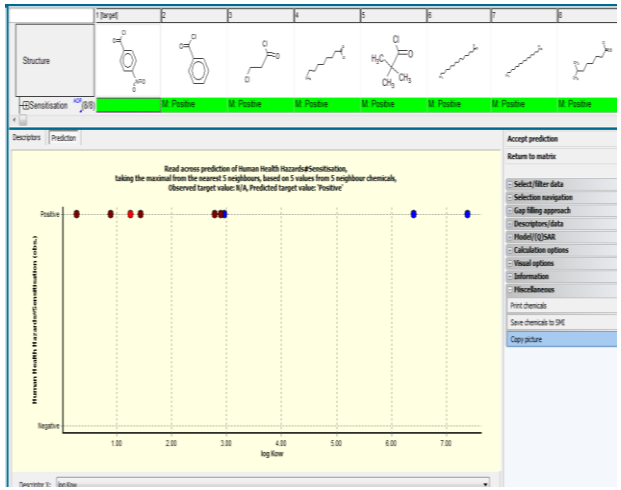
Step 5: Filling data gap - Predict missing data by read-across, trend analysis or QSAR models

Select a data gap by clicking in the corresponding empty cell in the data matrix, select one of the three data gap filling methods:

- Read-across: for "qualitative" endpoints (skin sensitisation 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.

→ 

The resulting graph proposes a prediction based on the available results for the analogues (or training set and test set in case of (Q) SAR models

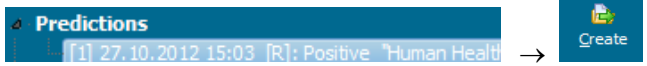


Once you are satisfied with a prediction, click **Accept prediction** and **Return to Matrix**.

To refine a prediction by subcategorisation or by filtering test results according to test conditions, use the functions under the menu **Select/filter data**

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

To obtain a report, select a prediction



→

Visit www.qsartoolbox.org for more detailed guidance documents.

QSAR TOOLBOX

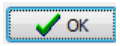
The OECD QSAR Toolbox for Grouping Chemicals into Categories

GETTING STARTED : QUICK REFERENCE GUIDE

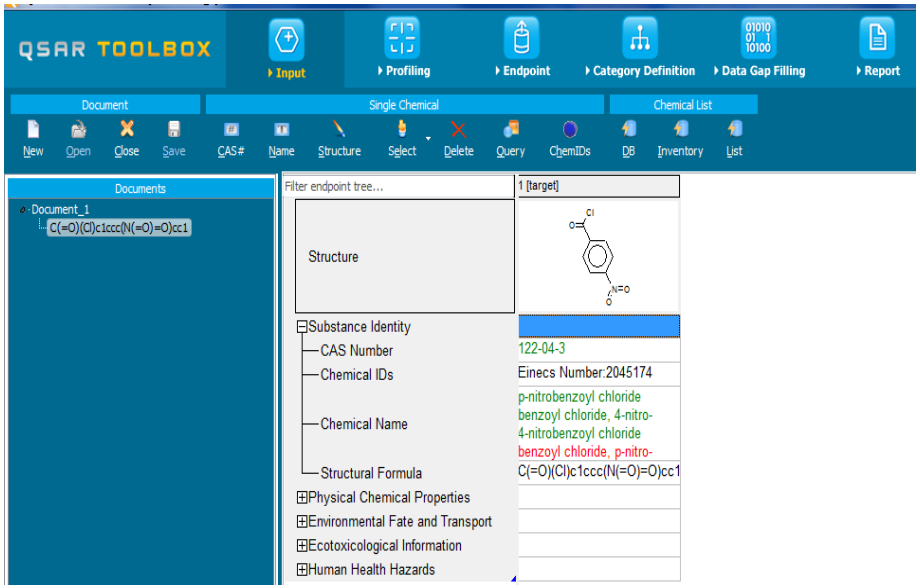
Step 1: Input - Define chemical of interest or "target chemical"

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

→ enter the number without hyphen,

→ the program displays the structure → 

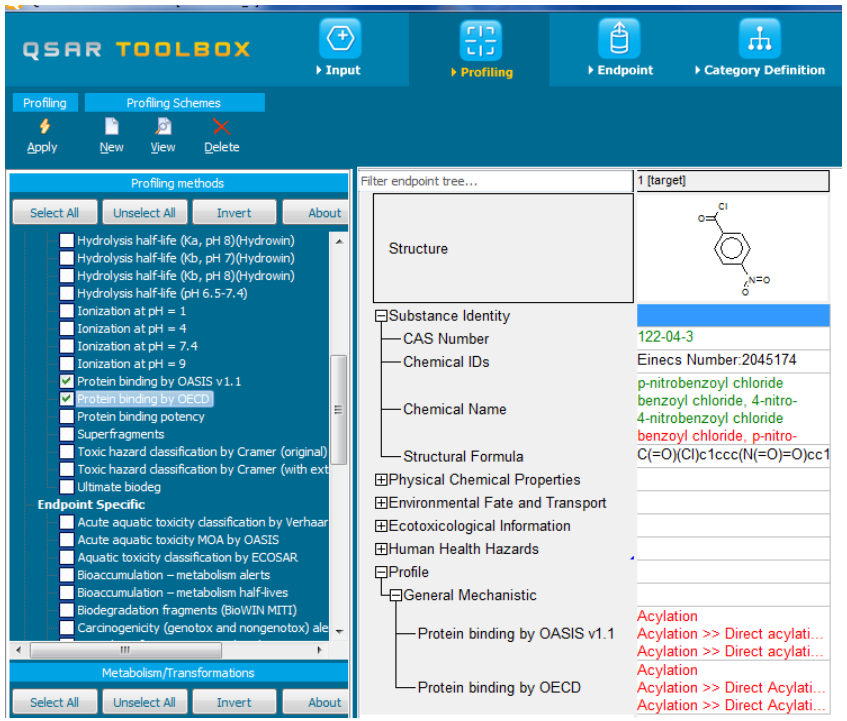
Click on **Substance identity** for details on the substance identity of the displayed substance.



Chemical names in green color indicate high quality in terms of identification of the right chemical. Double click for more information.

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

Select profilers by ticking the corresponding boxes (consult Manual for Getting Started to identify the most relevant profilers for any given endpoint) → Profiling Apply. The program establishes a "profile" of the chemical based on its structure.

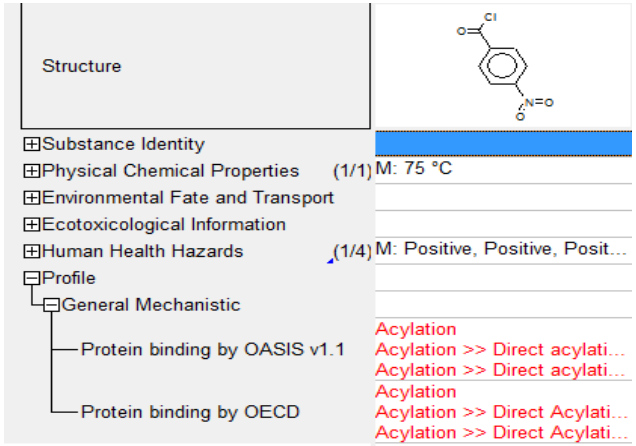


To obtain general background information on any profiler, right click on it and select **About**. To obtain scientific information on the functioning of a profiler, select it and click → View

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

Select databases by ticking the corresponding databases → Gather.

The retrieved information is displayed according to four sub-sections:



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.

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** and then click Define

You are prompted to confirm the query details, name of the category and retrieval of experimental data. Press OK each time.

If in the selected databases some experimental results are available more than once, the system identifies those multiple entries in a separate window. To keep only one result for multiple entries → Select one → OK

To refine the category, repeat the procedure by clicking on Subcategorize and selecting other grouping methods. In the subcategorisation procedure, the function Remove deletes chemicals with the highlighted profiles (i.e. by default chemicals that have profiles different from the target chemical).