



## GETTING STARTED: QUICK REFERENCE GUIDE FOR THE CLASSICAL USER INTERFACE

Choose which user interface you want to work with: *Simplified User Interface* or *Classical User Interface*.


**QSAR Toolbox Version 4.7, 2024**

Start with:

	<b>Simplified User Interface</b>	New QSAR Toolbox interface developed to perform basic tasks in a simplified environment
	<b>Classical User Interface</b>	The classical QSAR Toolbox interface with full functionalities


Remember the choice

After you select one of the interfaces from above, you can still switch between the two options later within the Toolbox

 If you want to use the same user interface everytime when you open the software then check **Remember the choice** checkbox before selecting one of the two interfaces.

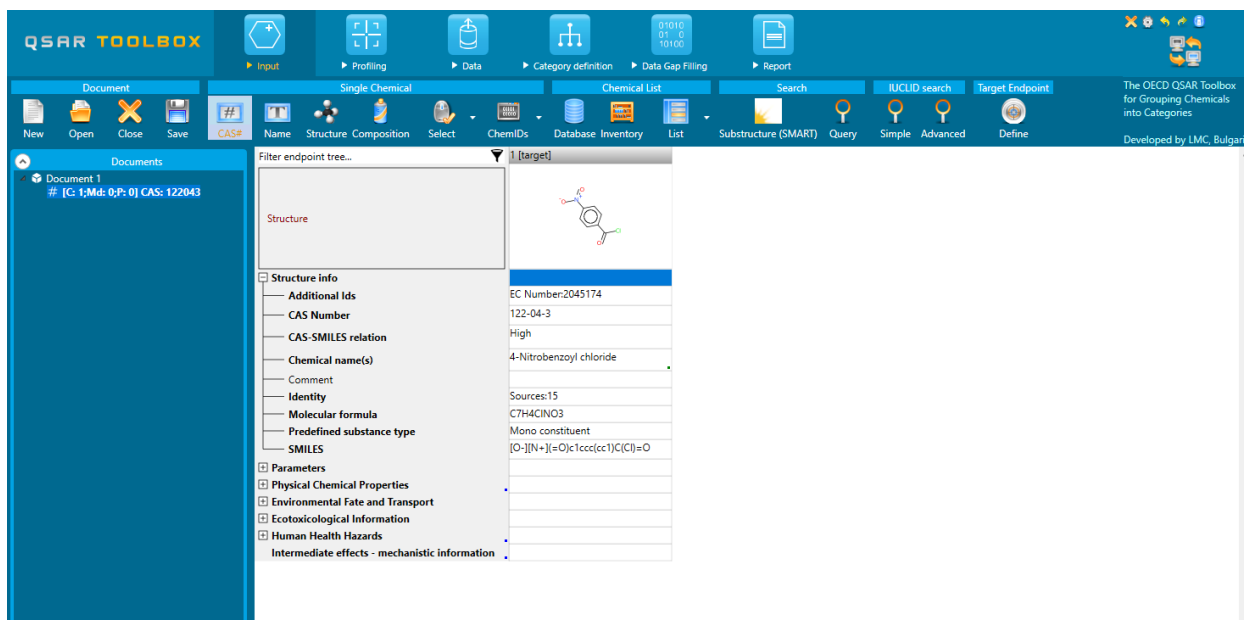
## Step 1: Input - Define chemical of interest or "target chemical"

Define your target chemical by Chemical Name, CAS number, SMILES, drawing the molecule or selecting it from a list. To define a chemical by CAS number:

Click  → enter the number, and then click

 → the program displays the structure → 

The structure is displayed on the data matrix.



The screenshot displays the QSAR TOOLBOX software interface. The top menu bar includes options like Document, Input, Profiling, Data, Category definition, Data Gap Filling, and Report. Below this, there are tabs for Single Chemical, Chemical List, Search, IUCLID search, and Target Endpoint. The 'Target Endpoint' tab is active, showing a search for a chemical with CAS number 122043. The interface displays the chemical structure of 4-Nitrobenzoyl chloride and its properties:


Structure info	Value
Additional Ids	EC Number:2045174
CAS Number	122-04-3
CAS-SMILES relation	High
Chemical name(s)	4-Nitrobenzoyl chloride
Comment	
Identity	Sources:15
Molecular formula	C7H4ClNO3
Predefined substance type	Mono constituent
SMILES	[O-][N+](=O)c1ccc(cc1)C(Cl)=O

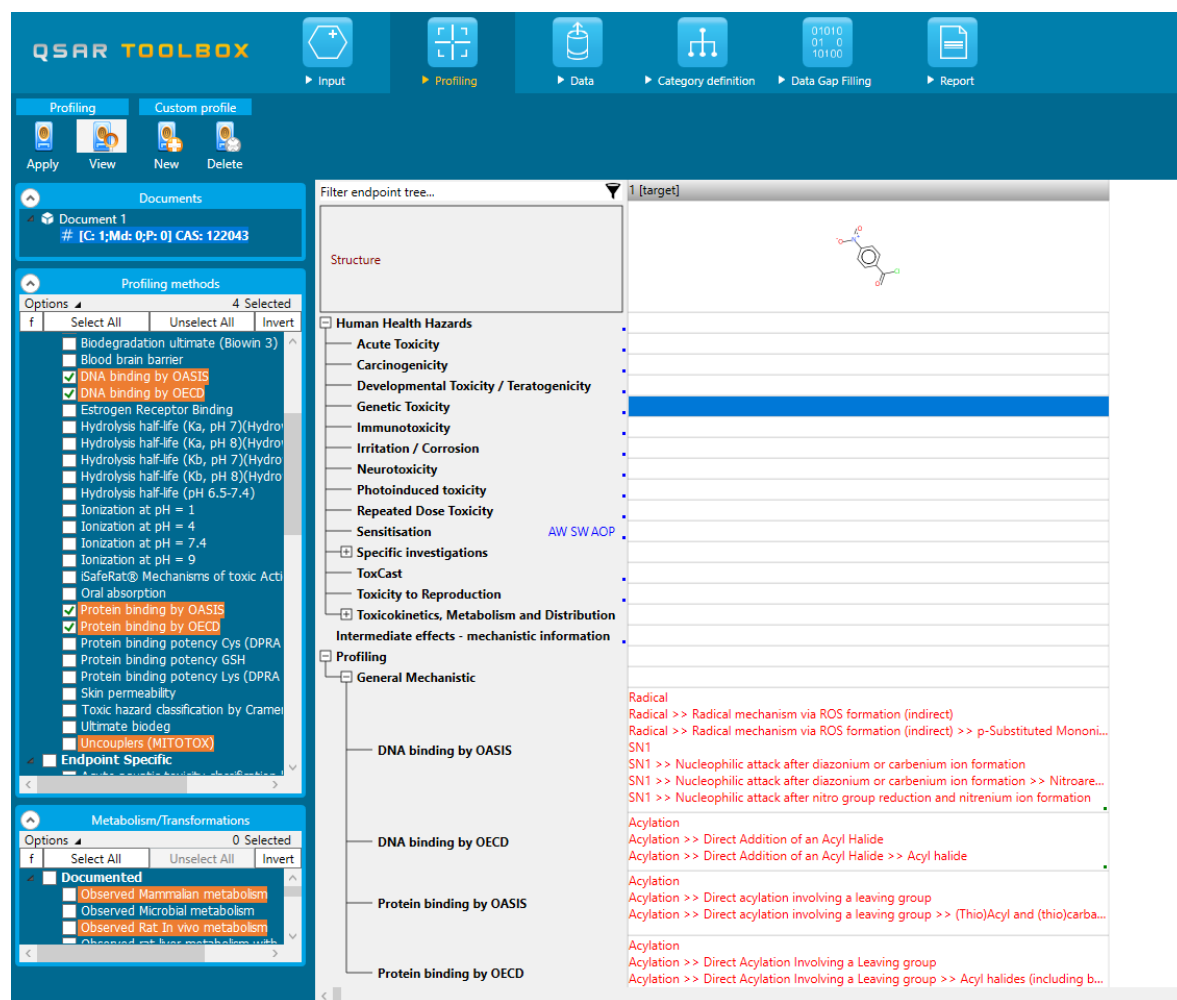



To define the target endpoint, which will be used for the predictions click




## Step 2: Profiling - Retrieve information based on the identity of the substance or its structure

Select profilers by ticking the corresponding boxes → . The program establishes a "profile" of the chemical based on its structure.



 To obtain the general background information on any profiler, right click on it and select **About**. To obtain the scientific information used to build the profiler, select

it and click .

 The highlighted profiles correspond to the selected endpoint in the data matrix or to the previously defined endpoint if any.

## Step 3: Endpoint - Retrieve experimental results from the resident databases




Select databases by ticking  the corresponding databases → . The retrieved information is displayed according to five subsections in the endpoint tree:

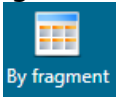
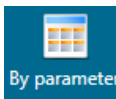
To open the data tree: left-click on the nodes. To access detailed information on the experimental results: double-click on the result in the matrix.

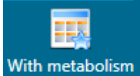
The highlighted databases correspond to the selected endpoint in the data matrix or to the previously defined endpoint if any.

## Step 4: Category definition - Identify chemicals which could form a category with the "target" chemical

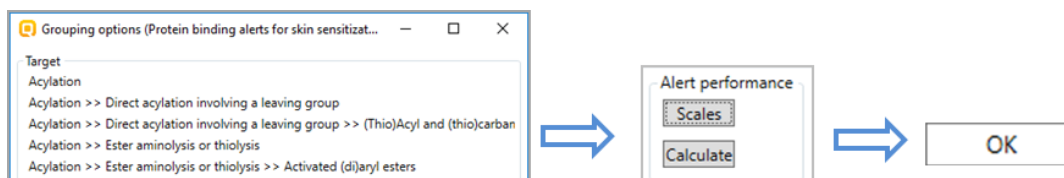
Select one of the grouping methods available in the **Categorization section**.

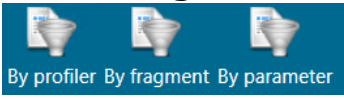
To collect analogues of a target chemical based on its profiling result, use →  **By profiler**.


Analogues of a target chemical could be searched also based on the fragment(s) defined by user →  **By fragment** or by a parametric criterion →  **By parameter**.


To identify the analogues of the target chemical accounting for its metabolic activation or based on specific criteria defined for the parent and/or generated metabolites, select →  **With metabolism**.


To check how much relevant to a target endpoint an alert is, once search **by profiler/with metabolism** is selected then calculate the Alert performance:




Select of the criteria available within the **Subcategorization section** to refine a chemical category on the data matrix →  **By profiler** **By fragment** **By parameter**.

To identify the subgroups within an existing category that are determined by the definitions of the currently selected profiling method →  **Clustering**.

To assess the consistency of the defined category →  **Category elements**.

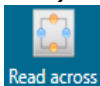
 The category consistency is endpoint specific. Four layers of information are considered important: Physicochemical similarity; Structural similarity and Mechanistic similarity and ADME similarity.

 The highlighted profiles correspond to the selected endpoint in the data matrix or to the previously defined endpoint if any.

## **Step 5: Data gap filling - Predict missing data by read-across, trend analysis, QSAR models or automated/standardized workflows**

Select data gap filling by clicking in the corresponding cell in the data matrix, and then select one of the data gap filling methods:

- Read-across: for “qualitative” endpoints (skin sensitization or mutagenicity e.g. positive, negative, equivocal) or for “quantitative endpoints” (e.g., 96h-LC50 for fish) if only very few analogues with experimental results are identified. →



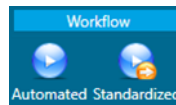
- Trend analysis: for “quantitative” endpoints if many analogues with experimental results are identified. →



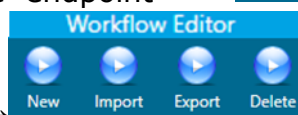
- (Q)SAR models: if no analogue with experimental results is identified or to build a weight of evidence case. →



- Standardized and Automated workflows: once started, they follow the implemented logic and finish with prediction. They include read-across or trend analysis method depending on the endpoint →



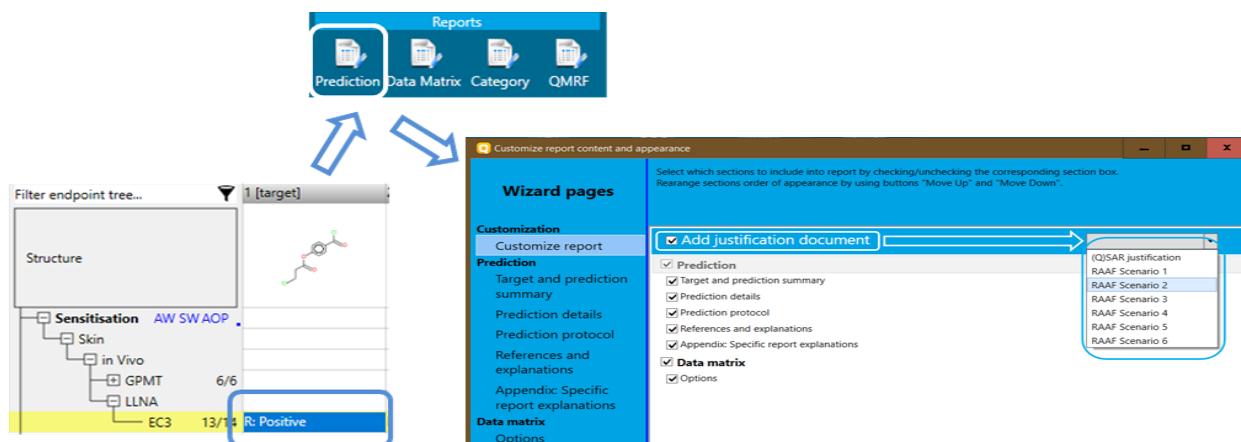
import/export your own workflows →



## **Step 6: Report – Obtain a detailed report for your prediction or category**

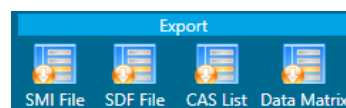
Prediction is needed to generate a *Prediction* report.

Read across Assessment Elements could be included in a separate justification document in case of regulatory interest, by selection of a **RAAF scenario**.



For predictions from a (Q)SAR model, the **(Q)SAR justification** document including (Q)SAR assessment elements, can be selected.

Four export types are also available in TB 4.7. →  
The Export allows exporting of various information from the current data matrix.



! Each of the above illustrated functionalities is explained in details in the F1 help file available with installation (press F1).