

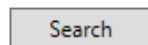
GETTING STARTED: QUICK REFERENCE GUIDE

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

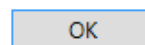
Define your target chemical by Chemical Name, CAS number, SMILES, drawing the molecule or selecting it from a list. To define a chemical by CAS number:



→ enter the number without hyphens,



→ the program displays the structure →



The structure is displayed on the data matrix.

The screenshot shows the QSAR Toolbox interface with the 'Define' button selected in the top right. The main window displays the chemical structure of Benzoyl chloride, 4-nitro- (CAS 122-04-3) and its corresponding data matrix. The data matrix includes the following information:


1 [target]
122-04-3
High
Benzoyl chloride, 4-nitro-
C7H4ClNO3
Unspecified
[O-][N+](=O)c1ccc(cc1)C(Cl)=O

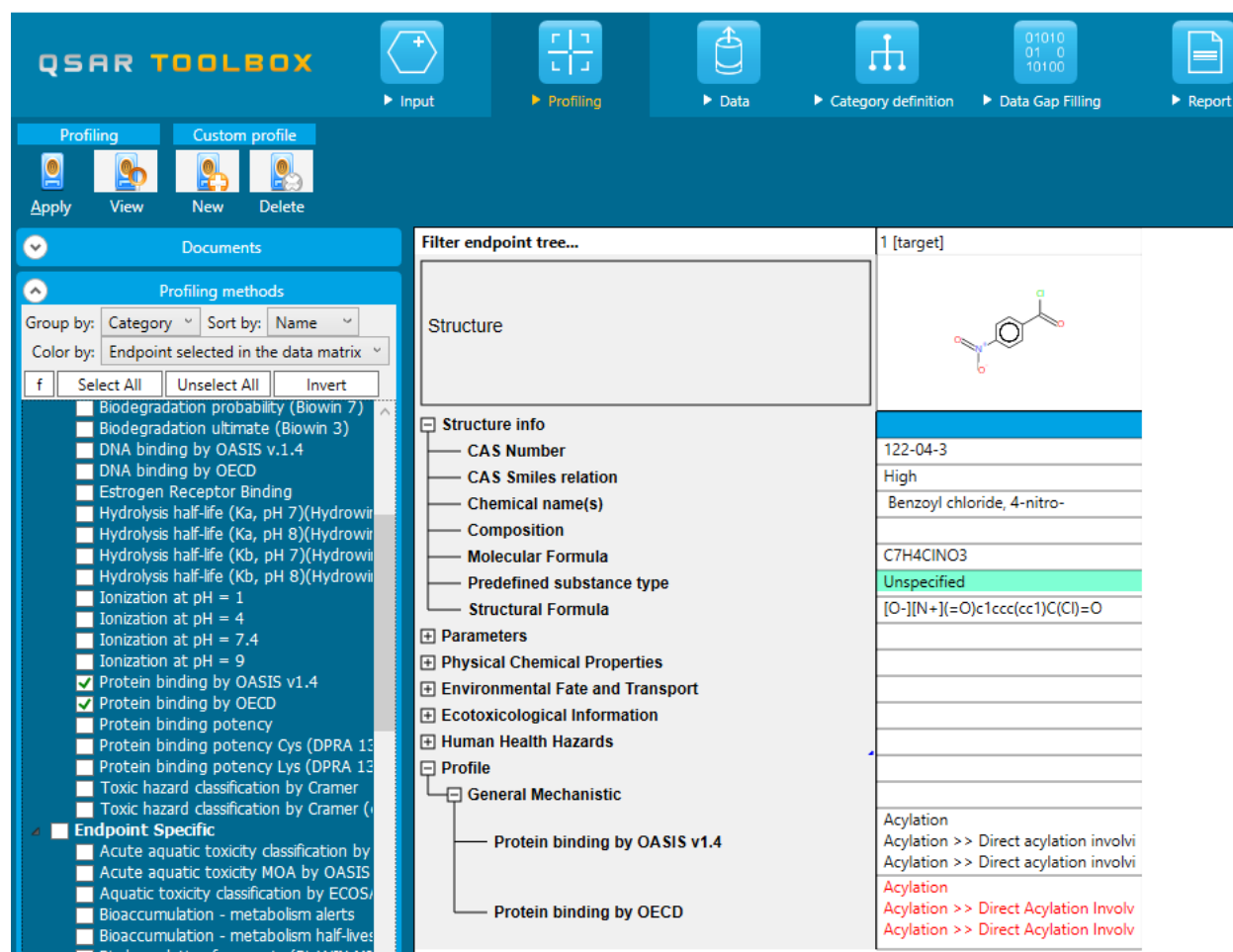


To define the target endpoint, which will be used for predictions click on





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.




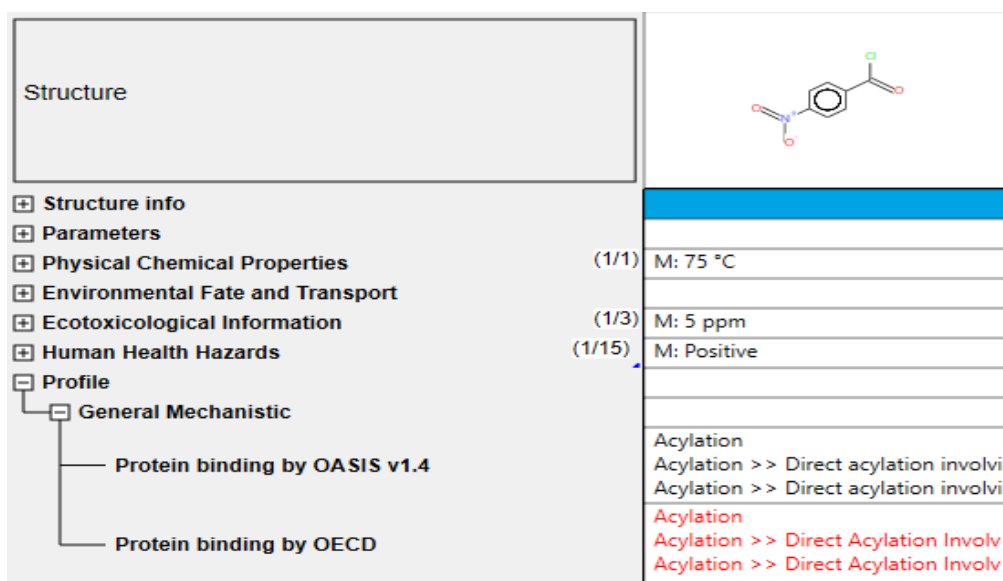
The screenshot displays the QSAR Toolbox interface during the Profiling step. The top navigation bar includes buttons for Input, Profiling, Data, Category definition, Data Gap Filling, and Report. The Profiling methods list on the left includes various endpoints, with 'Protein binding by OASIS v1.4' and 'Protein binding by OECD' checked. The 'Filter endpoint tree...' window shows a tree structure with 'Protein binding by OASIS v1.4' and 'Protein binding by OECD' selected. The 'Structure' window shows the chemical structure of Benzoyl chloride, 4-nitro- (SMILES: [O-][N+](=O)c1ccc(cc1)C(Cl)=O) and its corresponding profile information.

Structure info	Value
CAS Number	122-04-3
CAS Smiles relation	High
Chemical name(s)	Benzoyl chloride, 4-nitro-
Composition	
Molecular Formula	C7H4ClNO3
Predefined substance type	Unspecified
Structural Formula	[O-][N+](=O)c1ccc(cc1)C(Cl)=O
Parameters	
Physical Chemical Properties	
Environmental Fate and Transport	
Ecotoxicological Information	
Human Health Hazards	
Profile	
General Mechanistic	
Protein binding by OASIS v1.4	
Protein binding by OECD	

 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 on .

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 subsections in the endpoint tree:





The screenshot displays a software interface with a chemical structure on the right and a data matrix on the left. The chemical structure is 4-nitrobenzoic acid, with the SMILES string O=C(O)c1ccc([N+](=O)[O-])cc1. The data matrix is as follows:

Structure	
<input checked="" type="checkbox"/> Structure info	
<input checked="" type="checkbox"/> Parameters	
<input checked="" type="checkbox"/> Physical Chemical Properties	(1/1) M: 75 °C
<input checked="" type="checkbox"/> Environmental Fate and Transport	
<input checked="" type="checkbox"/> Ecotoxicological Information	(1/3) M: 5 ppm
<input checked="" type="checkbox"/> Human Health Hazards	(1/15) M: Positive
<input type="checkbox"/> Profile	
<input type="checkbox"/> General Mechanistic	
Protein binding by OASIS v1.4	
Protein binding by OECD	

Below the matrix, the following text is displayed:

Acylation
Acylation >> Direct acylation involvi
Acylation >> Direct acylation involvi
Acylation
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Acylation >> Direct Acylation Involv

 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.

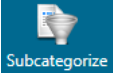
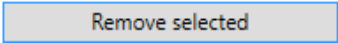
 The highlighted databases correspond to the selected endpoint in the data matrix or to the previously defined endpoint if any.


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

Select one grouping method according to the profile of your target chemical

in the window **Grouping methods** → .

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

To refine the category, repeat the procedure by clicking on  and selecting other grouping methods. In the subcategorization procedure, the function  deletes 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

Select data gap filling by clicking in the corresponding empty 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 → 

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

To obtain a report, select a prediction.

Click on the cell with the prediction → 