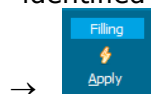


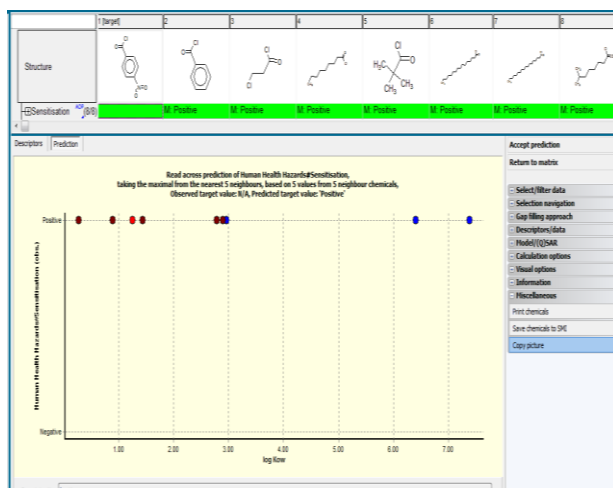
## Step 5: Filling data gap - Predict missing data by read-across, trend analysis or QSAR models

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

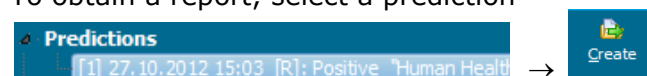


Once you are satisfied with a prediction, click **Accept prediction** and **Return to Matrix**.

! 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

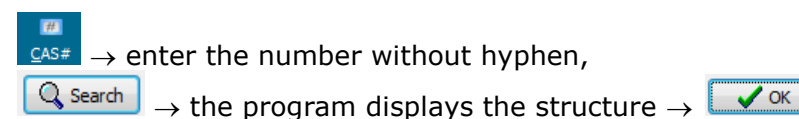


! Visit [www.qsartoolbox.org](http://www.qsartoolbox.org) for more detailed guidance documents.

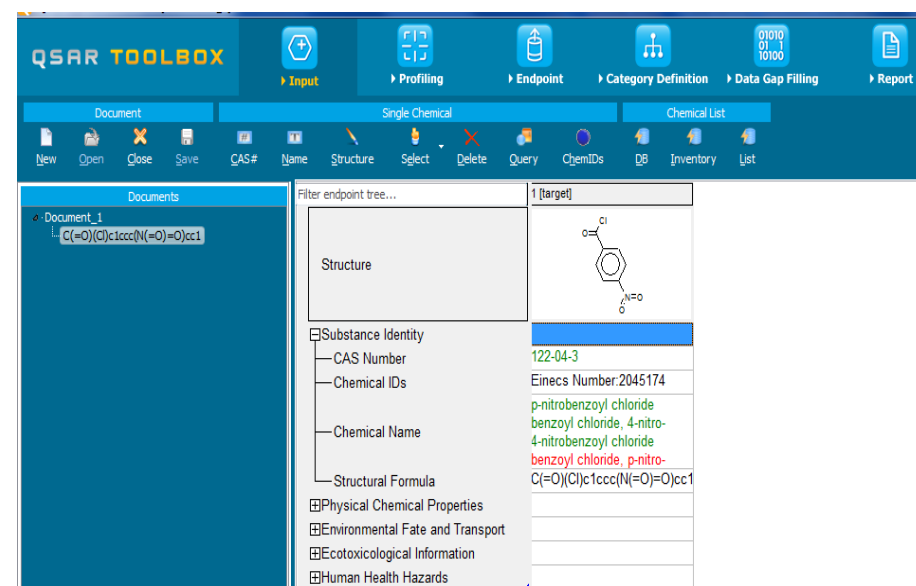
## GETTING STARTED : QUICK REFERENCE GUIDE

### 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:



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



Structure: C(=O)Cl


Substance Identity:

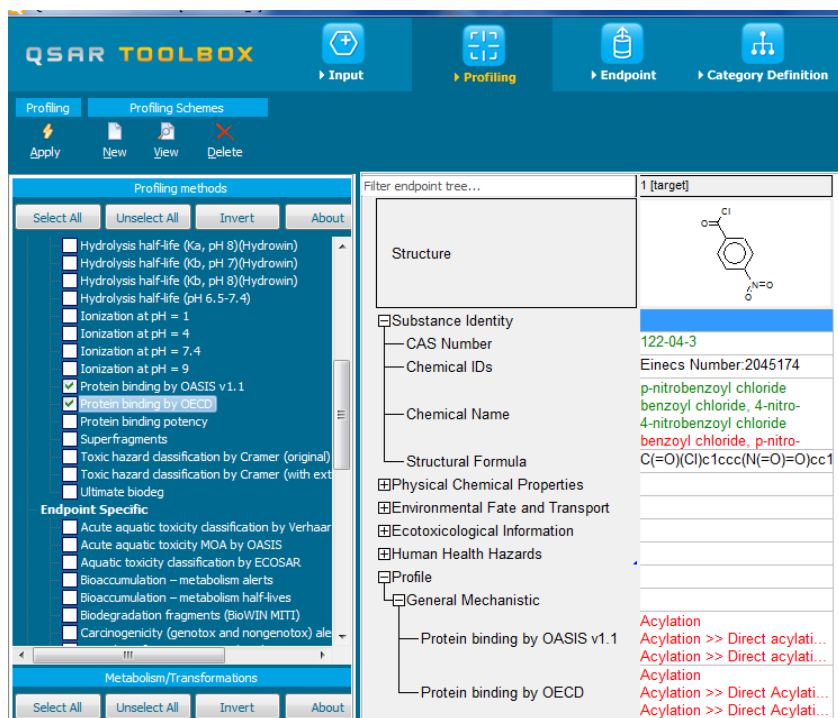
- CAS Number: 122-04-3
- Chemical IDs: EINECS Number: 2045174
- Chemical Name: p-nitrobenzoyl chloride, benzoyl chloride, 4-nitro-4-nitrobenzoyl chloride, benzoyl chloride, p-nitrobenzoyl chloride
- Structural Formula: C(=O)Cl
- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards


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



Filter endpoint tree...	1 [target]
Structure	
Substance Identity	
CAS Number	122-04-3
Chemical IDs	Einecs Number:2045174
Chemical Name	p-nitrobenzoyl chloride, 4-nitro-4-nitrobenzoyl chloride, p-nitrobenzoyl chloride, p-nitro-C(=O)(Cl)c1ccc(N(=O)=O)cc1
Structural Formula	
Physical Chemical Properties	
Environmental Fate and Transport	
Ecotoxicological Information	
Human Health Hazards	
Profile	
General Mechanistic	
Protein binding by OASIS v1.1	Acylation Acylation >> Direct acylati... Acylation >> Direct acylati...
Protein binding by OECD	Acylation Acylation >> Direct Acylati... Acylation >> Direct Acylati...

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

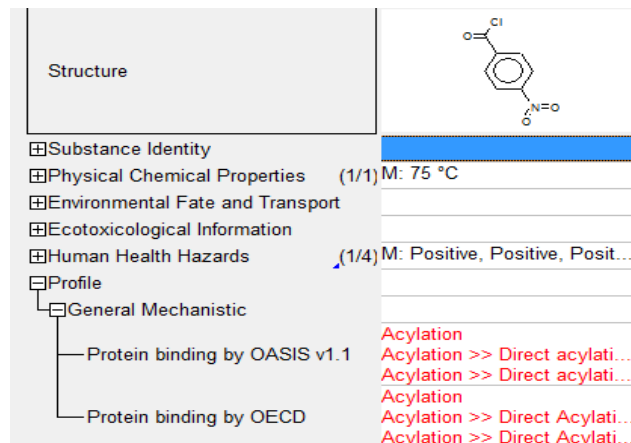
functioning of a profiler, select it and click → 

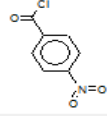
## Step 3: Endpoint - Retrieve experimental results from the resident databases

Select databases by ticking  the corresponding databases →



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



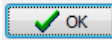
Filter endpoint tree...	1 [target]
Structure	
Substance Identity	
Physical Chemical Properties (1/1)	M: 75 °C
Environmental Fate and Transport	
Ecotoxicological Information	
Human Health Hazards (1/4)	M: Positive, Positive, Posit...
Profile	
General Mechanistic	
Protein binding by OASIS v1.1	Acylation Acylation >> Direct acylati... Acylation >> Direct acylati...
Protein binding by OECD	Acylation Acylation >> Direct Acylati... Acylation >> Direct Acylati...

! 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.

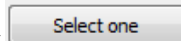

## Step 4: Category definition - Identify chemicals which could form a category with the "target" chemical

Select one grouping method according to the profile of your target


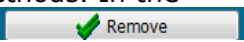
chemical in the window **Grouping methods** and then click 

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

 and selecting other grouping methods. In the subcategorisation procedure, the function  deletes chemicals with the highlighted profiles (i.e. by default chemicals that have profiles different from the target chemical).