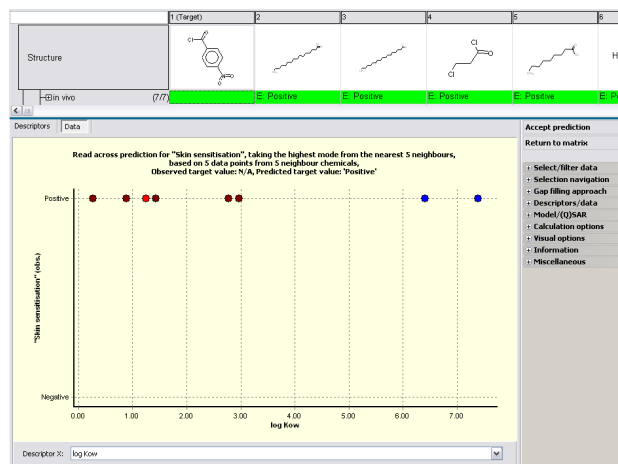


Step 5 : Filling data gap - Predict missing data by read-across, trend analysis or QSAR models

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.



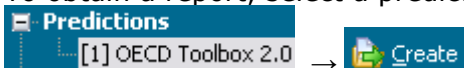
The resulting graph proposes a prediction based on the available results for the analogues (or training set and test set in case of (Q)SAR models).

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



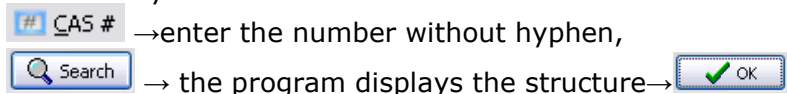
The report can then be saved in a number of formats (PDF, HTML, RTF).

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

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:




Double click on **Substance identity** for details on the substance identity of the displayed substance.

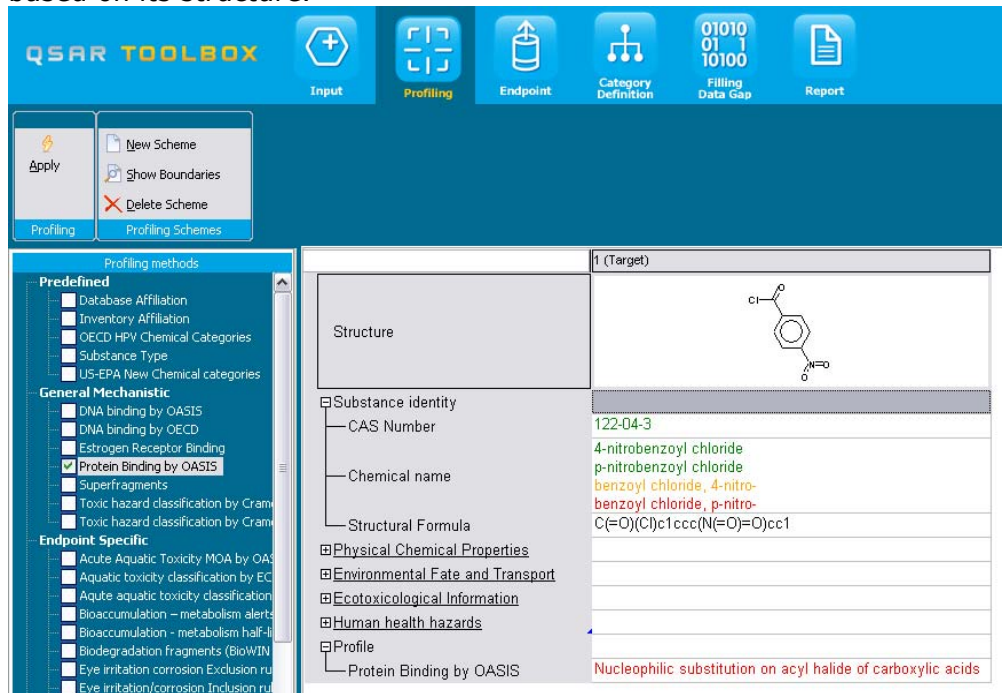
Document	1 (Target)
Structure	
Substance identity	
CAS Number	122-04-3
Chemical name	4-nitrobenzoyl chloride p-nitrobenzoyl chloride benzoyl chloride, 4-... benzoyl chloride, p-...
Structural Formula	C(=O)(Cl)c1ccc(N(=O)=O)cc1

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

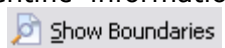
Step 2 : Profiling - Retrieve information based on the identity of the substance or its structure

Select profilers by ticking the corresponding boxes (consult Manual for Getting Started to identify the most relevant profilers for any given



endpoint) → . The program establishes a "profile" of the chemical based on its structure.



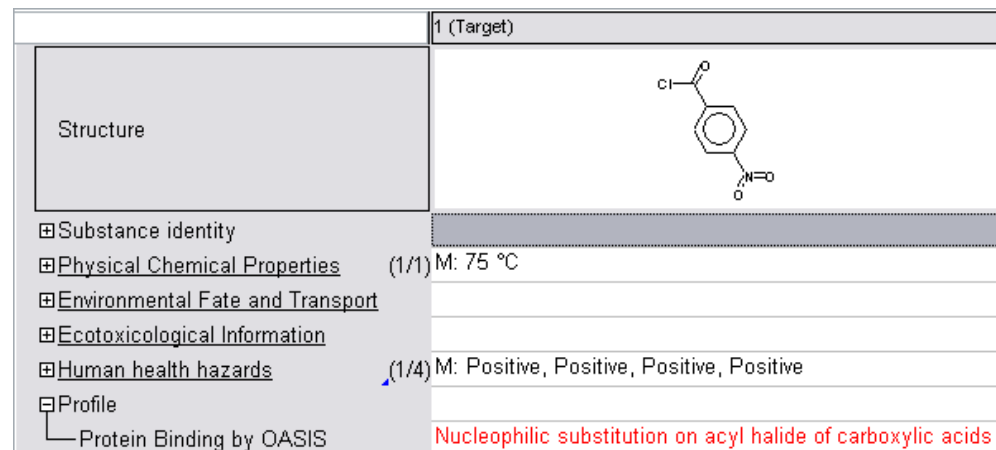
The screenshot displays the QSAR Toolbox Profiling interface. The top navigation bar includes 'Input', 'Profiling', 'Endpoint', 'Category Definition', 'Filling Data Gap', and 'Report'. The Profiling panel is active, showing a list of predefined methods on the left and a data table on the right. The 'Protein Binding by OASIS' method is selected. The data table shows the chemical structure of 4-nitrobenzoyl chloride and its profile: 'Nucleophilic substitution on acyl halide of carboxylic acids'.

! 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 .


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

Select databases by ticking  the corresponding databases → .

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



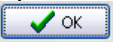


The screenshot displays the QSAR Toolbox data tree. The 'Structure' node is selected, showing the chemical structure of 4-nitrobenzoyl chloride. The data tree is expanded to show the 'Profile' section, which includes 'Protein Binding by OASIS' with the profile 'Nucleophilic substitution on acyl halide of carboxylic acids'.


! To open the data tree : double-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 . You are prompted to confirm the query details, name of the category and retrieval of experimental data. Press  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

→  → .

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).