QSAR TOOLBOX

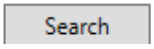
The OECD QSAR Toolbox for Grouping Chemicals into Categories

GETTING STARTED: QUICK REFERENCE GUIDE

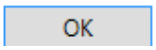
Step 1: Input - Define chemical of interest (target chemical)

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:

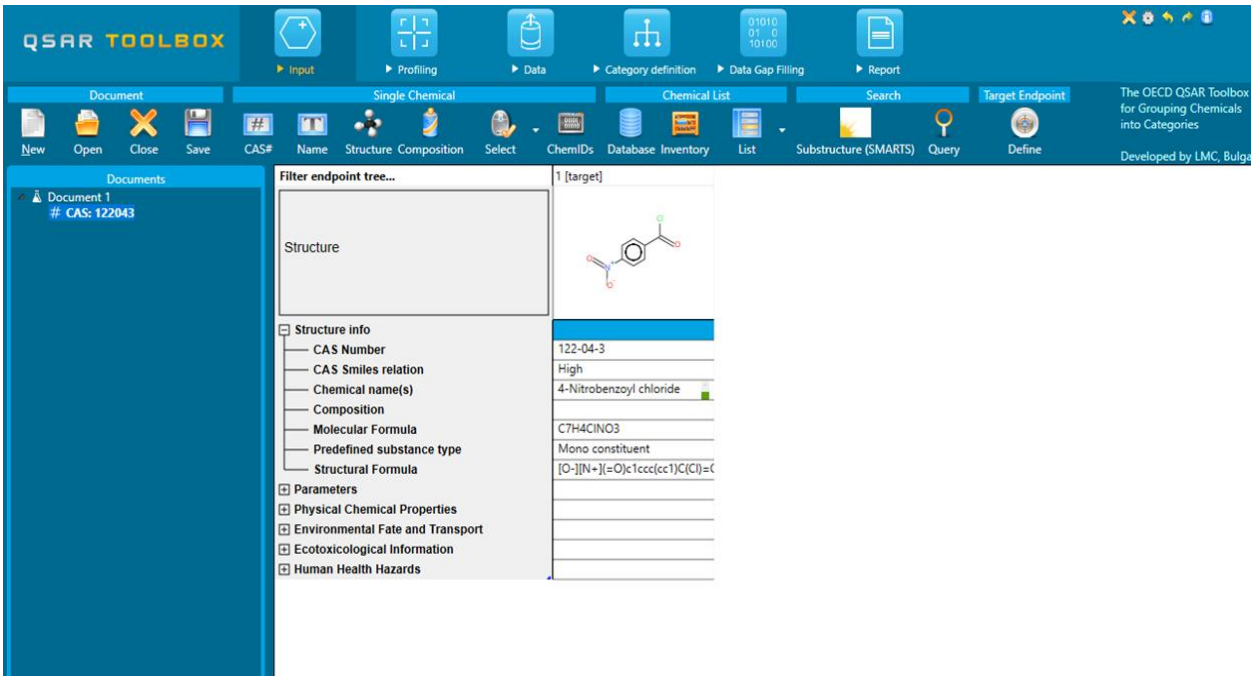
→ enter the number without hyphens,



→ the program displays the structure →



The structure is displayed on the data matrix.

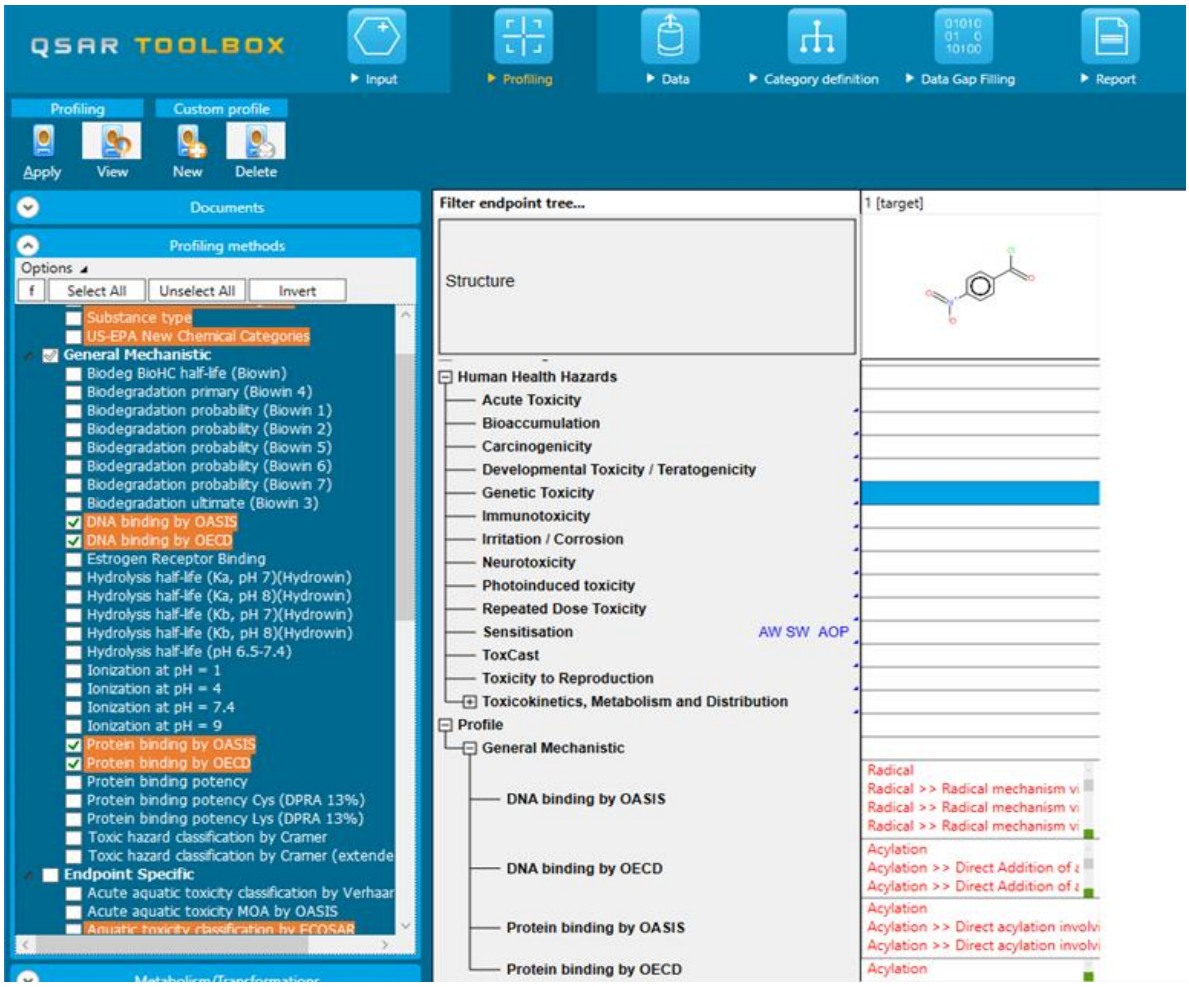


To define the target endpoint, which will be used for predictions click

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.



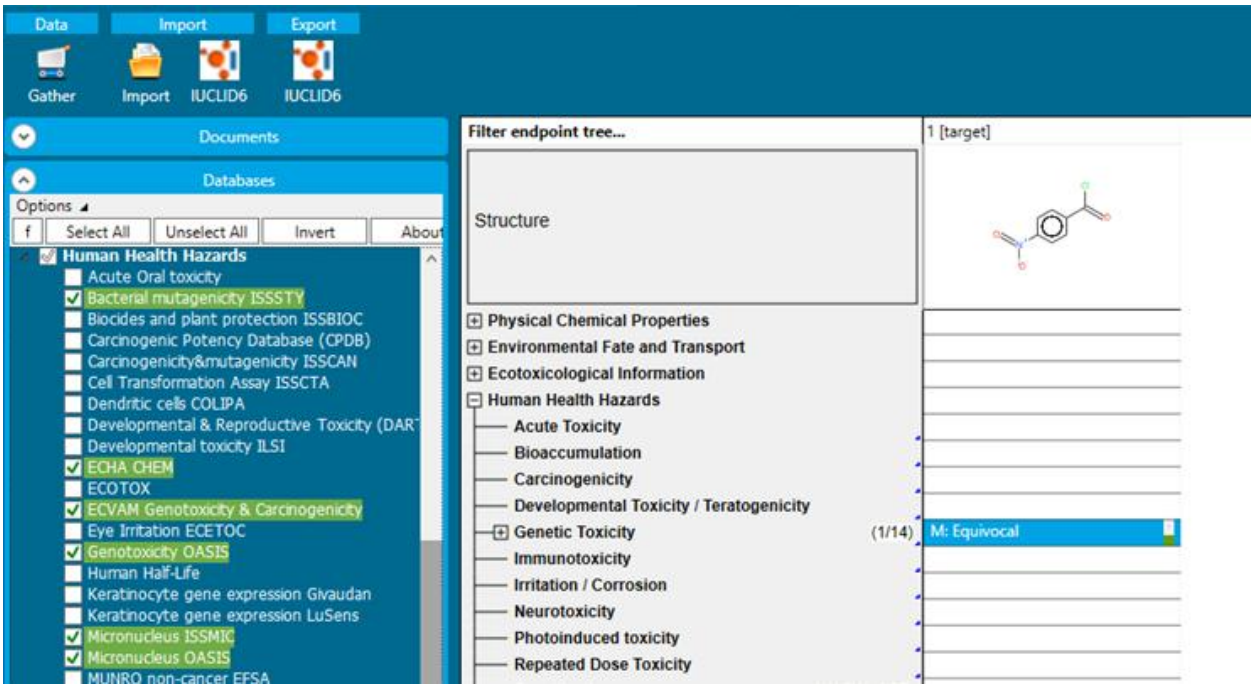
To obtain the general background information on any profiling scheme, right-click on it and select **About**. To obtain the scientific information used to build the profiling scheme, select it and click 

.

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

Step 3: Data - Retrieve experimental results from the resident databases

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



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

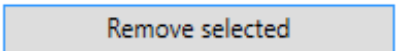
The highlighted databases correspond to the selected endpoint in the data matrix or to the previously defined endpoint if any.

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

Select one grouping method according to the profile of your target chemical in the window **Grouping methods** → Define.

You are prompted to confirm the query details and the retrieval of experimental data. Click OK each time.

To refine the category, repeat the procedure by clicking 

and selecting other grouping methods. In the subcategorization procedure, the function 

letes chemicals having different categories compared to the target.

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

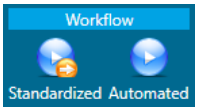
Step 5: Data gap filling - Predict missing data by read-across, trend analysis, QSAR models or automated/standardized workflows

Click the cell in the data matrix with missing experimental data, 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 → 

Step 6: Report – Obtain a detailed report for your prediction

Four type reports are available in TB 4.1. Prediction is needed only for the *Prediction* report. ->