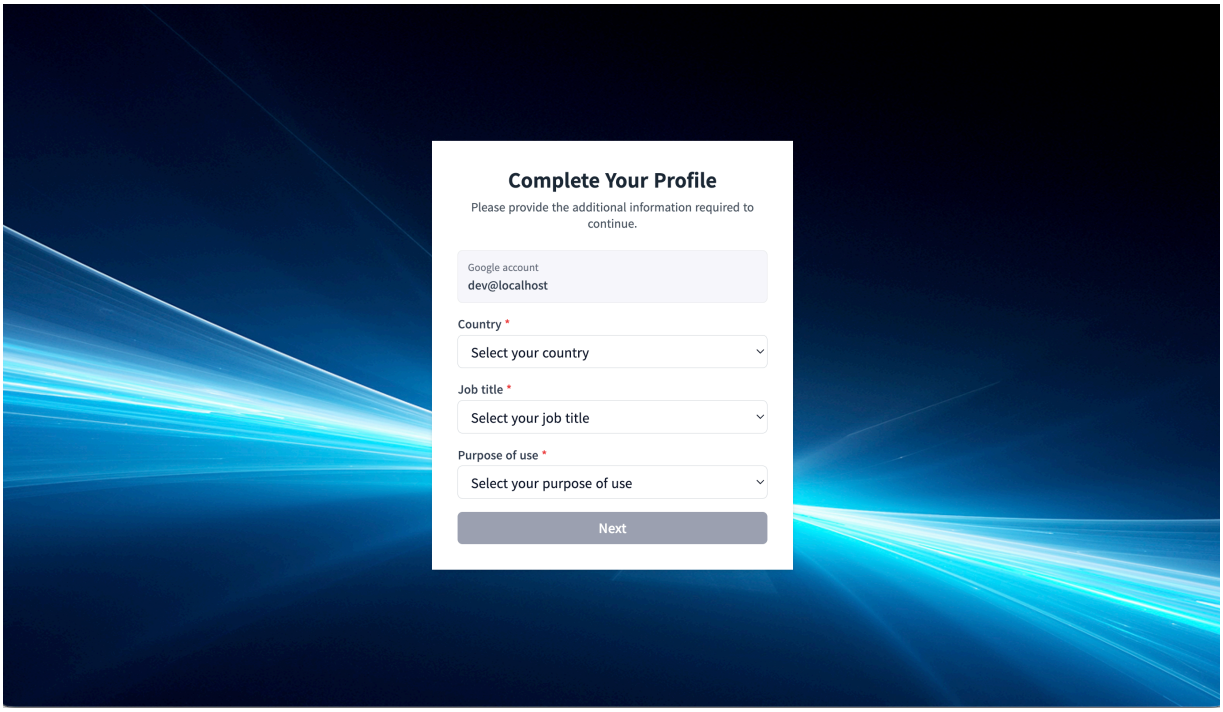


On the sign-in screen, tap the 'Sign in with Google' button to log in.

- You can sign in with your existing Google account — no need to create a separate new account.

4-3. Initial User Information and Terms Agreement

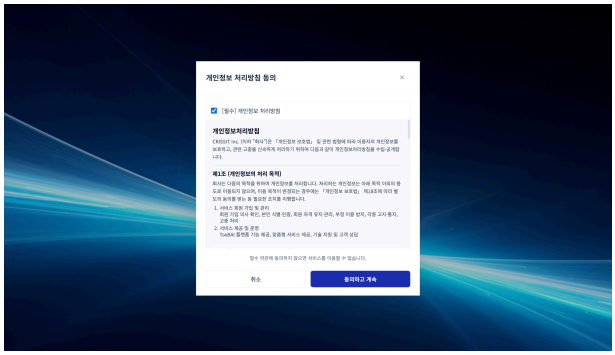
First-time users will see an additional information entry screen.

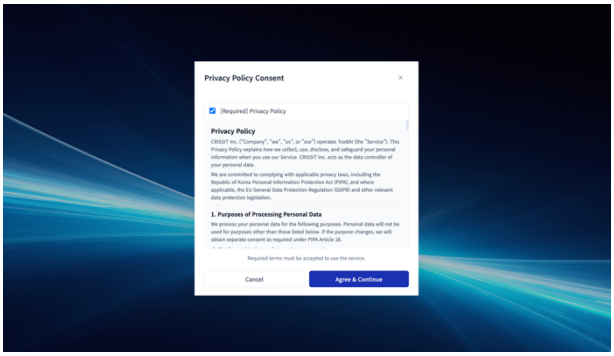


Fields to enter:

- Country
- Job title
- Purpose of use

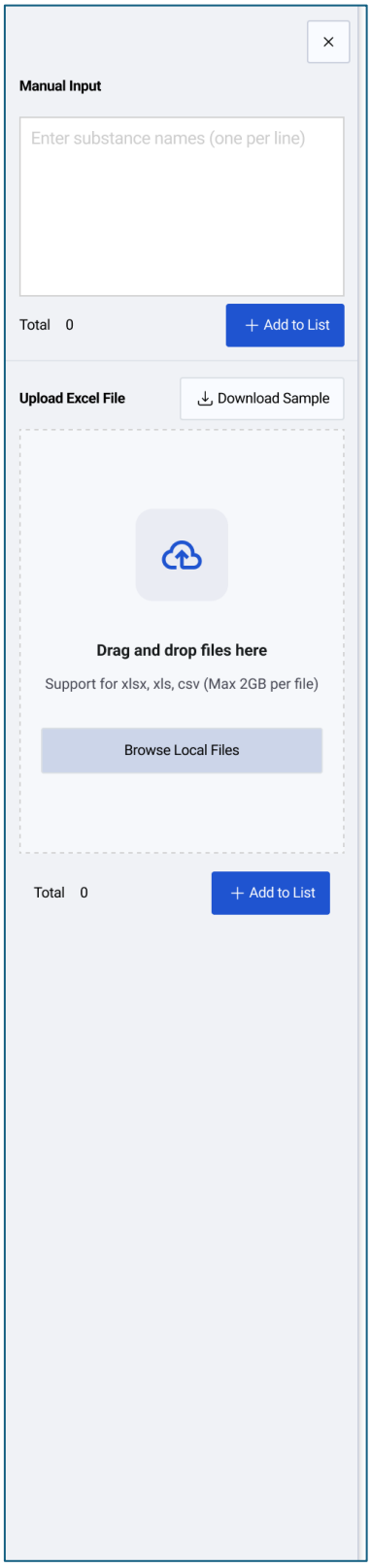
You only need to accept the terms once; after that you will be taken directly to the main screen.





5. Entering Substances

Substances can be entered by SMILES / CAS RN, and two input methods are provided.



5-1. Manual Input

Enter the substance name in the Manual Input area of the left panel.

- Enter one substance per line.
- When you finish entering, click the [Add to List] button.
- The Total number shows the current count of entries.

> Suitable for quickly entering a small number of substances.

5-2. Upload an Excel File

To enter multiple substances at once, use the Upload Excel File area.

How to upload:

- Drag and drop the file onto the screen
- Select a file using the [Browse Local Files] button

Additional features:

- You can download a sample file format with the [Download Sample] button.
- Enter CAS RN in column A and SMILES in column B. (Entering only one of the two is also fine.)

- After uploading, you can quickly check the file name and the list of loaded items.
- After reviewing, click [Add to List] to proceed to the next step.

> Suitable for quickly entering a large number of substances.

6. Input Validation

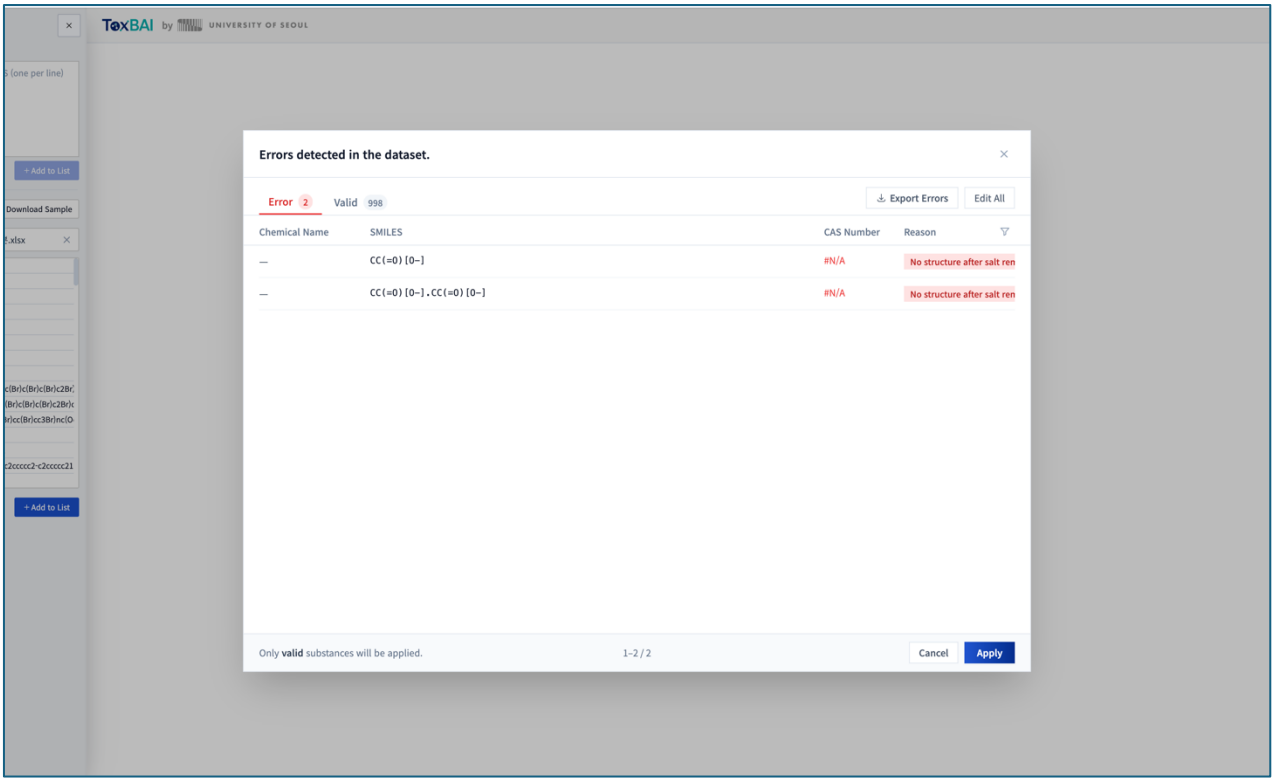
When you add substances, the system automatically checks the input. Validation results fall into two categories.

✓ Valid

Items that can be used as-is. They are included when running the prediction model.

✗ Error

Items that need correction or cannot be used. After excluding the error items, only valid items are applied.



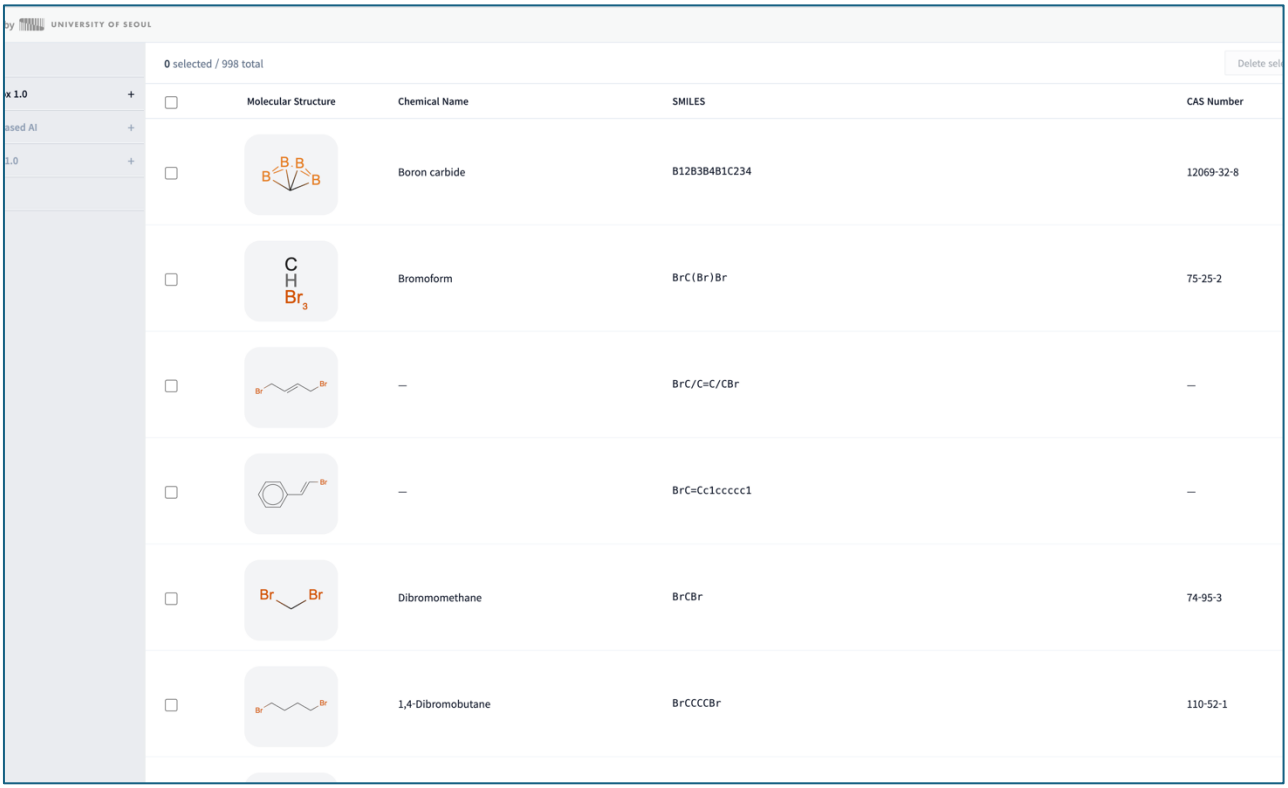
- If there are errors, error items and valid items are displayed separately.
- If no matching entry exists in the current database, the item is marked as an Error; you can correct the error items and check again. If you proceed as-is, error items are excluded and only valid items are applied to the list.

Notes

- Substances already in the list are not added again as duplicates.

7. Reviewing the Substance List

Substances that pass validation are shown in the list on the main screen.



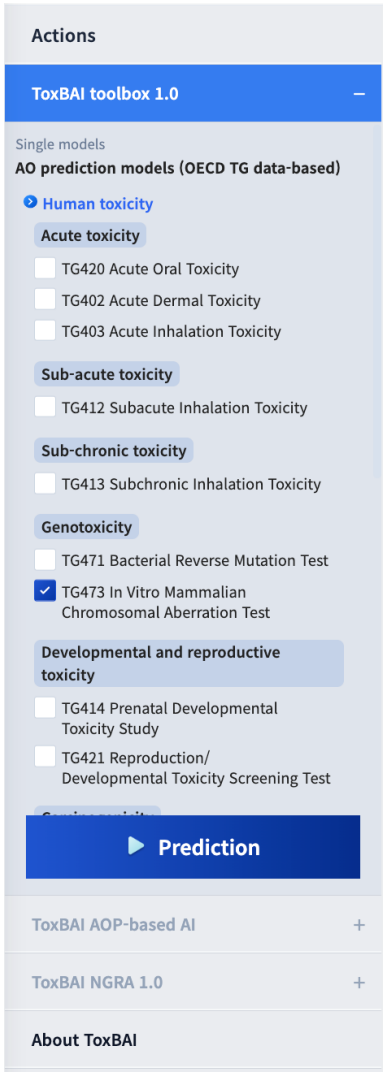
Information displayed:

- Molecular structure
- Substance name
- SMILES
- CAS Number

- If there are duplicate substances, a warning message is shown and you can view the details.
- If the list is empty, a guidance message is shown.

8. Prediction – Selecting a Prediction Model

In the Actions panel, click [ToxBAI toolbox] to open the prediction model selection area.



Currently available model categories:

Model name	Description
AO prediction models	Prediction model based on OECD TG data
Mechanism prediction models	Prediction model based on ToxCast data

Conditions for enabling the Prediction button:

- At least one substance must be in the list.
- At least one prediction model must be selected.

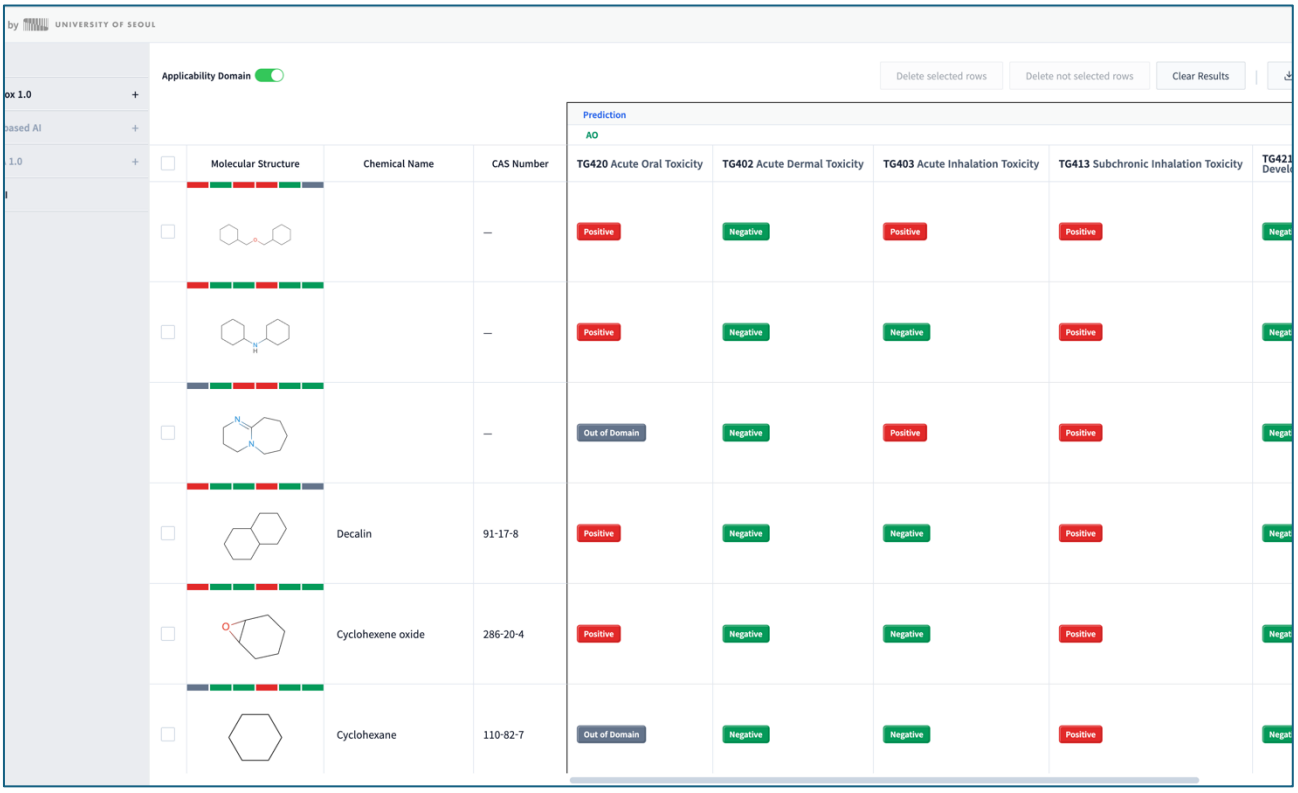
Once you finish selecting models, click the [Prediction] button at the bottom to start prediction.

- A progress window is shown while running.
- You can check the progress in real time based on the selected models.

> *Molecular Properties and Find Analogs features will be released later.
>
> *AOP-based AI and ToxBAI NGRA 1.0 models will be released later.

9. Prediction – Reviewing Results

When prediction is complete, you can review all results in table form on the Results screen.

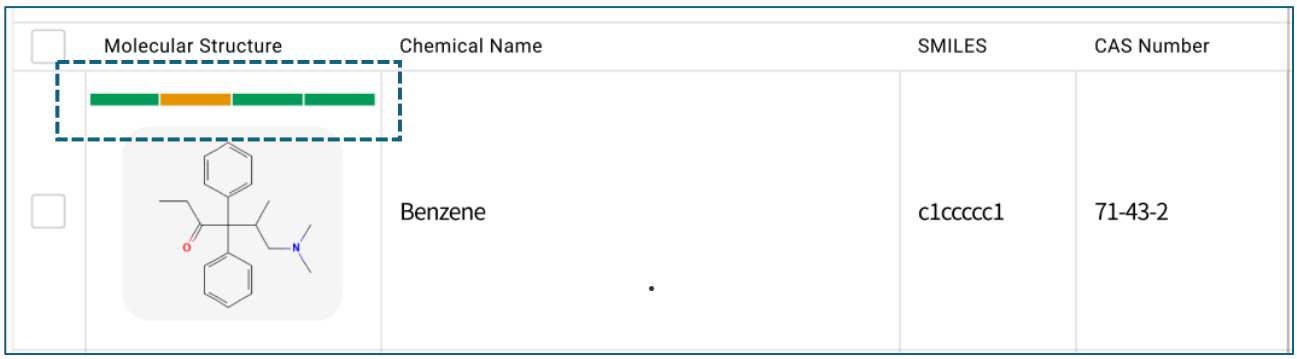


Screen layout:

- Basic substance information (molecular structure, substance name, CAS RN, SMILES) is pinned on the left.
- Prediction results by model are displayed horizontally on the right.
- Toggle the Applicability Domain button in the upper-left corner to apply the Applicability Domain to the prediction results displayed in the table. If a substance falls outside the applicability domain for all models, it will be displayed as Out of Domain.

Features:

- Row selection / Select all / Delete selected rows / Delete unselected rows / Clear all results.
- Click the prediction result summary bar above the substance molecular structure to jump to the corresponding result column.

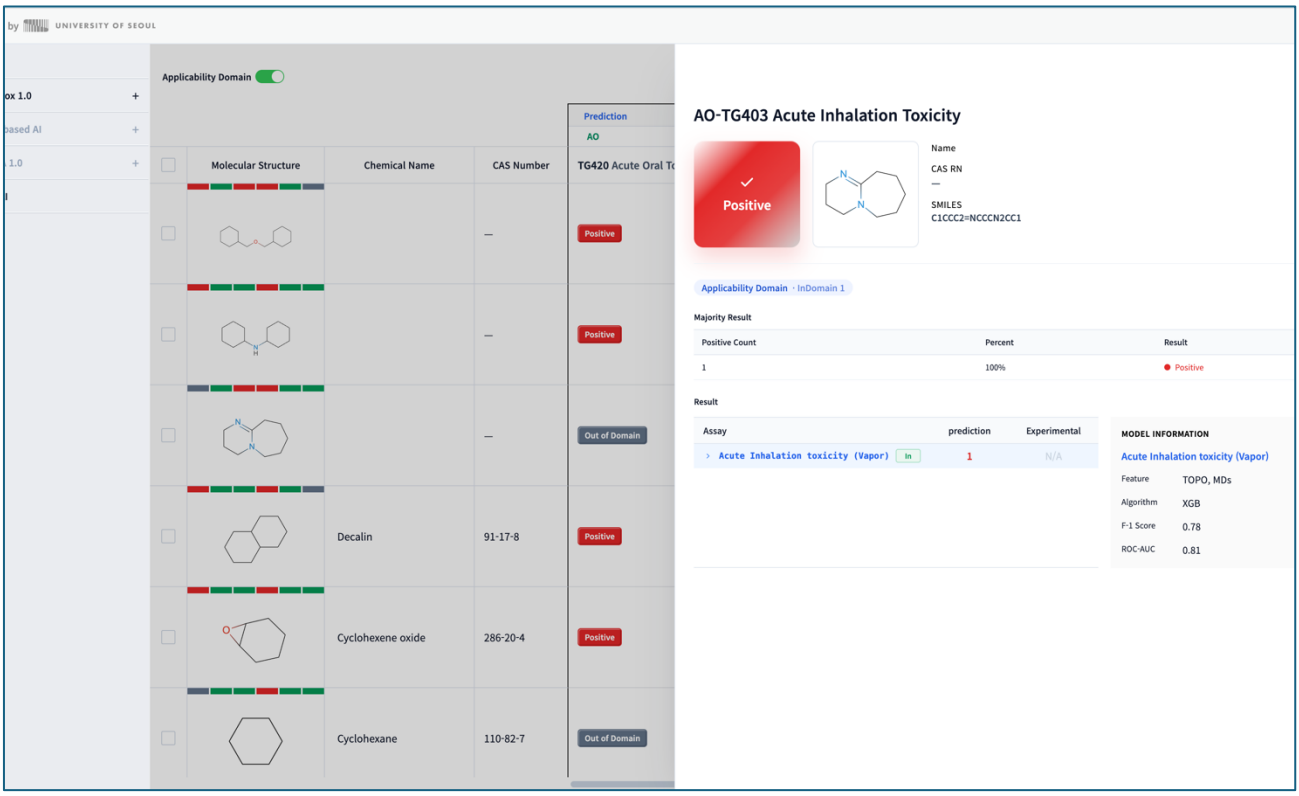


- You can copy the substance name, CAS, or SMILES values by clicking them.

> **Workflow** While reviewing the results screen, you can add new substances in the left panel or change the prediction model selection in the Actions panel and run prediction again.

10. Prediction – Reviewing Detailed Results

When you select a specific prediction item in the results table, the detail panel opens.



Information available on the detail screen:

- Name of the selected prediction model
- Basic information for the substance
- Summary of the prediction result
- Detailed description based on the model type
- Applicability Domain status for each model (In/Out)

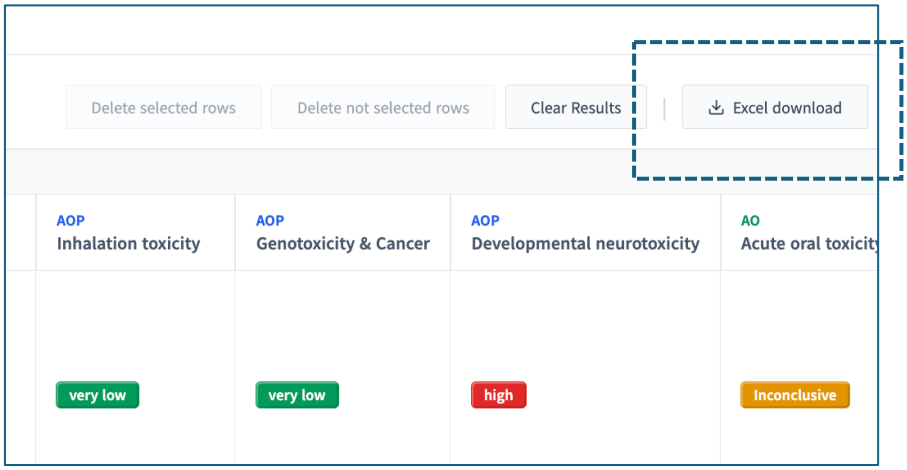
Closing the panel:

- Click the [X] button at the top right.
- Click the existing results screen on the left.
- Press the keyboard back button.

*This screen also provides the copy function for Name, CAS RN, and SMILES.

11. Prediction – Excel Download

Click the [Excel Download] button at the top right of the results screen to export the results. A single Scoring-format Excel file is generated and downloaded immediately; there is no format selection dialog.

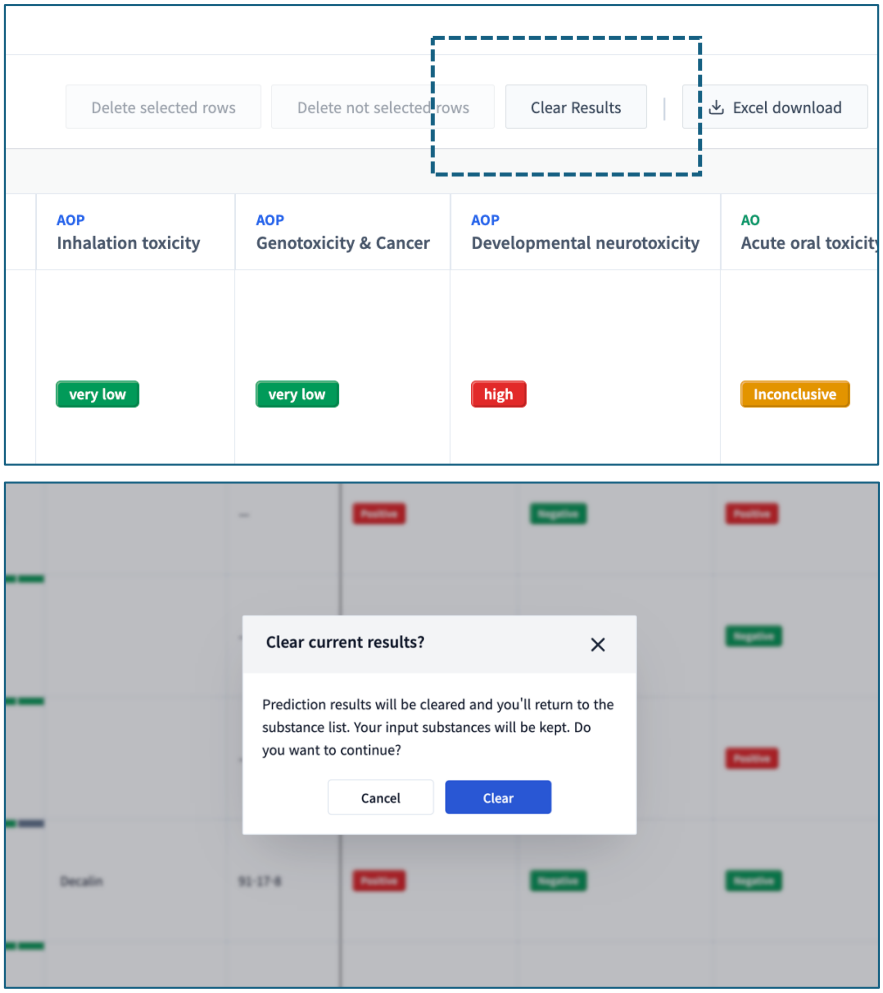


Format	Contents
Full Data	Download the full dataset including more detailed prediction information

Select the format you need and proceed with the download.

12. Prediction – Clearing Results and Starting a New Task

To clear the current work and start over from the beginning, use [Clear Results].



Items deleted together when clearing:

- Results list
- Entered substance list
- Selected prediction models
- Validation-related temporary state

> Caution Once clearing is complete, you are returned to the home screen, and the previous work cannot be restored. Please download any results you need before starting a new task.