QSAR TOOLBOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

OECD (Q)SAR Toolbox v.4.4.1

Predicting acute aquatic toxicity to fish of *Dodecanenitrile (CAS 2437-25-4)* by taking into account tautomerism

Outlook

- **Background**
- Keywords
- Objectives
- The exercise
- Workflow
- Save prediction

Background

- This is a step-by-step presentation designed to take the user of the Toolbox through the workflow for filling a data gap for acute aquatic toxicity to fish taking into account tautomerism of the target chemical.

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Keywords

TARGET CHEMICAL - chemical of interest

MODULE – a Toolbox module is a section dedicated to specific actions and options

WORKFLOW – the use, in combination, of the different modules (e.g. prediction workflow: from input to report)

PROFILER - algorithm (rule set) for the identification of specific features of the chemicals. Several types of profilers are available, such as structural (e.g. Organic functional groups), mechanistic (e.g. Protein binding by OECD) and endpoint-specific (e.g. in vitro in vitro mutagenicity (Ames test) alerts by ISS) profilers.

ALERT - the profilers consist of sets of rules or alerts. Each of the rules consists of a set of queries. The queries could be related to the chemical structure, physicochemical properties, experimental data, comparison with the target or list with substances and external queries from other predefined profilers (reference queries).

CATEGORY – "group" of substances sharing same characteristics (e.g. the same functional groups or mode of action). In a typical Toolbox workflow, it consists of the target chemical and its analogues gathered according to the selected profilers

ENDPOINT TREE – Endpoints are structured in a branched scheme, from a broader level (Phys-Chem properties, Environmental Fate and transport, Ecotoxicology, Human health hazard) to a more detailed one (e.g. EC3 in LLNA test under Human health hazard-Skin sensitization)

TAUTOMER – Tautomers are structural isomers which are in dynamic equilibrium due to the migration of a proton, accompanied by a switch of a single bond and adjacent double bond.

DATA MATRIX – Table reporting the chemical(s) and data (experimental results, profilers outcomes, predictions). Each chemical is in a different column and each data in a different row

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Objectives

- **This presentation reviews a number of functionalities of the Toolbox:**
  - Providing tautomeric set for the target chemical
  - Identify analogues for the active tautomeric form
  - Retrieve experimental results available for those analogues
  - Perform trend analysis for the active tautomeric form
  - Assigning of the prediction for the active tautomer to the target chemical
  - Saving the prediction result

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The Exercise

- In this exercise we will predict *LC50* for fish: *P.promelas* for target chemical *Dodecanenitrile (CAS 2437-25-4)*
- Set of simulated tautomers for the target chemical will be provided
- Analyze the profilers of the tautomeric forms within tautomeric set
- Filling data gaps for active tautomer by trend analysis
- Assign prediction for the tautomeric forms to the target chemical

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Workflow

- **As you know the Toolbox has 6 modules which are typically used in sequence:**
  - Chemical Input
  - Profiling
  - Data
  - Category Definition
  - Data Gap Filling
  - Report

Chemical Input
Ways of Entering a Chemicals

User Alternatives for input of Chemical:

A. Single target chemical

- Chemical Name
- Chemical Abstract Services (CAS) number (#)
- SMILES (simplified molecular information line entry system) notation/InChi
- Drawing chemical structure
- Select from User List/Inventory/Databases

B. Group of chemicals

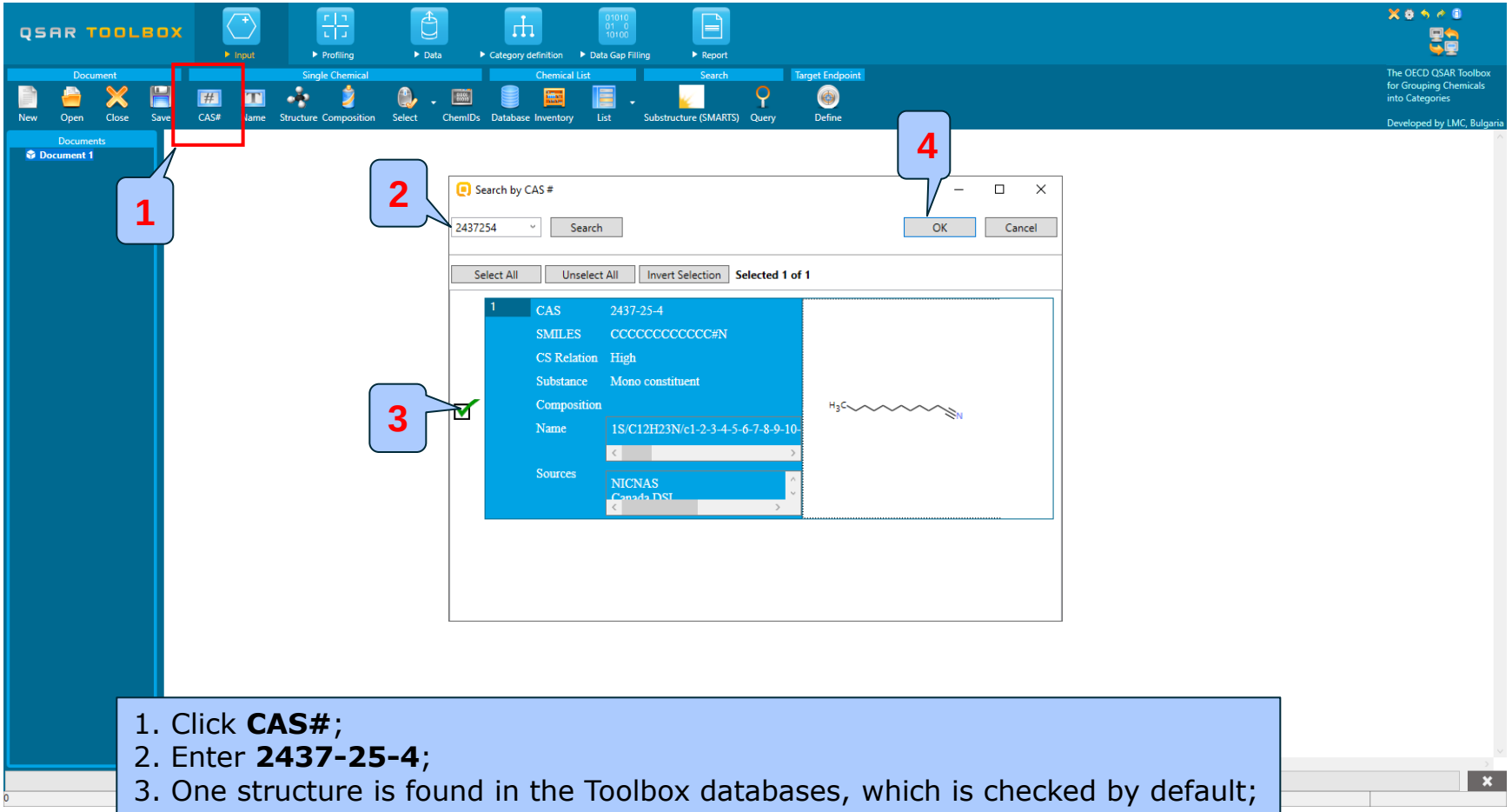
- User List/Inventory
- Specialized Databases

Chemical Input
Input Screen

- Open the Toolbox.
- The six modules in the workflow are seen listed next to "(Q)SAR TOOLBOX" title.
- Click on "Input" (see next screen shot)

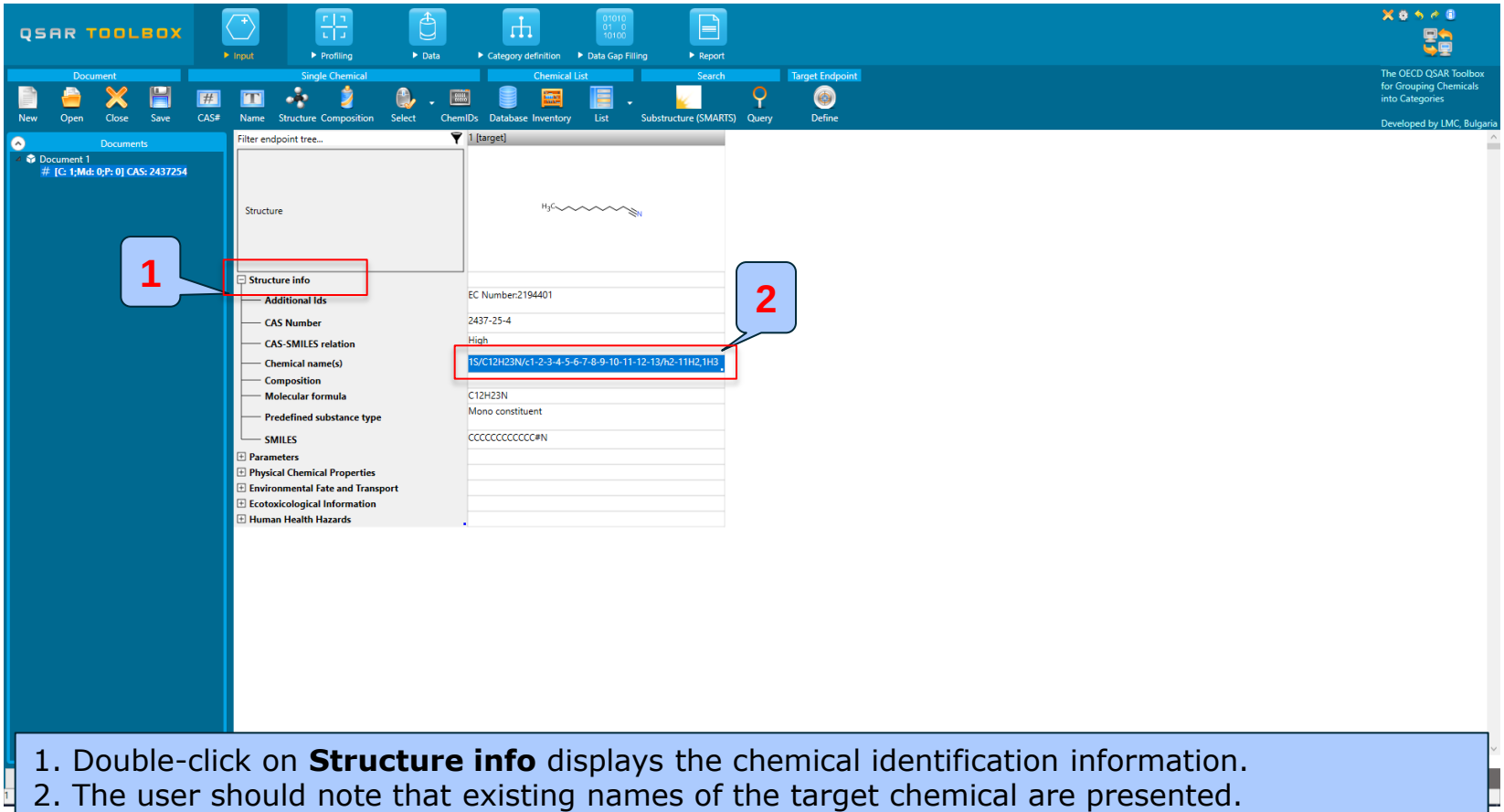
Chemical Input

Input target chemical by CAS#



1. Click **CAS#**;
2. Enter **2437-25-4**;
3. One structure is found in the Toolbox databases, which is checked by default;
4. Click **OK.**

Chemical Input
Target chemical identity



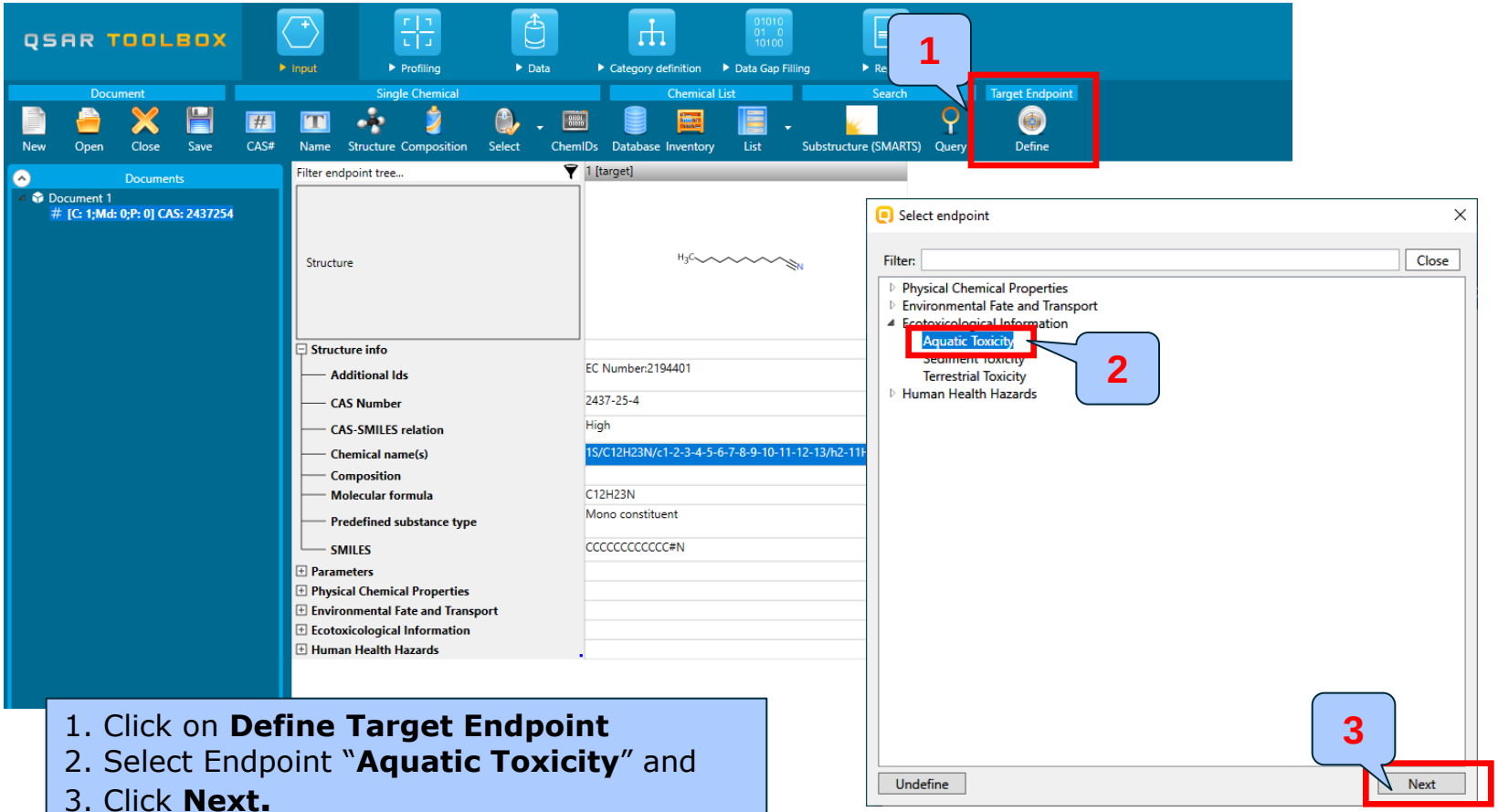
1. Double-click on **Structure info** displays the chemical identification information.
2. The user should note that existing names of the target chemical are presented.

The workflow on the first module is now complete, and the user can proceed to the next module.

Outlook

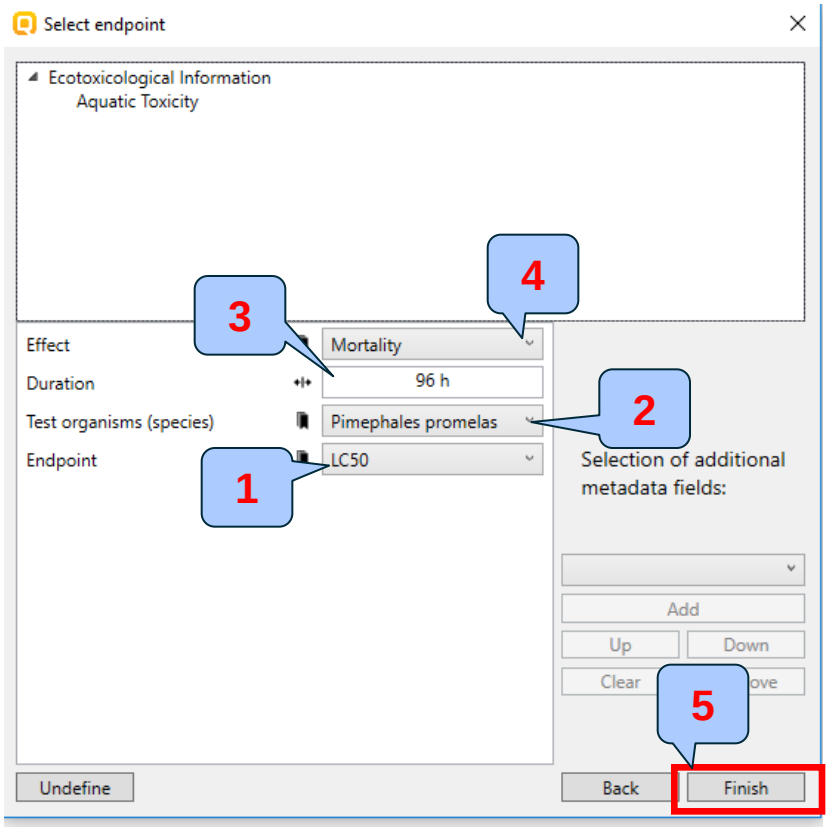
- Background
- Keywords
- Objectives
- The exercise
- **Workflow**
  - Input
  - **Define Target Endpoint**

Define target endpoint
Overview



1. Click on **Define Target Endpoint**
2. Select Endpoint "**Aquatic Toxicity**" and
3. Click **Next.**

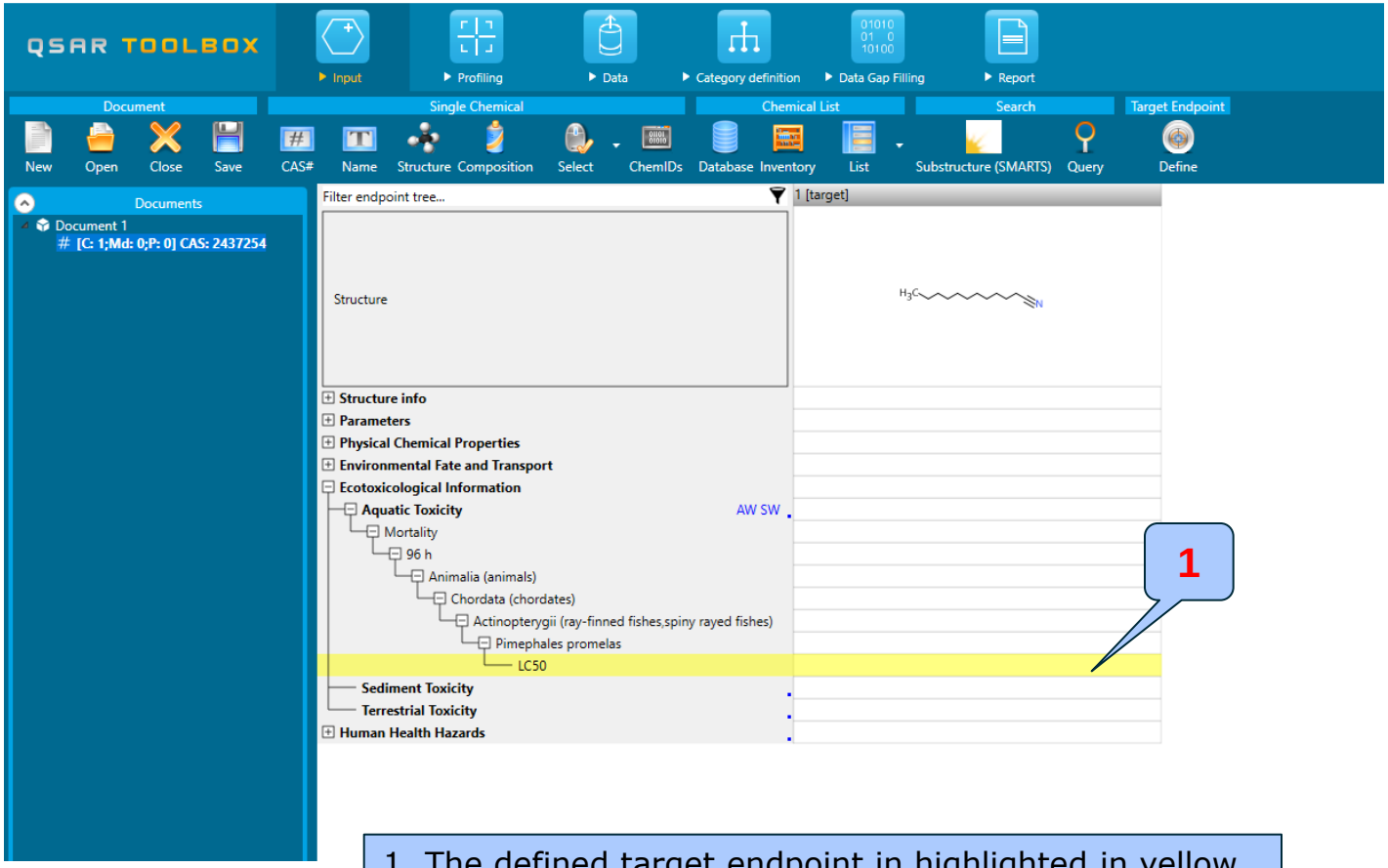
Define target endpoint
Overview



1. First select "LC 50" from drop- down menu of **Endpoint** field, then consecutively select the following metadata:
2. Field **Test organism (species)** – Pimephales promelas;
3. Field **Duration** – 96 h.
4. Field **Effect** – Mortality
5. Click **Finish.**

Define target endpoint

Overview



1. The defined target endpoint in highlighted in yellow

Outlook

- Background
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- **Workflow**
  - Input
  - Define Target Endpoint
  - **Profiling**

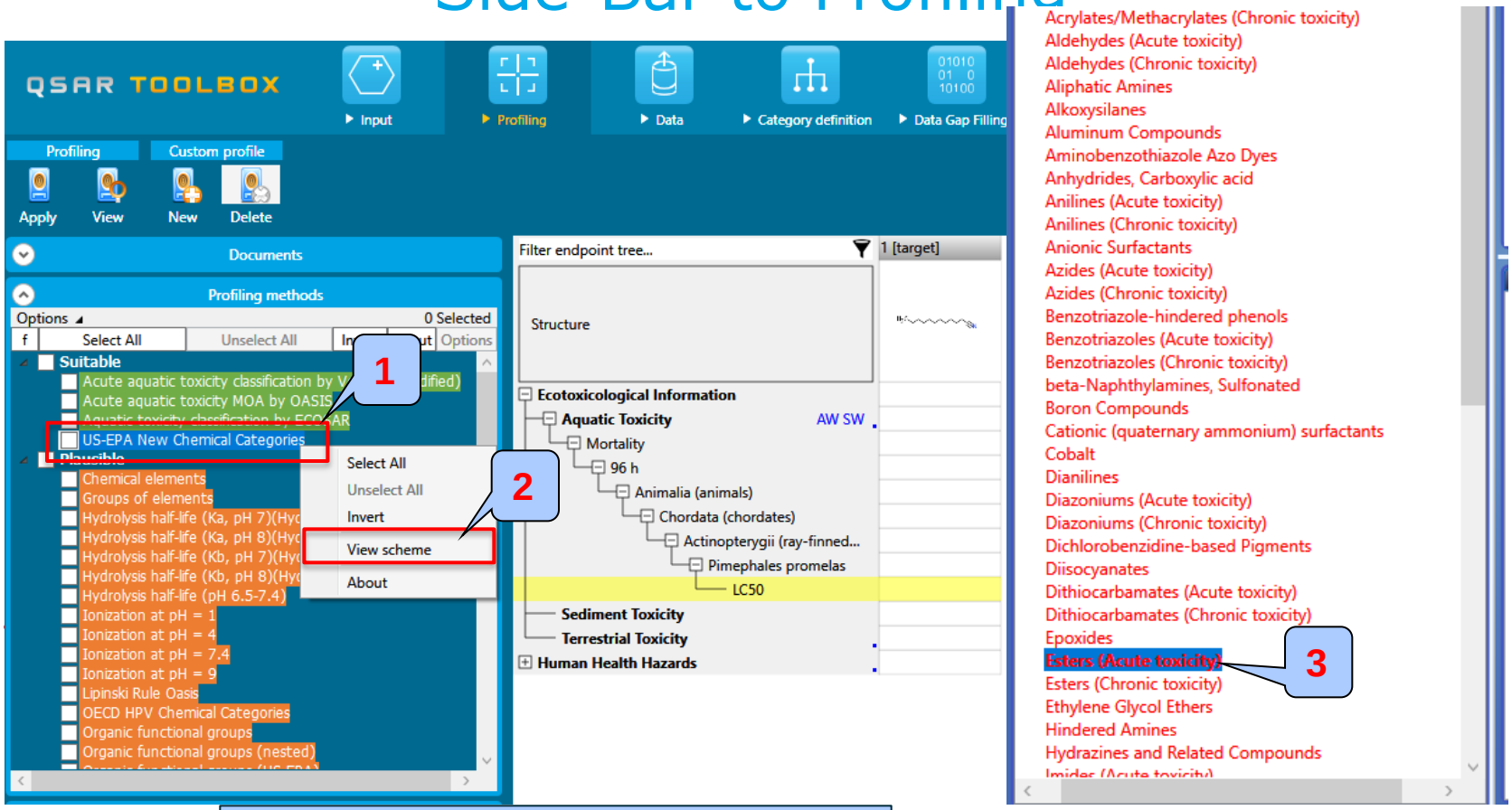
Profiling
Overview

- "Profiling" refers to the electronic process of retrieving relevant information on the target compound, other than environmental fate, ecotoxicity and toxicity data, which are stored in the Toolbox database.
- Available information includes likely mechanism(s) of action, as well as observed or simulated metabolites.

Profiling
Side-Bar to Profiling

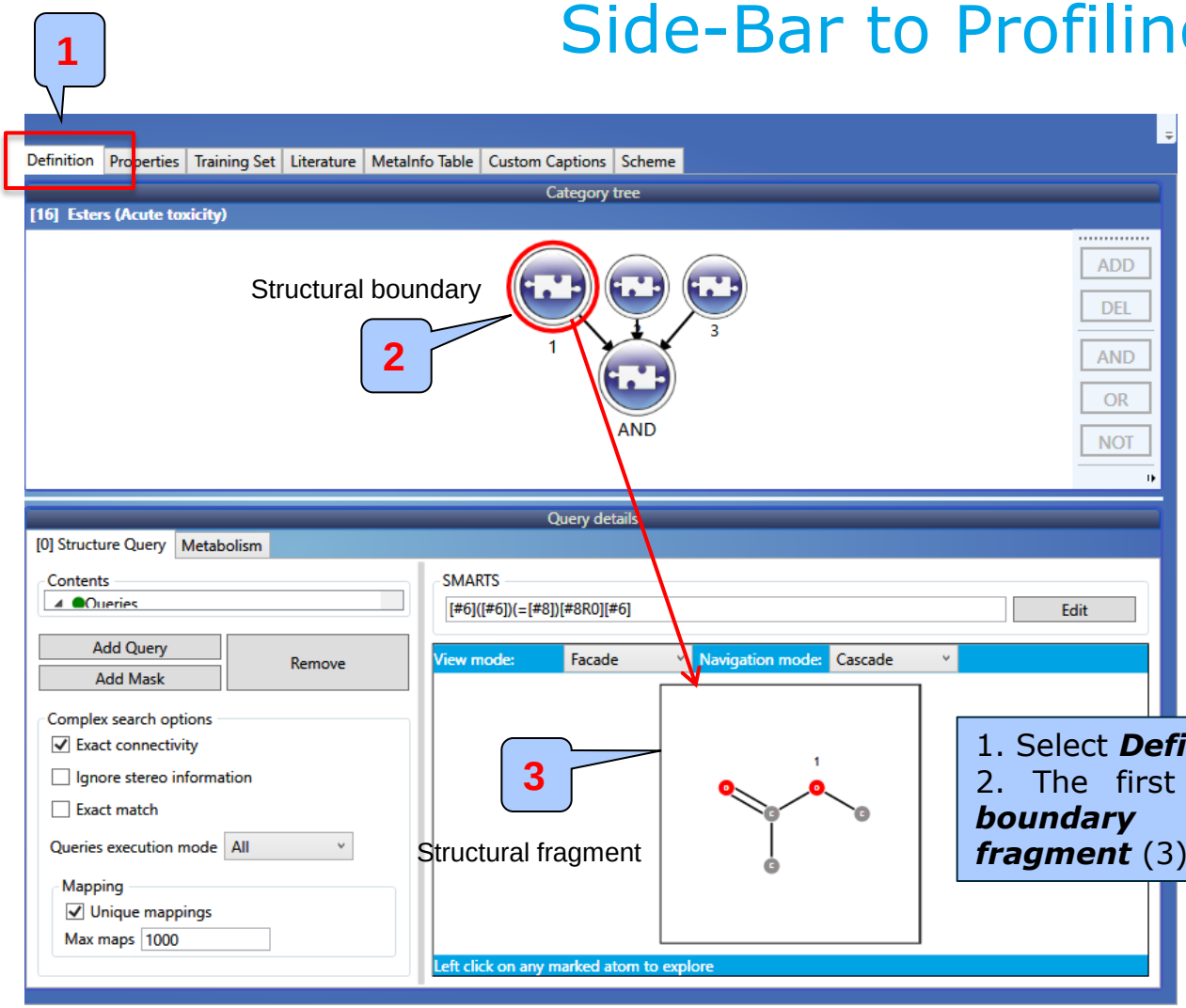
- For most of the profilers, background information can be retrieved by highlighting one of the profilers (for example, US-EPA New Chemical categories and clicking on “View” (see next screen shot).

Profiling
Side-Bar to Profiling



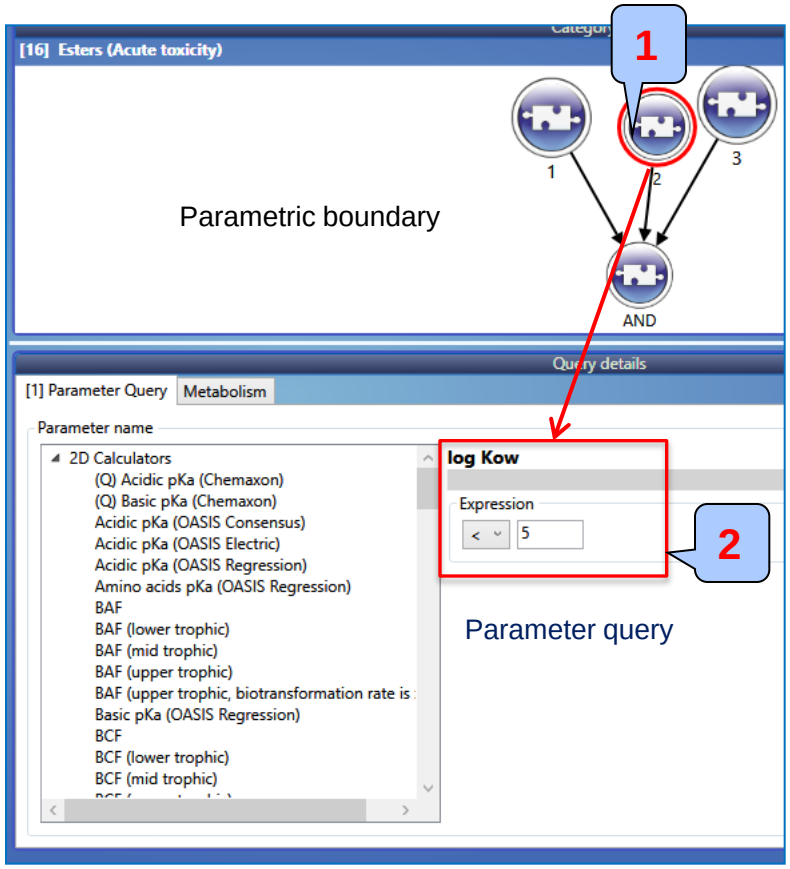
1. Select US-EPA New Chemical categories
2. **Click** View
3. **Select** "Esters(Acute toxicity)"

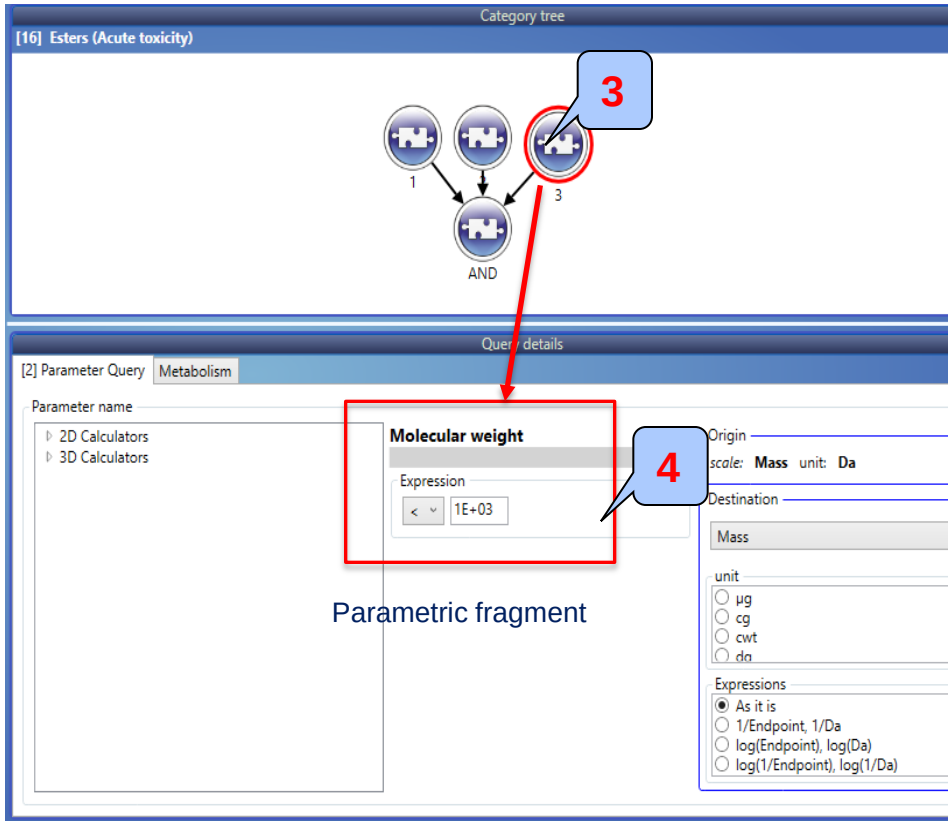
Profiling
Side-Bar to Profiling



1. Select ***Definition*** tab;
2. The first boundary is a ***structural boundary*** containing a ***structural fragment*** (3).

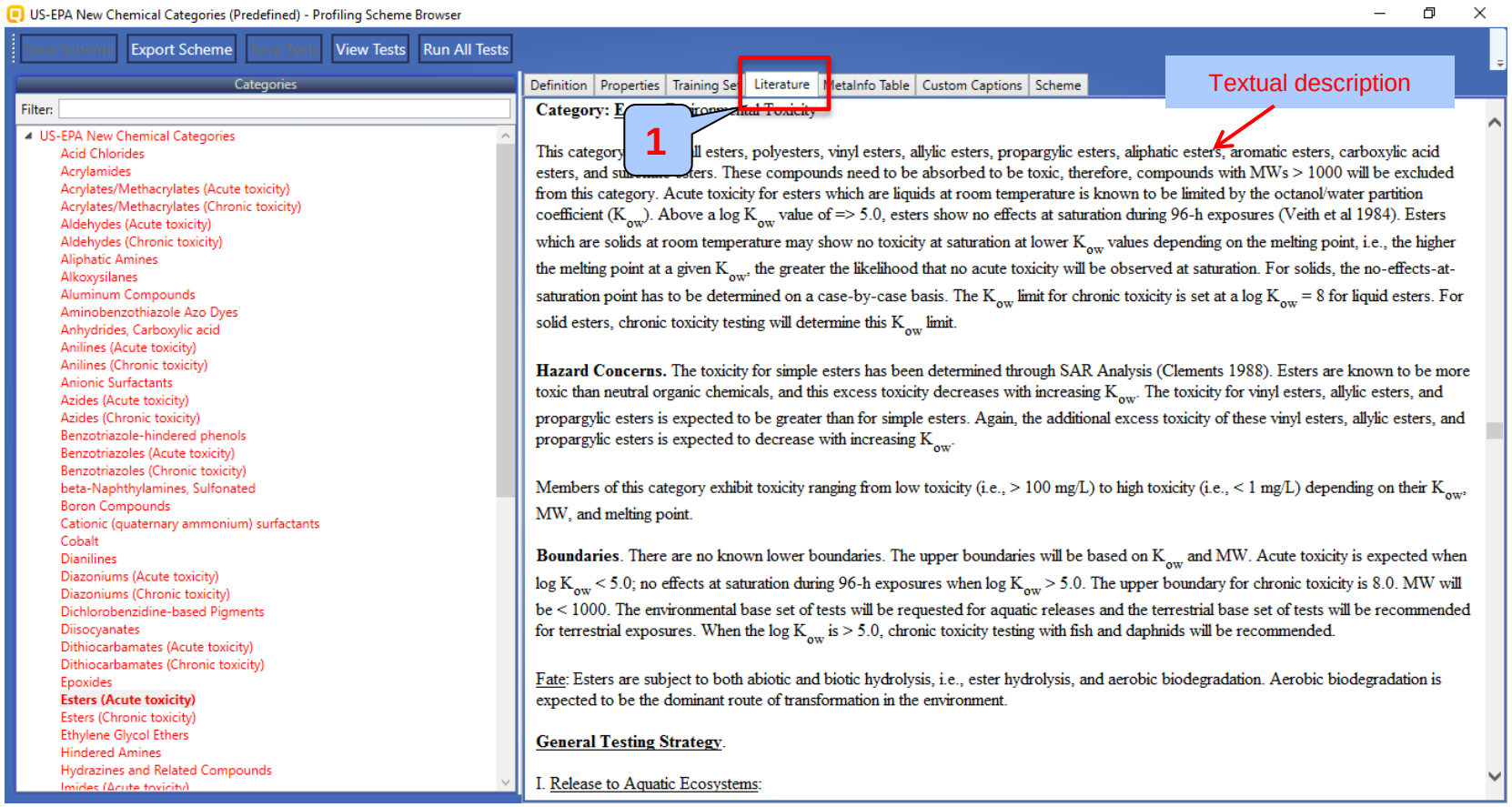
Profiling
Side-Bar to Profiling





The second boundary (1) is a parameter query containing expression for logKow (2); The third boundary (3) is a parameter query containing expression for Molecular weight (4).

Profiling
Side-Bar to Profiling



1. **Click on Literature** tab to see mechanistic justification of the category

Profiling

Profiling the target chemical

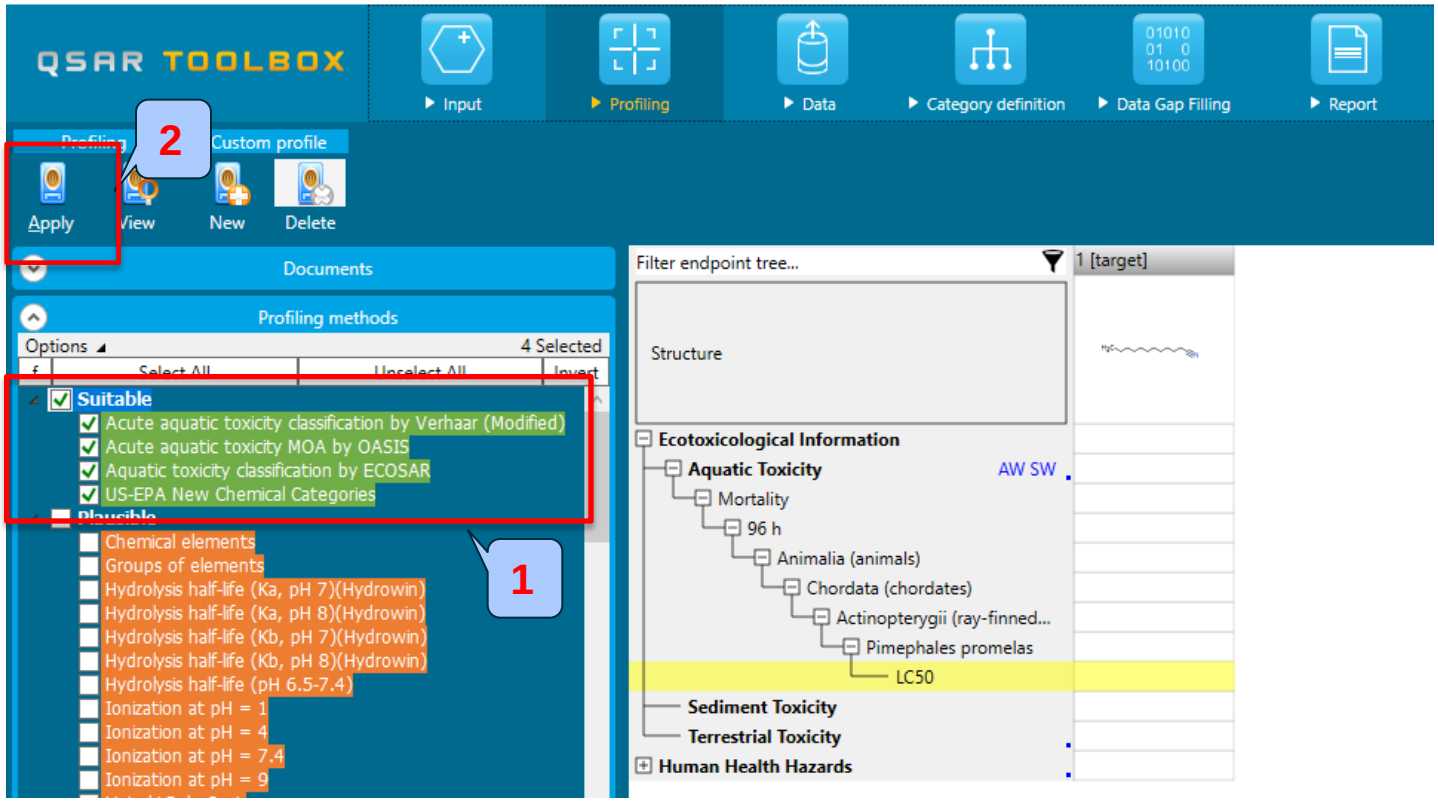
- The outcome of the profiling determines the most appropriate way to search for analogues
- The following profiling schemes are relevant to the **Acute aquatic toxicity**:
  - Aquatic toxicity classification by ECOSAR
  - Acute aquatic toxicity MOA by OASIS
  - Acute aquatic toxicity classification by Verhaar (Modified)
  - US-EPA New Chemical Categories
- More details about profiling schemes used for categorization and collection of analogues is provided in stage "Category formation" on slide 51

Profiling
Profiling the target chemical

- Select the "Profiling methods" related to the target endpoint by clicking the box next to the profilers name;
- This selects (a **green** check mark appears) or deselects (**green** check mark disappears) profilers.
- For this example, go through the general and endpoint specific profiling mechanisms and highlight those that apply to acute aquatic toxicity(see next screen shot).

Profiling

Profiling the target chemical



1. Check all **green highlighted profilers;**
2. Click **Apply.**

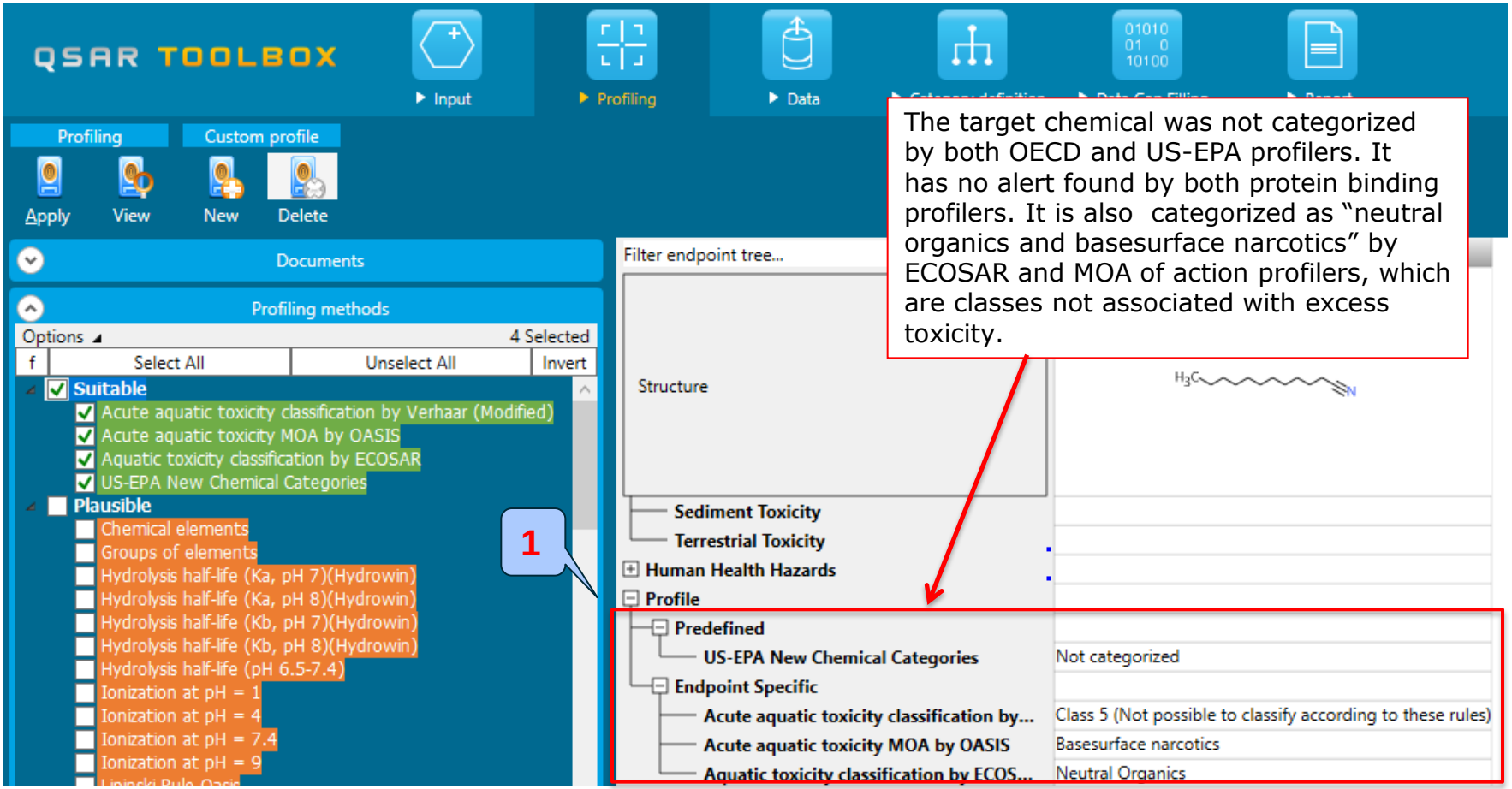
Profiling
Profiling the target chemical

- The actual profiling will take up to several seconds depending on the number and type of profilers selected
- The results of profiling automatically appear as a dropdown box under the target chemical (see next screen shot)
- Please note the endpoint specific profilers and structure based profilers such as US-EPA and ECOSAR
- No structural and endpoint specific alerts have been found for the test compound.

(see next screenshot)

Profiling

Profiling the target chemical



1. Double click on **Profile** node to review the profiling results.

Outlook

- Background
- Keywords
- Objectives
- The exercise
- **Workflow**
  - Input
  - Define Target Endpoint
  - Profiling
  - **Data**

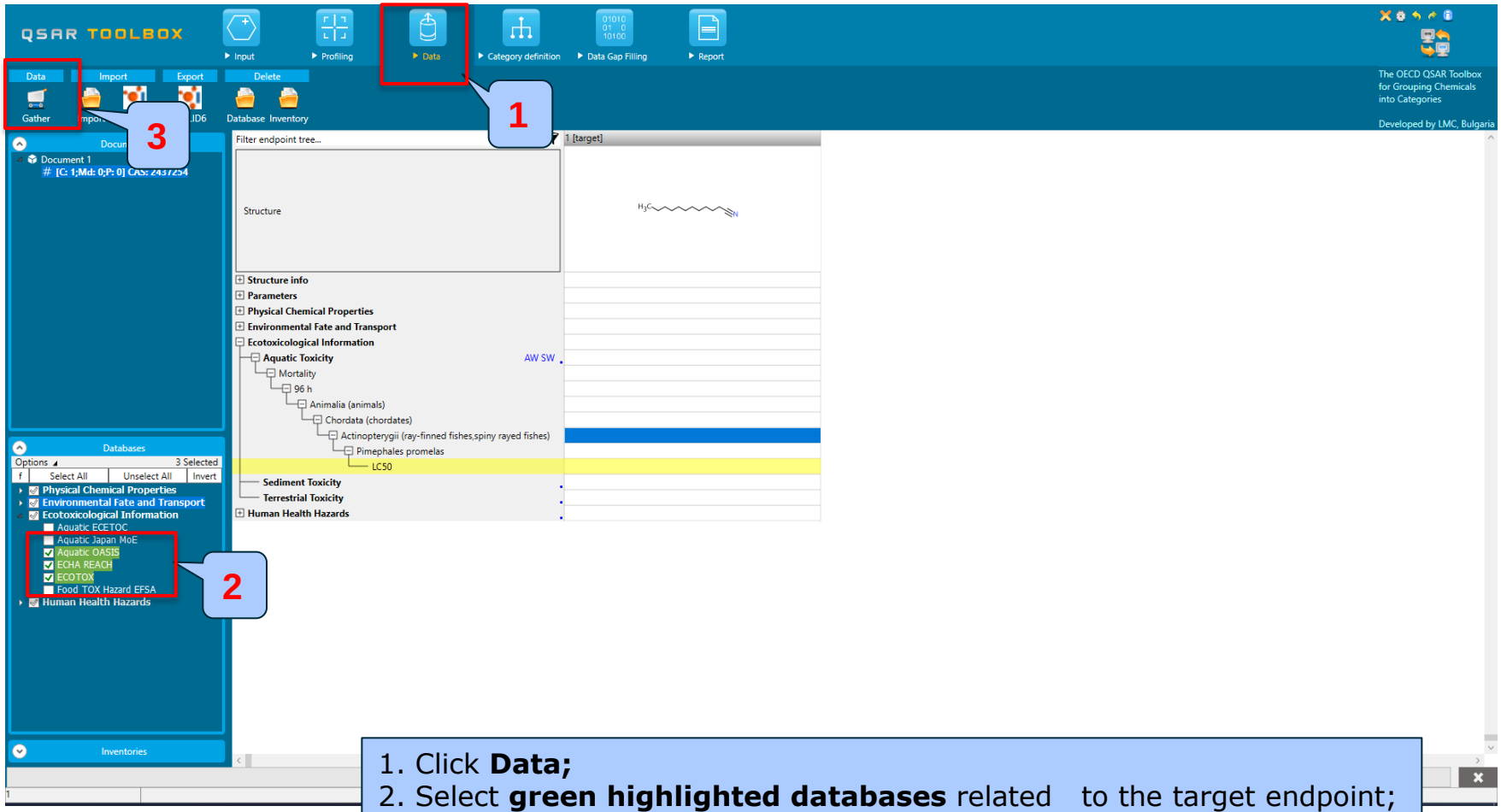
Data
Overview

- "Data" refers to the electronic process of retrieving the environmental fate, ecotoxicity and toxicity data that are stored in the Toolbox.
- Data gathering can be executed in a global fashion (i.e., collecting all data for all endpoints) or on a more narrowly defined basis (e.g., collecting data for a single or limited number of endpoints).

Data
Case study

- In this example, we limit our data gathering to a single toxicity endpoint (acute aquatic toxicity).
- In this example, we collect data from the databases containing experimental results for acute aquatic toxicity (Aquatic toxicity OASIS; ECOTOX and ECHA REACH).
- Click on "Data" in the Toolbox workflow.
- Expand the "Ecotoxicological information" section
- Click on the box to select the relevant databases.
- Click on "Gather data" (see next screen shot).

Data
Gather data



1. Click **Data;**
2. Select **green highlighted databases** related to the target endpoint;
3. Click **Gather.**

Data
Gather data

- Toxicity information on the target chemical is electronically collected from the selected dataset(s)

- It should be kept in mind that the search for data and analogues is performed only among the chemicals which are listed in the selected databases, which in this example are Aquatic toxicity OASIS; ECOTOX and ECHA REACH.

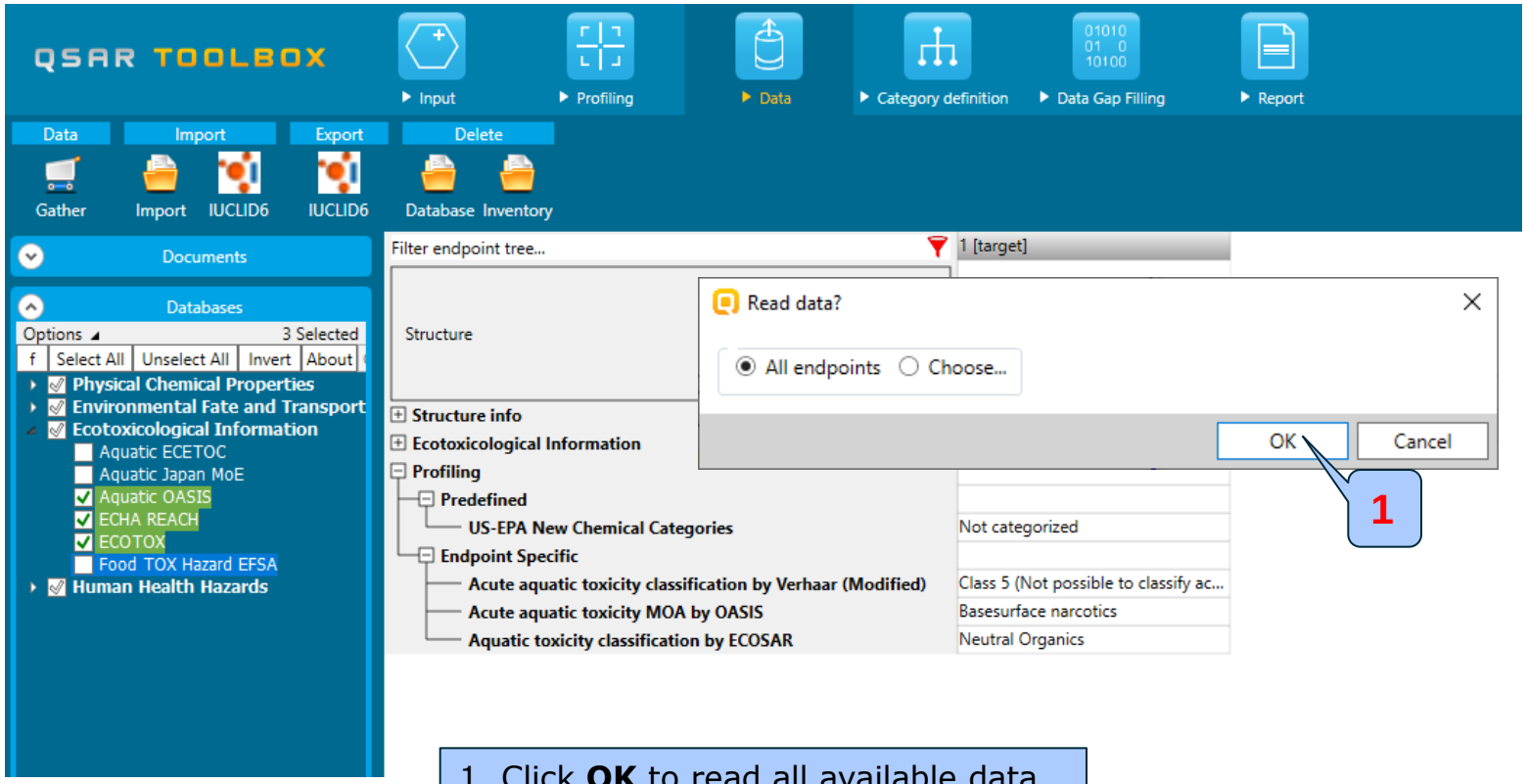
- In this example, there is LC50 experimental data for *P. promelas* (96h) for the target chemical (see next screen shots)

- The experimental data for the investigated endpoint falls within the toxic range (less than 1mg/l[1])

[1] Globally Harmonized System of Classification and Labeling of Chemicals (GHS):
https://www.unece.org/fileadmin/DAM/trans/danger/publi/ghs/ghs_rev04/English/ST-SG-AC10-30-Rev4e.pdf

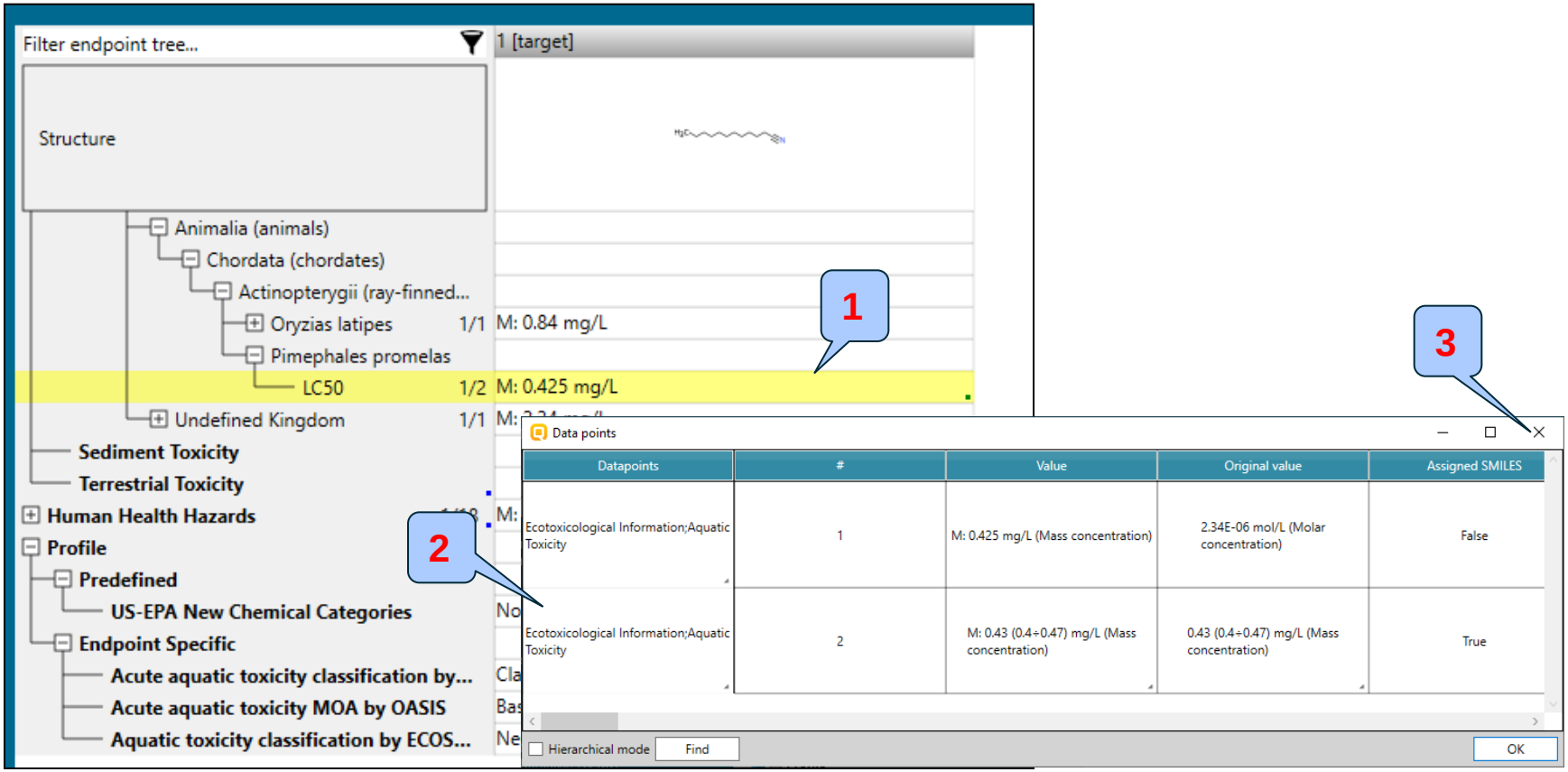
Data
Gather data

Toxicity information on the target chemical is electronically collected from the selected datasets. A Read data?" window appears. Now the user could choose to collect "all" or "endpoint specific" data for the target chemical.



1. Click **OK** to read all available data.

Data
Gather data



1. Double-click on **the cell** displays metadata information for the observed data (2)
2. Click on the **X** to close the window.

Recap

- The first module, which introduces the target chemical, ensure correctness of the structure;
- In the second module the target endpoint was defined.
- The third module shows that there is no structural or endpoint specific alerts for target chemical
- In the fourth module, you have found that the target chemical has experimental data for the investigated endpoint
- The study continues with accounting for tautomersim of target chemical trying to explain toxic experimental data of the target chemical (see next slides).

Outlook

- Background
- Keywords
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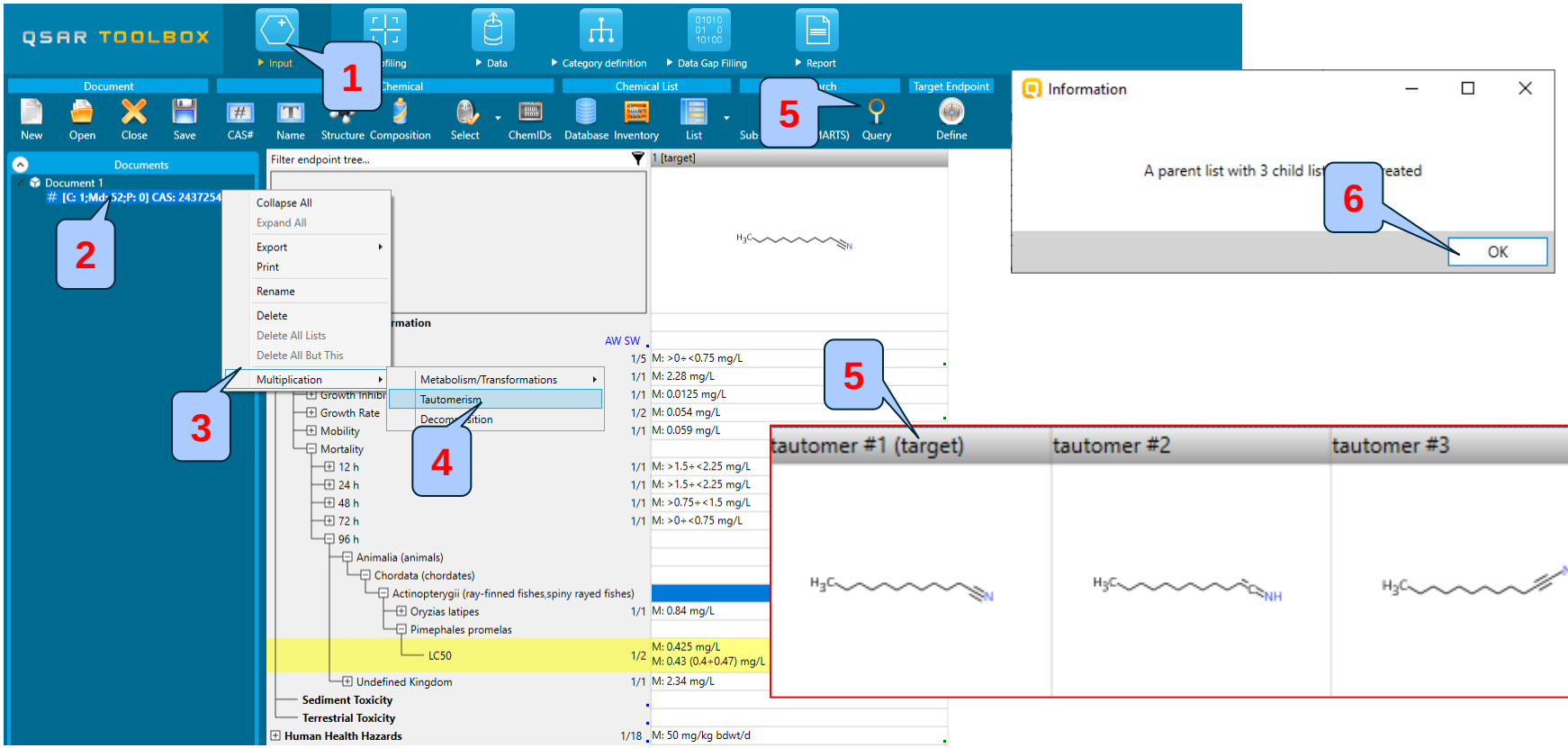
- The exercise
- **Workflow**
  - Input
  - Define Target Endpoint
  - Profiling
  - Data
  - **Handling of tautomerism of target chemical**

Handling of tautomerism of target chemical



1. Go to **Input**
2. Right click over the node with **CAS#** and select **Multiplication** (3) and then **Tautomerism** (4)
5. Three tautomeric forms are generated for the target chemical;
6. Click **OK**.

Outlook

- Background
- Keywords
- Objectives
- The exercise
- **Workflow**
  - Input
  - Profiling
  - Data
  - Handling of tautomerism of target chemical
    - **Profiling set of tautomers**

Handling of tautomerism of target chemical
Profiling set of tautomers

- This module identifies profilers of target chemical and its tautomeric forms
- Endpoint specific and structurally based profiles related to acute aquatic toxicity are applied on the set of tautomers
- Profiling results of tautomers are illustrated in Single Component mode
- Click on “Profiling" to go to the required module (see next screen shots)

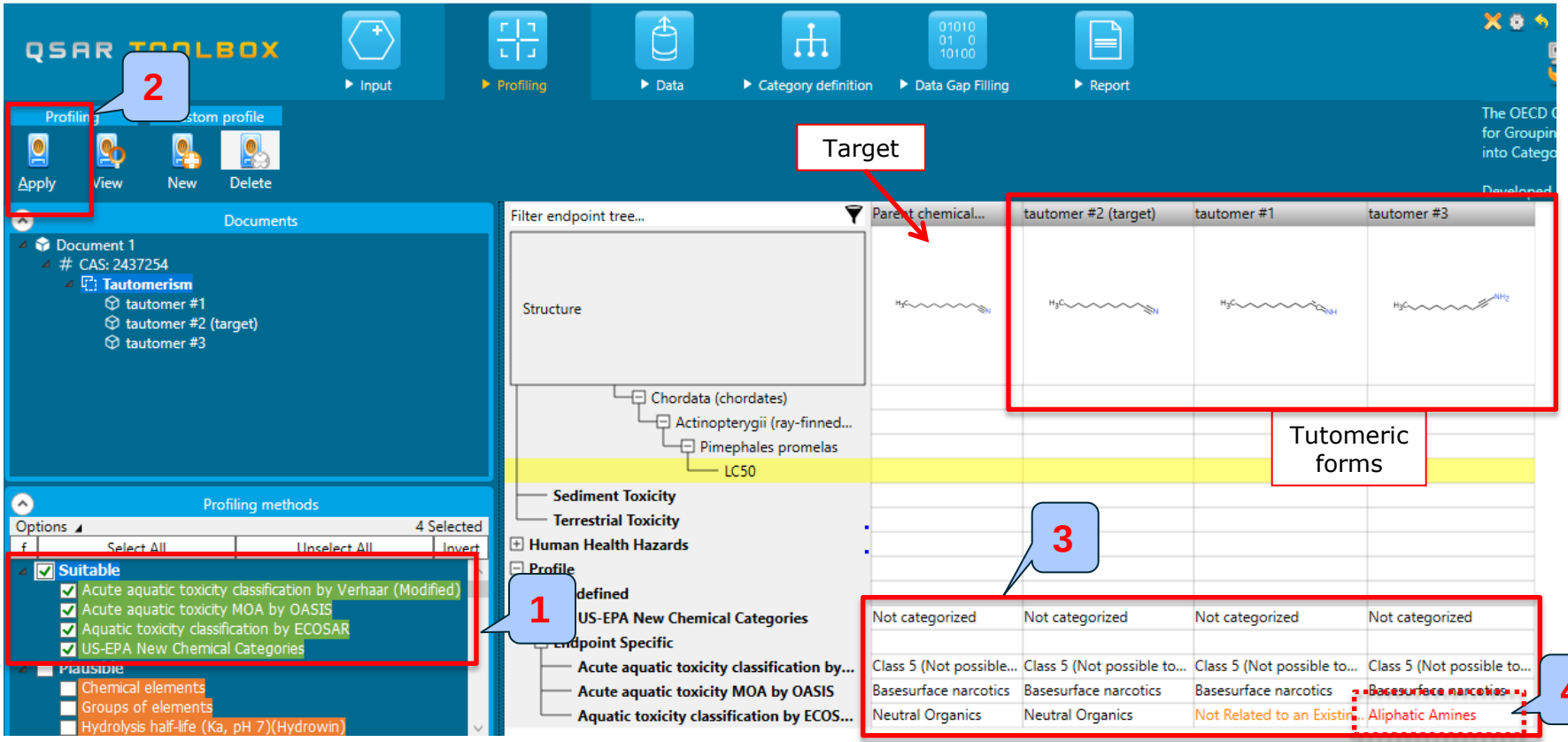
Handling of tautomerism of target chemical
Profiling set of tautomers

- The following primary profilers relevant to the aquatic toxicity are used in this example (see next screenshot):
  - US-EPA New chemical category
  - Aquatic toxicity classification by ECOSAR
  - Acute aquatic toxicity MOA by OASIS
  - Acute aquatic toxicity classification by Verhaar

- Select the Profilers highlighted in green which are related to the target endpoint by ticking the boxes next to the profilers name.

Handling of tautomerism of target chemical

Profiling set of tautomeric forms



1. Check the **profilers related to acute aquatic toxicity** (highlighted in green)
2. Click **Apply**

The profiling results **(3)** indicates no alerts found for the target chemical. Also classes associated with baseline toxicity (not excess toxicity) have been found for the target. However, there is an endpoint specific alert (Aliphatic amines) **(4)** for one of the simulated tautomeric form. This tautomer has been used in further trend analysis

Handling of tautomerism of target chemical
Recap

- The profiling results indicates no endpoint specific or active structural alerts for target chemical
- One of the simulated tautomeric form has positive endpoint specific alert identified by ECOSAR
- The active tautomer is used for further trend analysis
- The next two parts of the exercise will focus the active tautomer and identify the category of similar analogues (see next screenshots).

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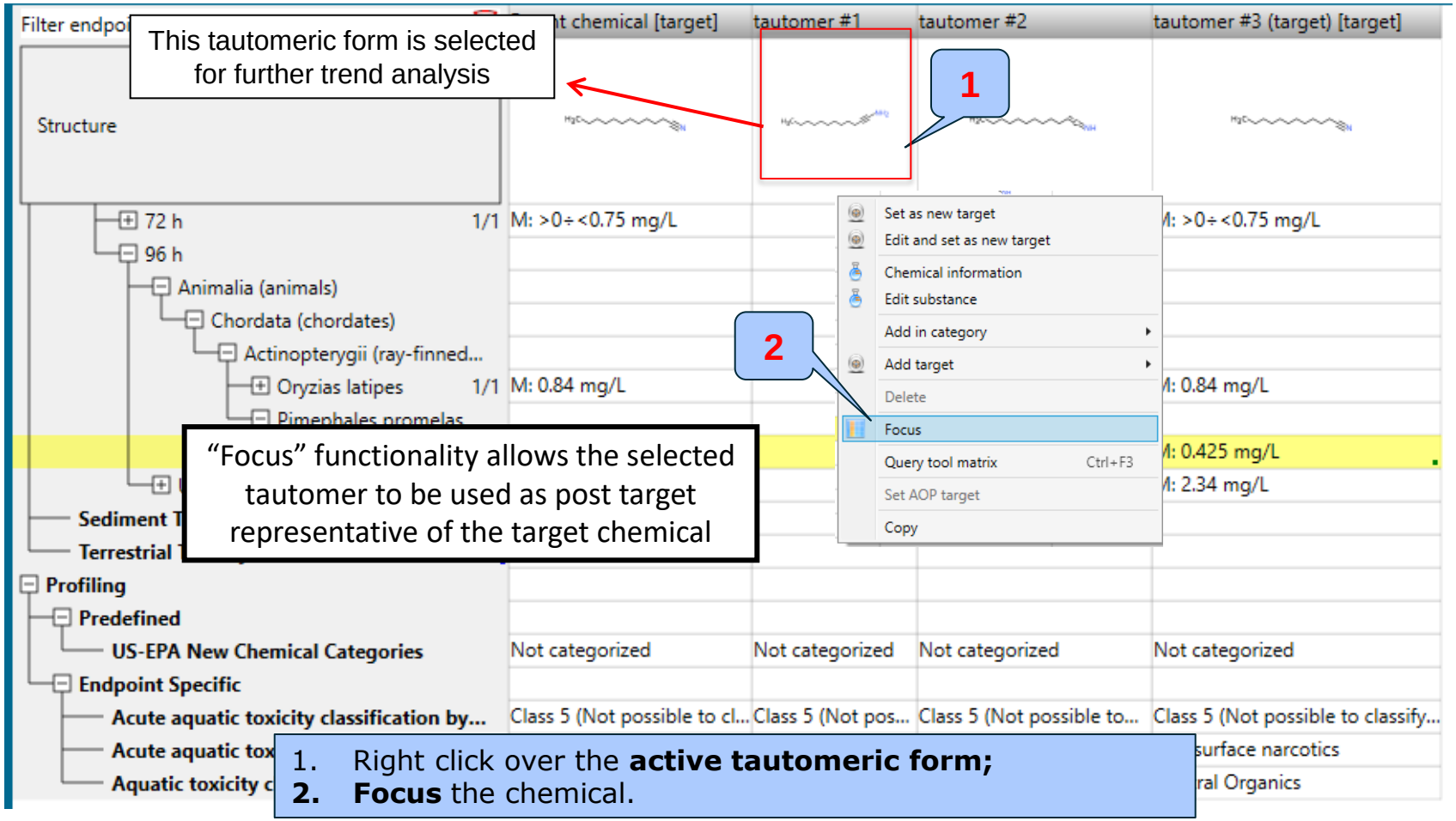
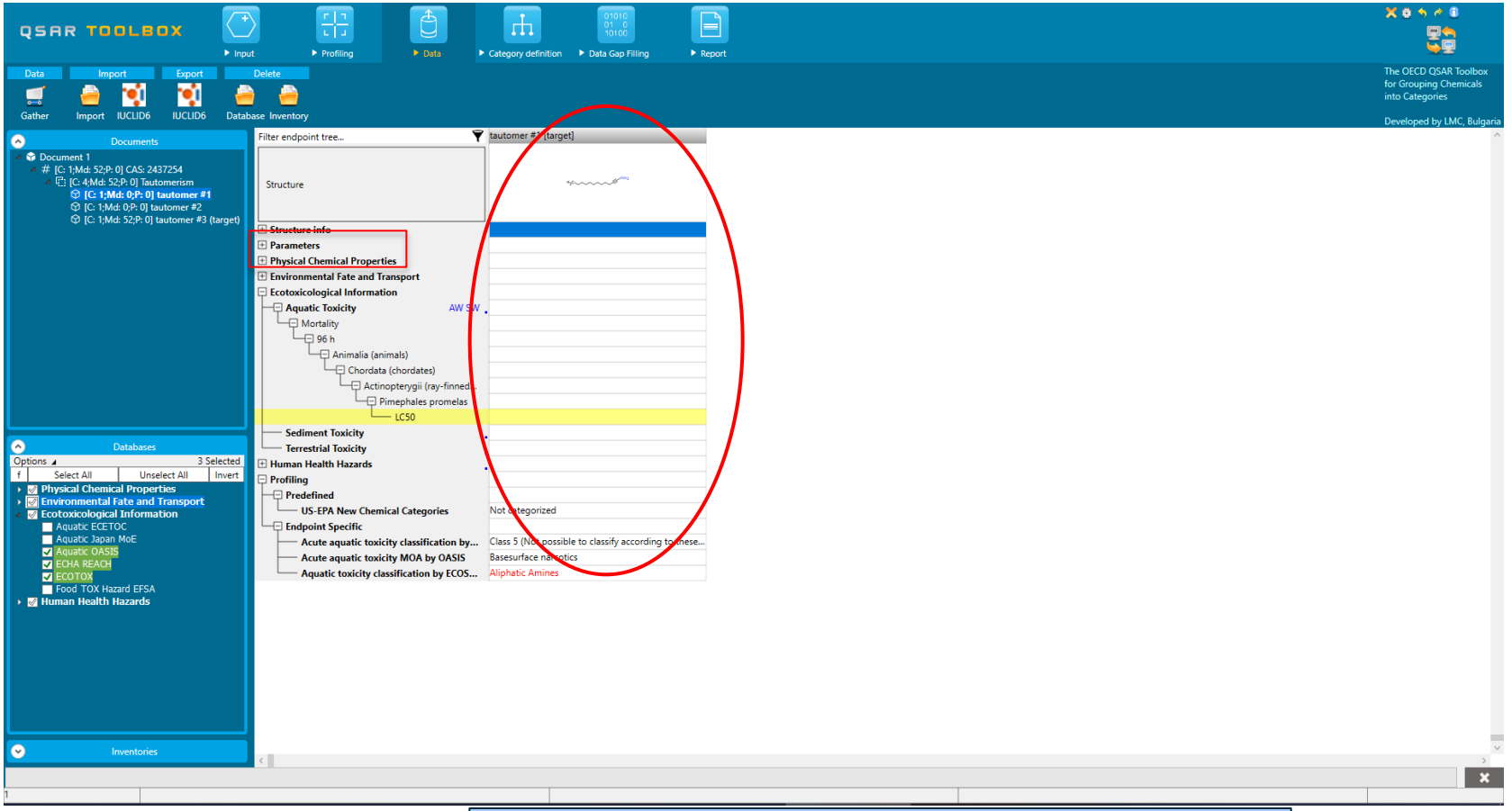
- **Workflow**
  - Input
  - Profiling
  - Data
  - Handling of tautomerism of target chemical
    - Profiling set of tautomers
    - **Focus active tautomer**

Handling of tautomerism of target chemical
Focus of active tautomer



Handling of tautomerism of target chemical
Focus of active tautomer



The selected tautomer appears in a new data matrix.

Outlook

- Background
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- The exercise
- **Workflow**
  - Input
  - Profiling
  - Data
  - Handling of tautomerism of target chemical
    - Profiling set of tautomers
    - Focus active tautomer
    - **Defining category for active tautomer**

Category Definition
Grouping methods

- The different grouping methods allow the user to group chemicals into chemical categories according to different measures of "similarity" so that within a category data gaps can be filled by read-across/trend analysis.

Basic guidance for category formation and assessment

Usually, a three stages procedure is recommended for building categories for read-across, in Toolbox. The categorization phases could be organized as follows:

- Stage I: Broad and endpoint non-specific primary categorization of chemicals based on their belonging to common chemical classes, predefined categories or being structurally similar
- Stage II: Subcategorization based on mechanisms conditioning the target endpoint thus coming to endpoint specific subset of chemicals reacting by same interaction mechanisms.
- Stage III: Further narrowing down the category based on elimination of chemicals most dissimilar to target one by using additional structure-related profilers

This sequence of stages is not mandatory and depends on the specificity and number of the chemical analogues and target endpoint. Moreover, some of the stages could be skipped if consistency of category members is reached earlier. It is also recommended only primary categorization to be applied in the Category Definition phase of the Toolbox workflow whereas the subcategorization to be applied at Data gap filling phase; thus, one could follow up the effect of subcategorization on the read-across results (having visualization of the endpoint vs. parameter relationship).

The structural similarity is not recommended to be applied as primary categorization. However, often it is needed to be used in the last stage of the subcategorization – for eliminating most dissimilar chemicals. This holds for read-across implementation for any endpoint.

Graphical illustration of suitable categorization phases is shown on next slide

Suitable Categorization/Assessment Phases

Phase I. Structure based

- US EPA Categorization
- OECD Categorization
- Organic functional group
- Structural similarity
- ECOSAR

Broad grouping
Endpoint Non-specific

Repeating Phase I due to Multifunctionality of chemicals

Phase II. Mechanism based*

- DNA binding mechanism
- Protein binding mechanism
- Genotoxicity/carcinogenicity
- Cramer rules
- Verhaar rule
- Skin/eye irritation corrosion rules

Subcategorization
Endpoint Specific

Metabolism accounted for

Phase III. Eliminating dissimilar chemicals

Apply Phase I – for structural dissimilarity
Filter by test conditions – for Biological dissimilarity

Subcategorization
Endpoint Specific

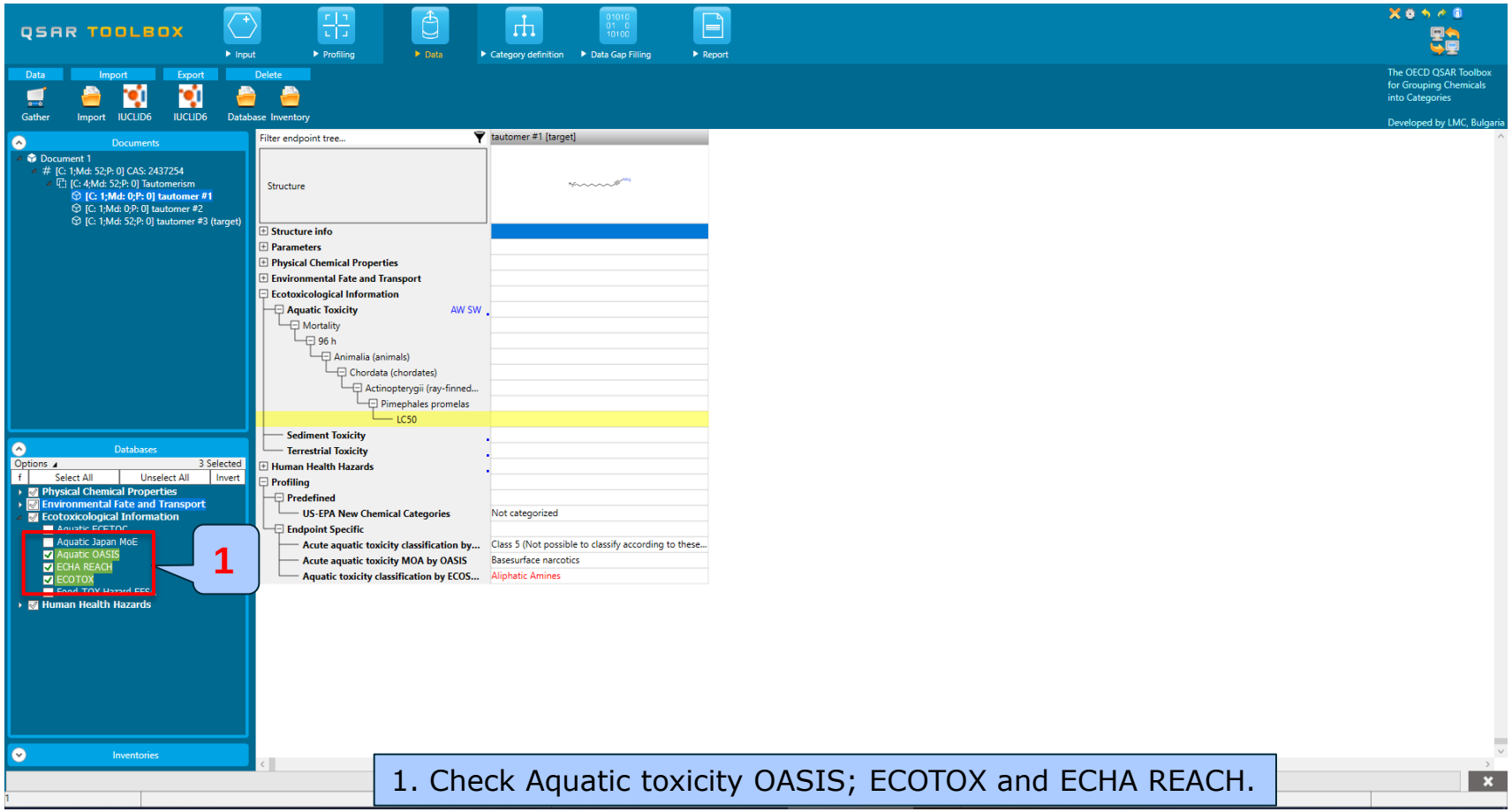
*General strategy not specific to the investigated acute aquatic tox endpoint

Handling of tautomerism of target chemical
Category definition for active tautomeric form

- In this exercise, the active tautomer is classified as: Aliphatic amine by ECOSAR category (phase I)
- Searching for similar analogues of the selected active tautomeric form is accomplished using ECOSAR category
- Searching for similar analogues is accomplished using four acute aquatic toxicity databases: Aquatic toxicity OASIS; ECOTOX and ECHA REACH.
- Before defining the category make sure that three aquatic aquatic databases (1) have been selected (see next screenshot)

Handling of tautomerism of target chemical

Check databases

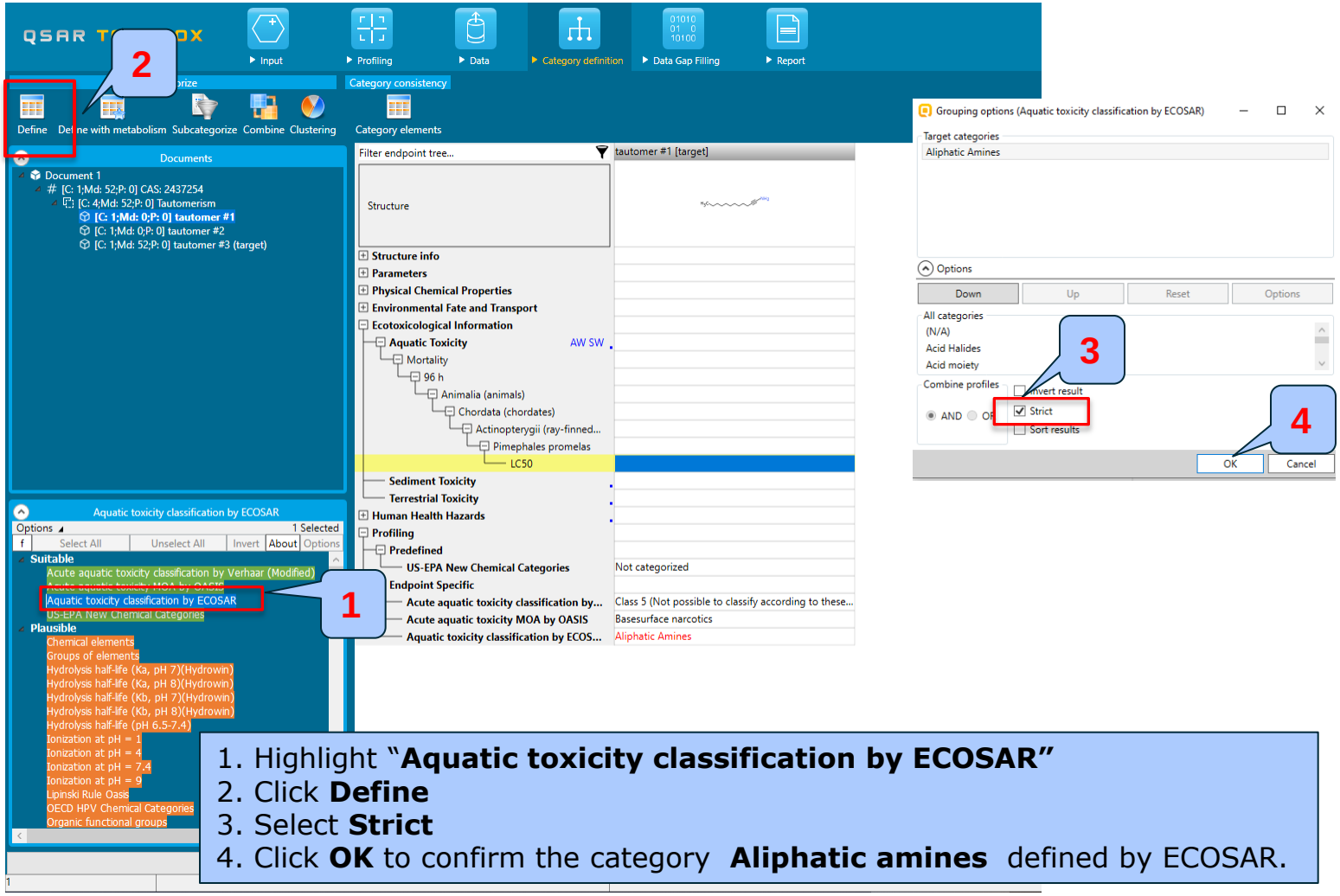


Handling of tautomerism of target chemical
Defining ECOSAR category

- The category ECOSAR (strict) is used;
- **Strict** functionality means that the software will identify analogues having ONLY the categories of the target (e.g. aliphatic amines) and will exclude the analogues having any other categories
- Select Aquatic toxicity classification by ECOSAR category
- Click Define (see next screen shots)

Handling of tautomerism of target chemical

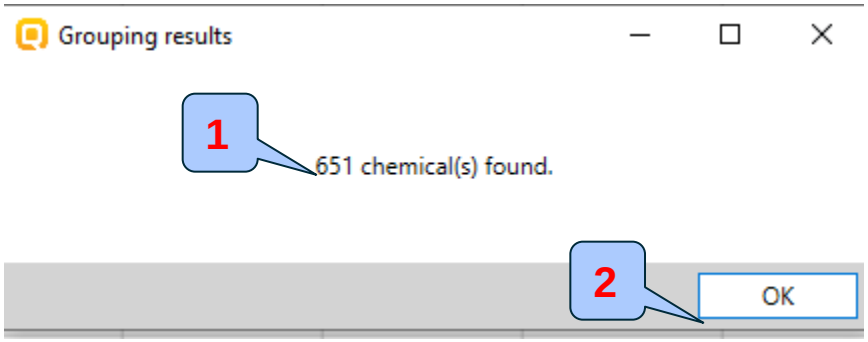
Defining ECOSAR category



1. Highlight "**Aquatic toxicity classification by ECOSAR**"
2. Click **Define**
3. Select **Strict**
4. Click **OK** to confirm the category **Aliphatic amines** defined by ECOSAR.

Handling of tautomerism of target chemical

Defining ECOSAR category



1. 651 chemicals having Aliphatic amines category are found in the selected databases.
2. Click **OK**

Handling of tautomerism of target chemical
Category analogues

- The Toolbox now identifies all chemicals corresponding to *Aliphatic amines* by ECOSAR listed in the four aquatic databases.

- 651 analogues including the target chemical are identified; they form a mechanistic category named "**Aliphatic amines**", which will be used for further data gap filling.

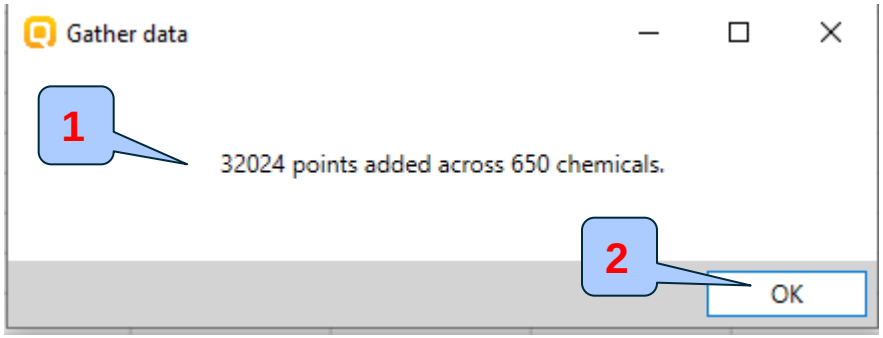
- The experimental data for analogues in the category appears on datamatrix

Handling of tautomerism of target chemical
Read data for Analogues

- The Toolbox automatically requests the user to select the endpoint that should be retrieved.
- The user can either select the specific endpoint or by default choose to retrieve data on all endpoints (see below).

- In this example, since only databases that contain information for ecotoxicological endpoints are selected, both options give the same results.
- As the Toolbox must search the database, this may take some time.

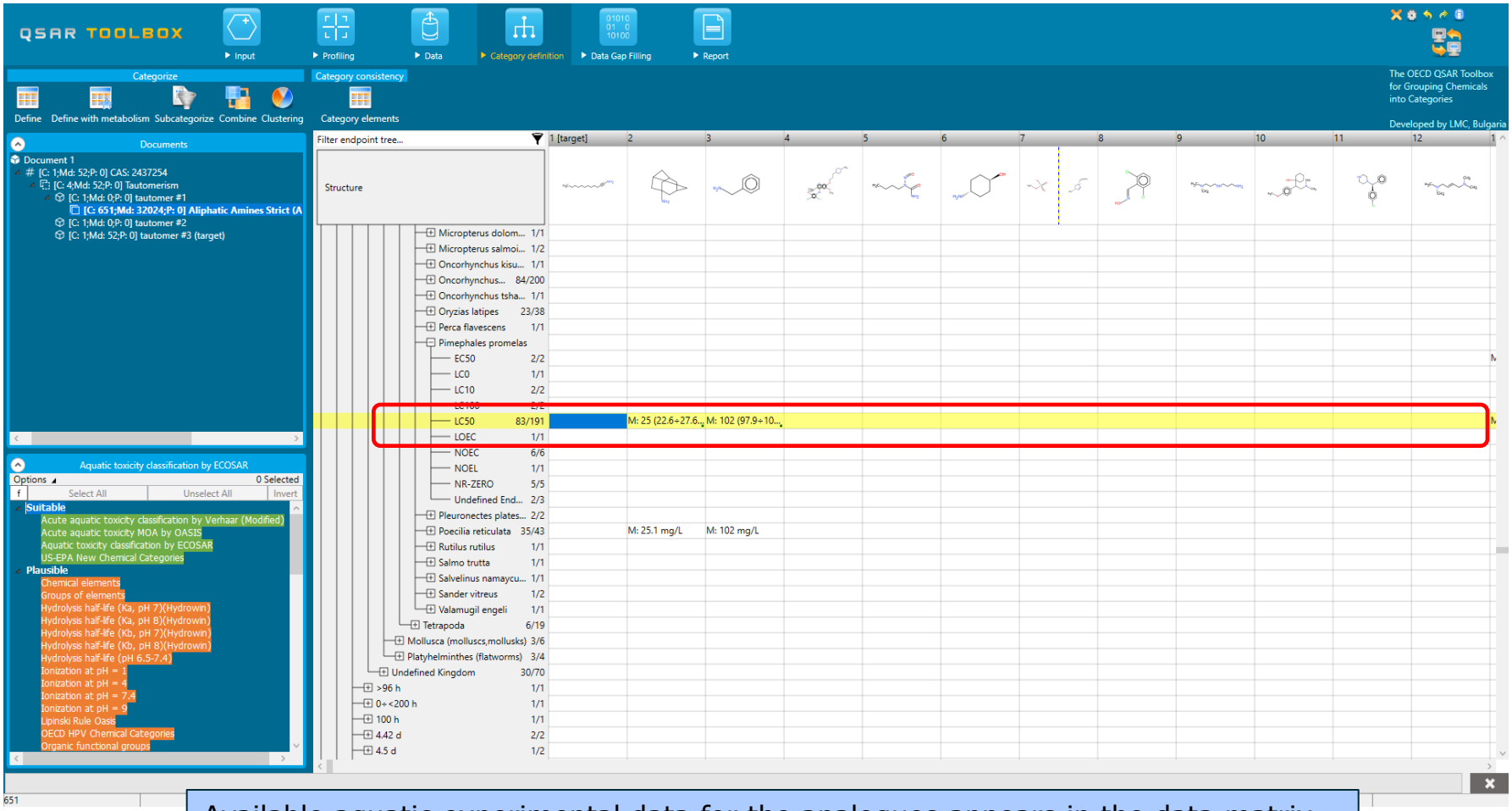
Handling of tautomerism of target chemical
Read data for Analogues



1. 32024 data values across 650 chemicals are found.
2. Click **OK.**

Handling of tautomerism of target chemical

Summary information for Analogues



Available aquatic experimental data for the analogues appears in the data matrix.

Recap

- You have identified a category (“Aliphatic amines”) with the “Acute aquatic toxicity classification by ECOSAR” profiler for the target chemical *Dodecanenitrile (CAS 2437-25-4)*

- The available experimental results for these 650 analogues have been collected from the selected databases (Aquatic ECETOC, ECOTOX and ECHA REACH).

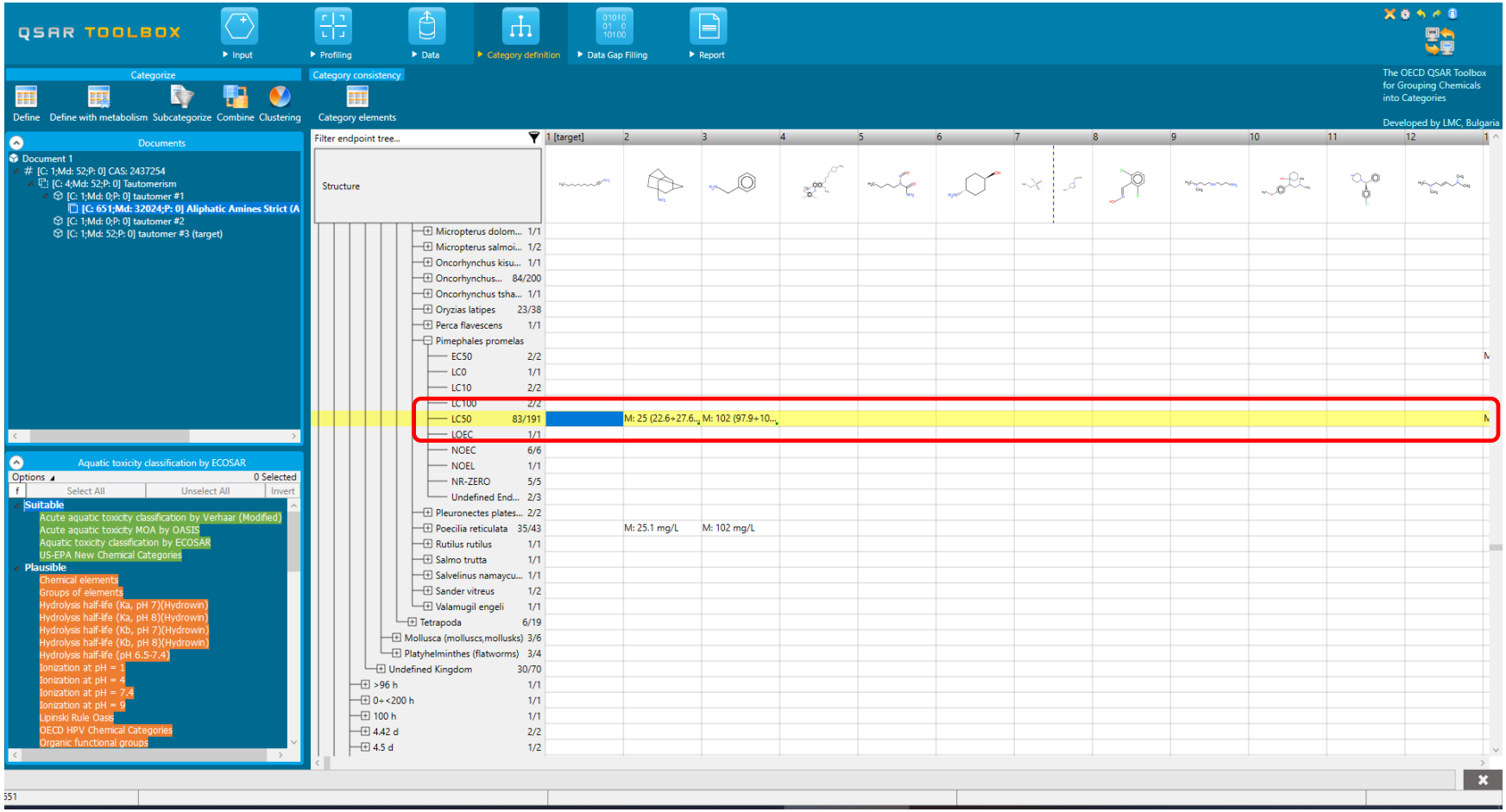
- But before the user can proceed with the “Data Gap Filling” module, he/she should navigate through the endpoint tree and find the specific gap that will be filled.

Handling of tautomerism of target chemical
Navigation through the endpoint tree

- The user can navigate through the data tree by opening (or closing) the nodes of the tree.
- The data tree is extensive but logically constructed; it can be mastered with a practice.
- In this example, the "96 h LC50 Mortality for *Pimephales promelas*" is the target endpoint.
- You can navigate through the endpoint tree by typing the species "*Pimephales promelas*" in the "Filter endpoint tree…" box and double click on Aquatic Toxicity, Mortality, LC50, 96 h, Animalia, etc to *Pimephales promelas* - the specific endpoint (see next screenshot)

Handling of tautomerism of target chemical

Navigation through the endpoint tree



Recap

- You have now retrieved the available experimental data on aquatic toxicity for 83 analogue chemicals of focused tautomeric form classified as “Aliphatic amines” by the “ECOSAR” profiler.

- You have identified the target endpoint of “96 h LC50 Mortality for *Pimephales promelas*”.

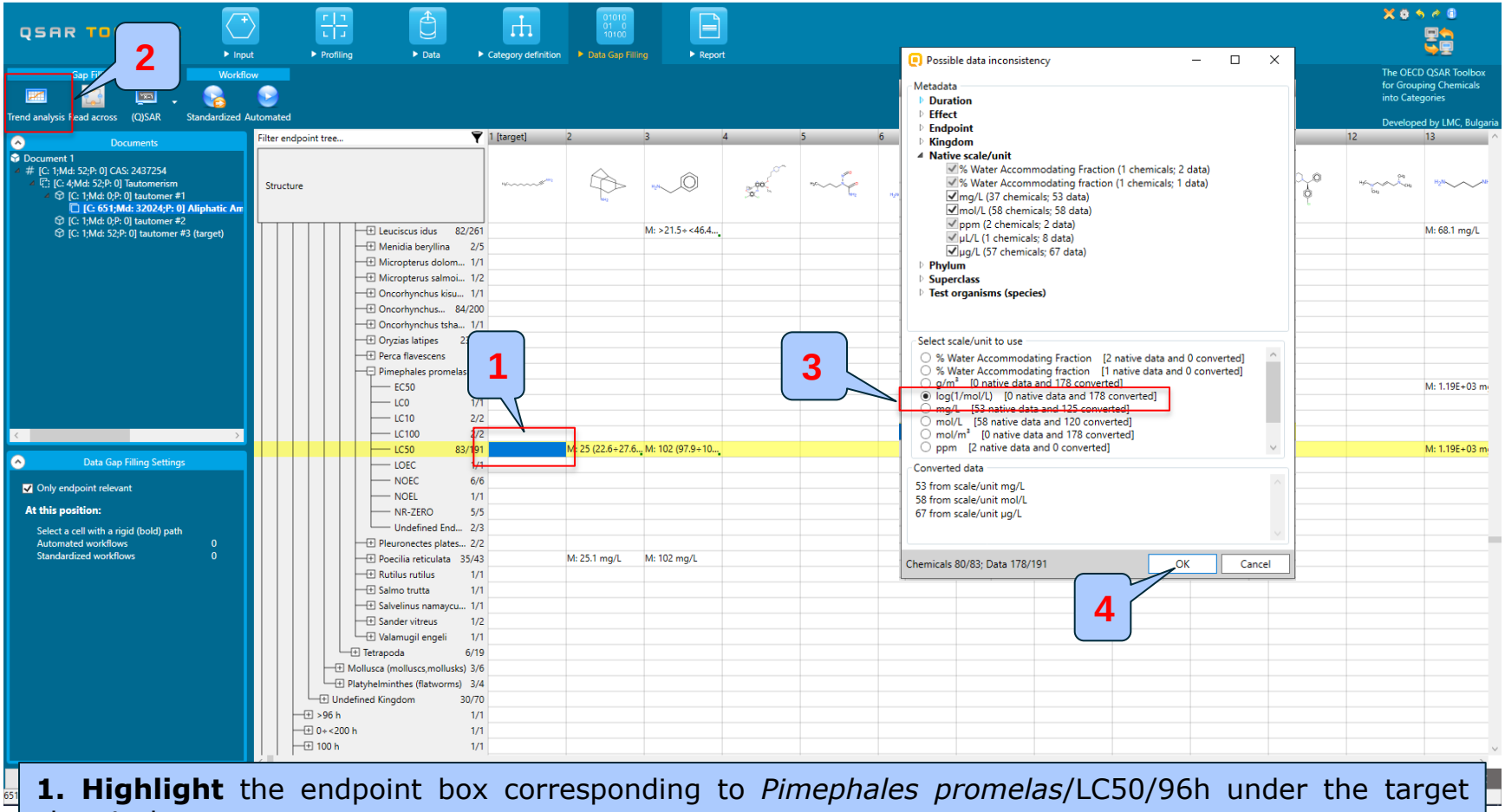
- You are ready to fill in the data gap so click on “Data Gap Filling” (see next screen shots).

Outlook

- Background
- Keywords
- Objectives
- The exercise
- **Workflow**
  - Input
  - Profiling
  - Data
  - Handling of tautomerism of target chemical
    - Profiling set of tautomers
    - Focus active tautomer
    - Defining category for active tautomer
    - **Trend analysis of the focused tautomer**

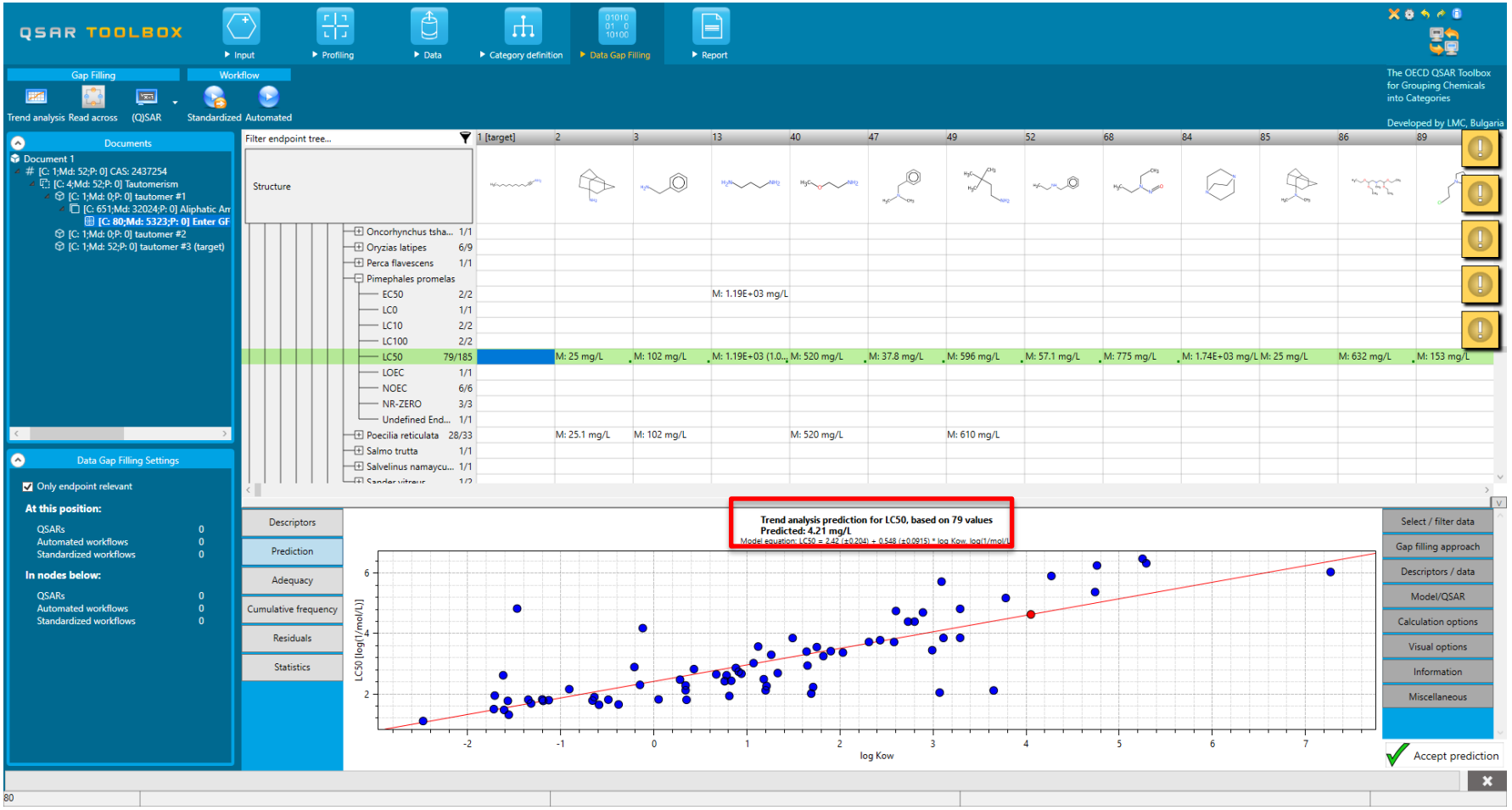
Data Gap Filling

Apply Trend analysis



1. Highlight the endpoint box corresponding to *Pimephales promelas*/LC50/96h under the target chemical.
2. Select **Trend analysis** 3. Select **scale** – log(1 mol/l) 4. Click **OK.**

Data Gap Filling
Results of Trend analysis



Data Gap Filling
Side-Bar of Subcategorisation

- In this example, the following subcategorizations are applied in order to eliminate dissimilar analogues (phase II):
  - Chemical elements

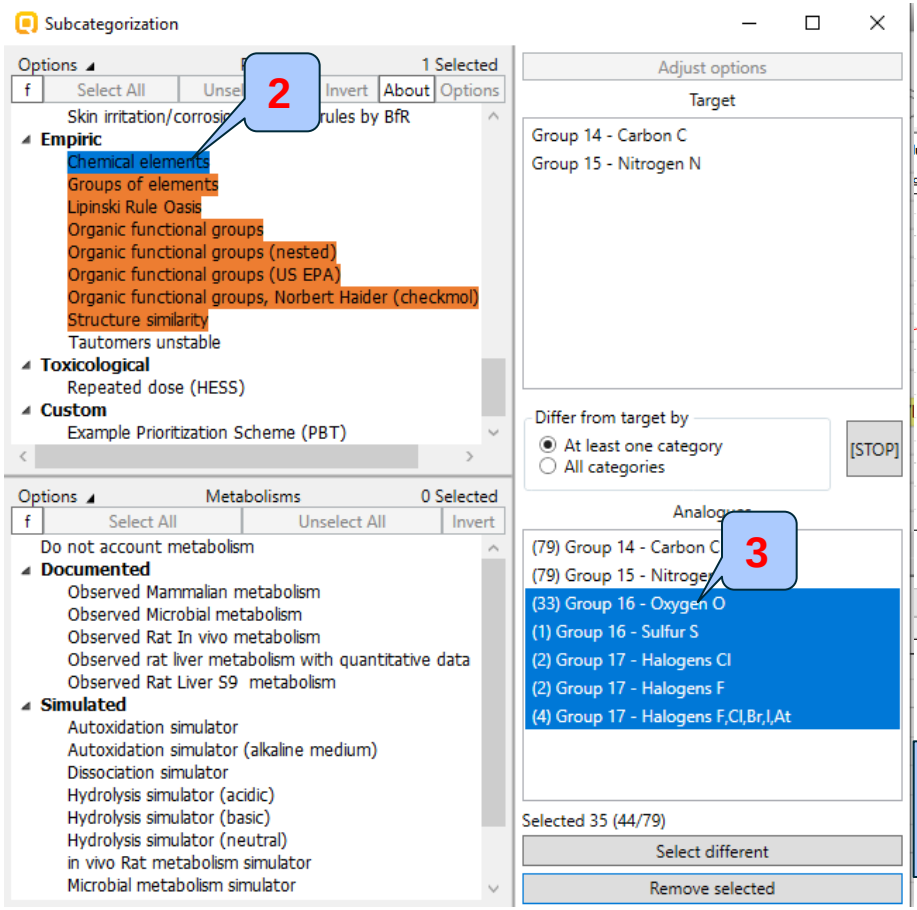
    The categorisation based on Chemical elements allows keeping among the analogues only those that have the same chemical elements as the target chemical (target tautomeric form).
  - Organic functional groups (nested)

    Subcategorization by OFG (nested) eliminates dissimilar analogues with respect to structural functionalities. This subcategorization will eliminate structurally dissimilar analogues such as aromatic amines.

    Subcategorisation steps are demonstrated on the next slides.

Data Gap Filling

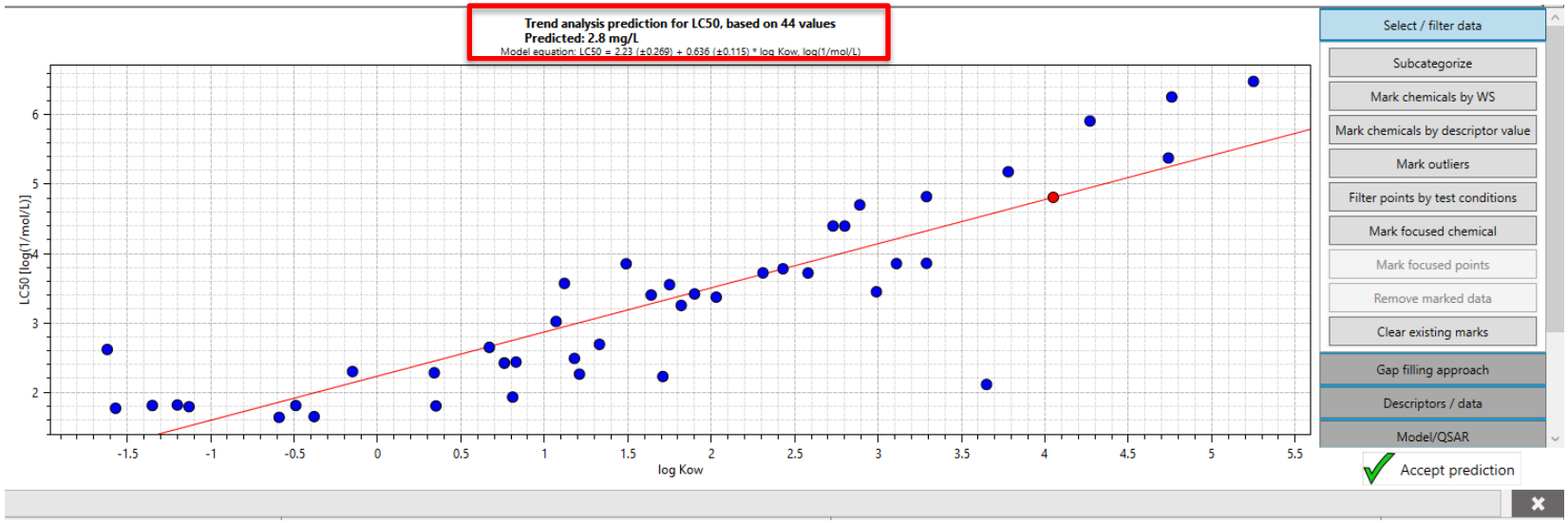
Subcategorisation 1 by Chemical elements



1. Click Subcategorize
2. Select **Chemical elements**
3. Click **Remove** to eliminate dissimilar analogues

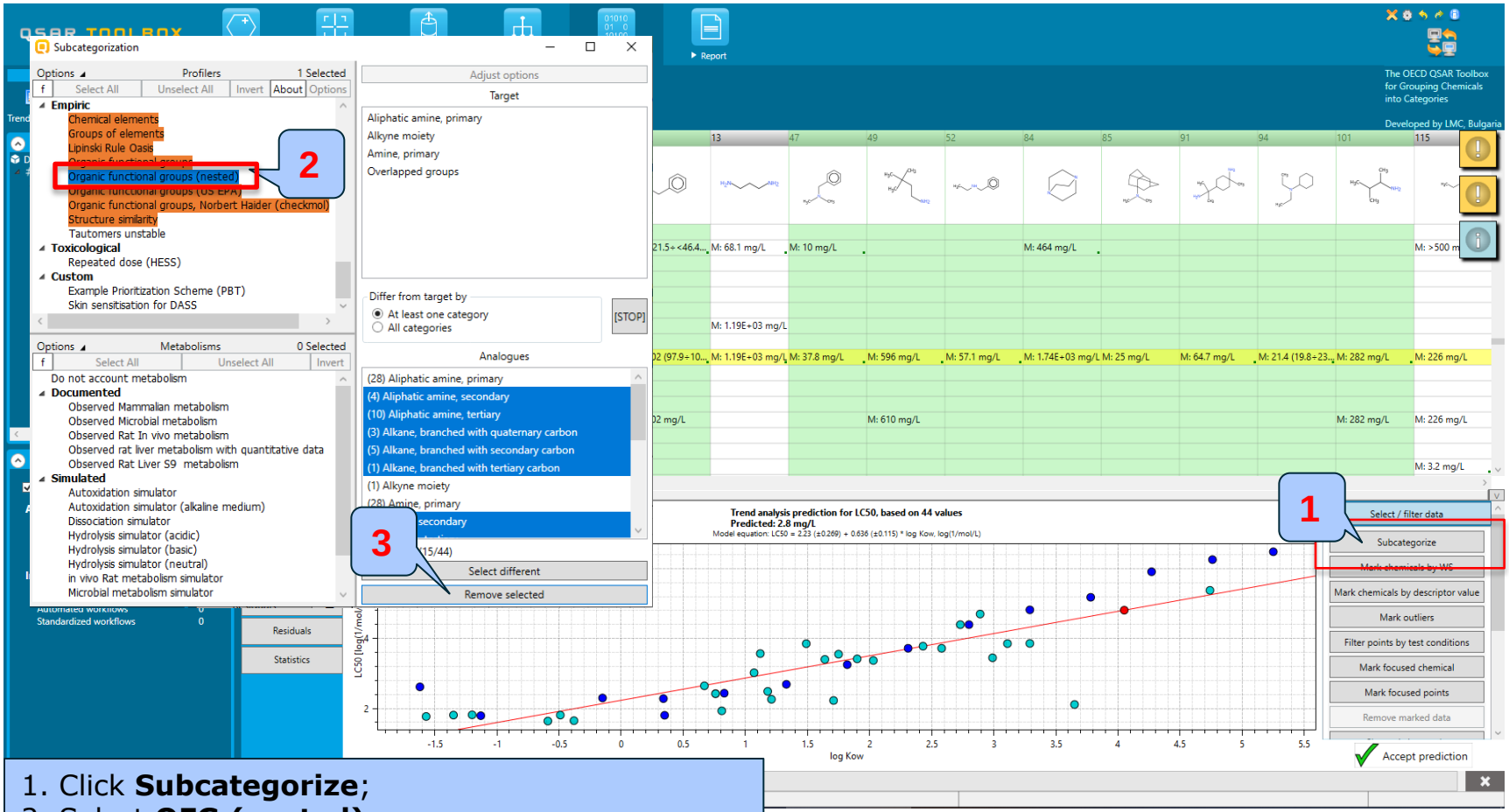
Data Gap Filling

Result of Subcategorisation 1 by Chemical elements



Data Gap Filling

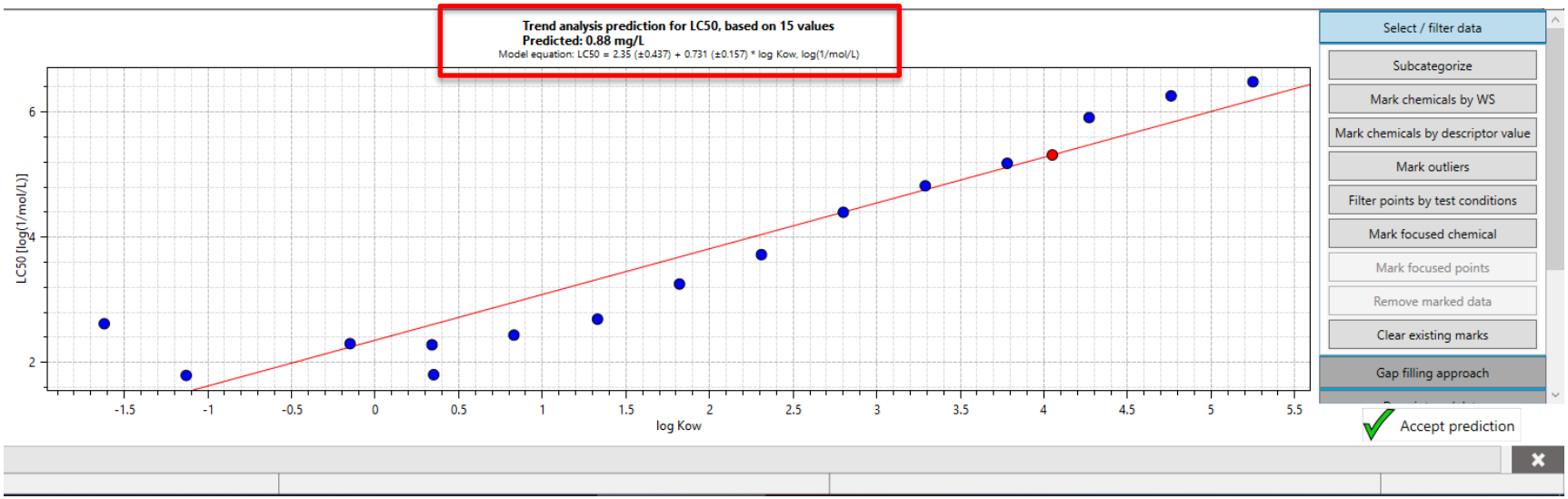
Subcategorisation 2 by OFG (nested)



1. Click **Subcategorize**;
2. Select **OFG (nested)**;
3. Click **Remove** to eliminate dissimilar analogues.

Data Gap Filling

Result of Subcategorisation by OFG (nested)



Data Gap Filling
Side-Bar of Subcategorisation

The last subcategorisation procedure aims to check and eliminate structurally dissimilar chemicals based on structural similarity

- Structural similarity

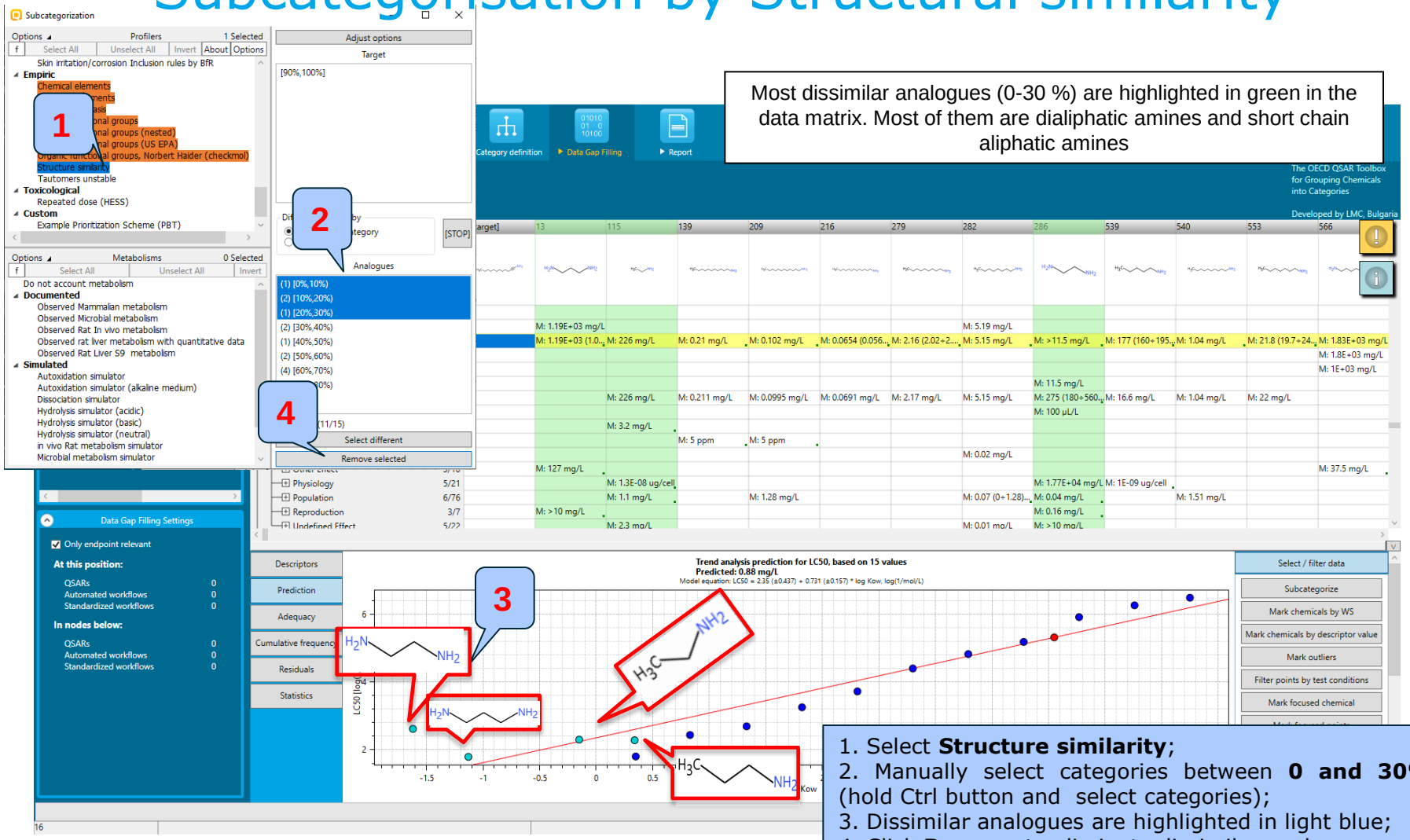
  The options of structural similarity used in the last subcategorization step are as follows: Dice, Atom centred fragments(ACF), atom features: Atom type; Count H attached; Hybridizations;

Analogues with similarity less than 30 % have been eliminated.

See next two slides.

Data Gap Filling

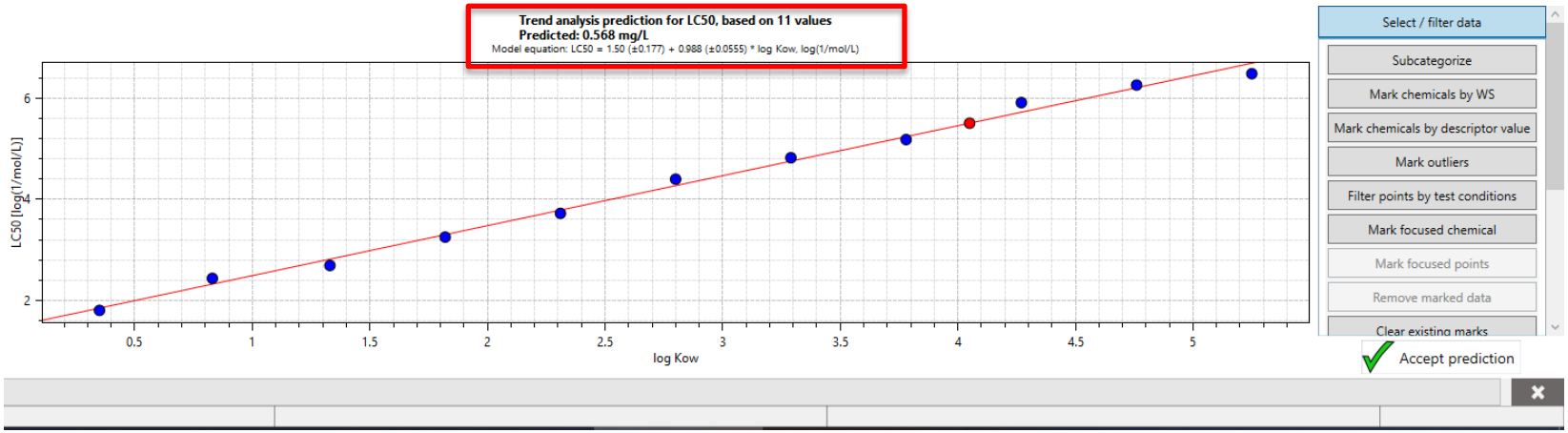
Subcategorisation by Structural similarity



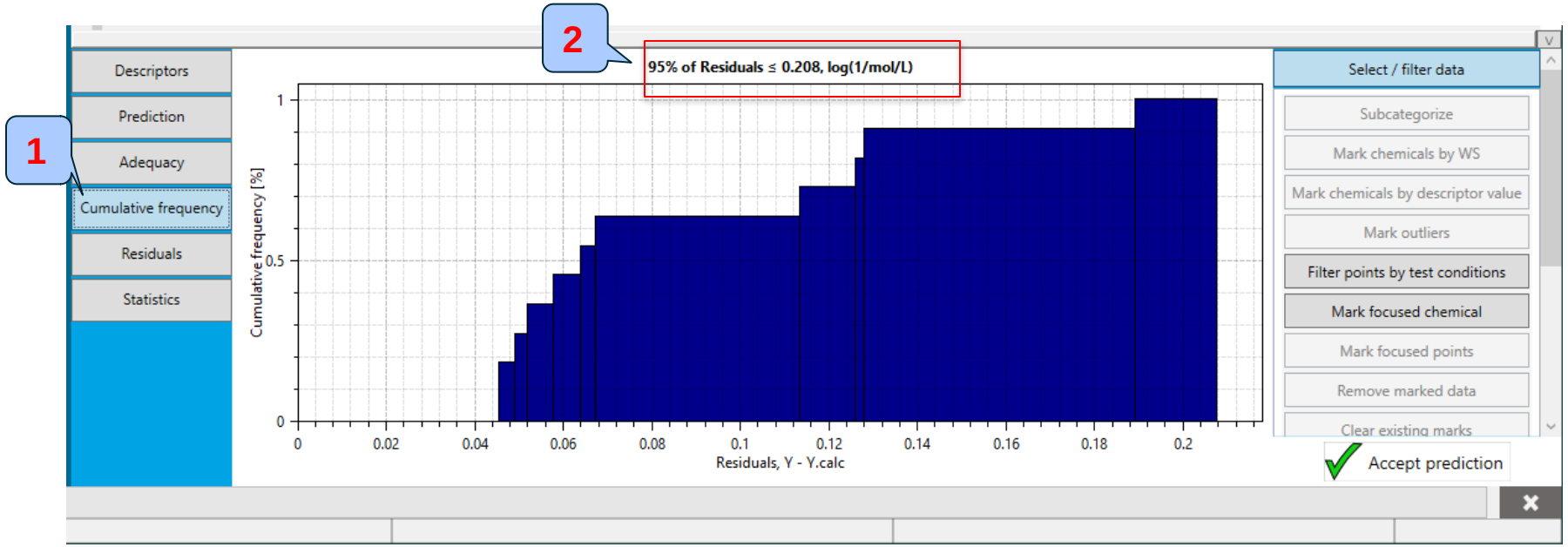
1. Select **Structure similarity**;
2. Manually select categories between **0 and 30%** (hold Ctrl button and select categories);
3. Dissimilar analogues are highlighted in light blue;
4. Click **Remove** to eliminate dissimilar analogues

Data Gap Filling
Result

Predicted value:
0.57 mg/l

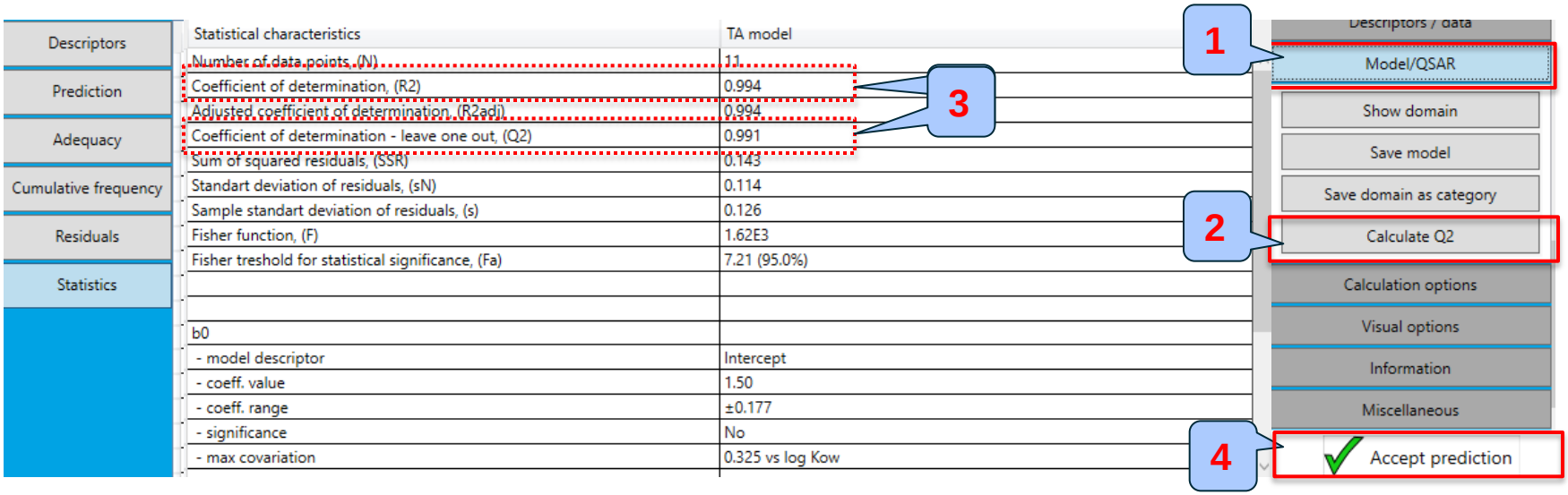


Data Gap Filling
Cumulated frequency



1. Click **Cumulative frequency**;
2. 95% of residuals are in the range of experimental error

Data Gap Filling
Statistics



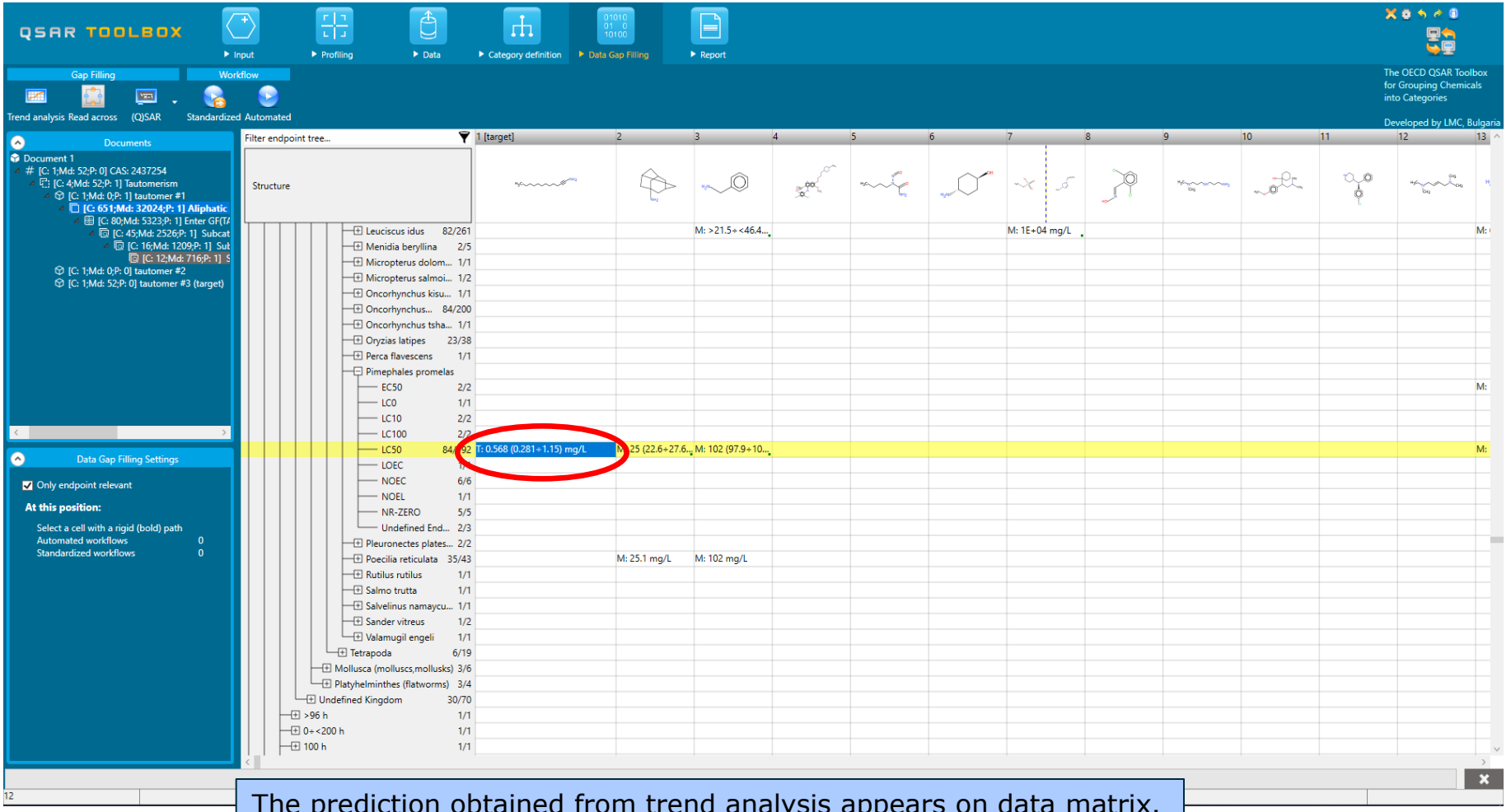
1. Select **Model (Q)SAR;**
2. Calculate **Q2;**
3. The high **R2** and **Q2** support the reliability of the prediction;
4. **Accept prediction.**

Data Gap Filling
Result of trend analysis

- The analysis of trend analysis shows:
  - The predicted acute aquatic toxicity value is 0.57 mg/l;
  - The remaining analogues form robust category of structurally similar analogues (aliphatic amines);
  - The 95% of residuals are in the range of experimental error;
  - The high R2 and Q2 coefficient values support the reliability of the prediction;

Data gap filling for focused tautomer

Trend analysis



The prediction obtained from trend analysis appears on data matrix.

Data gap filling for focused tautomer
Interpreting Read-across

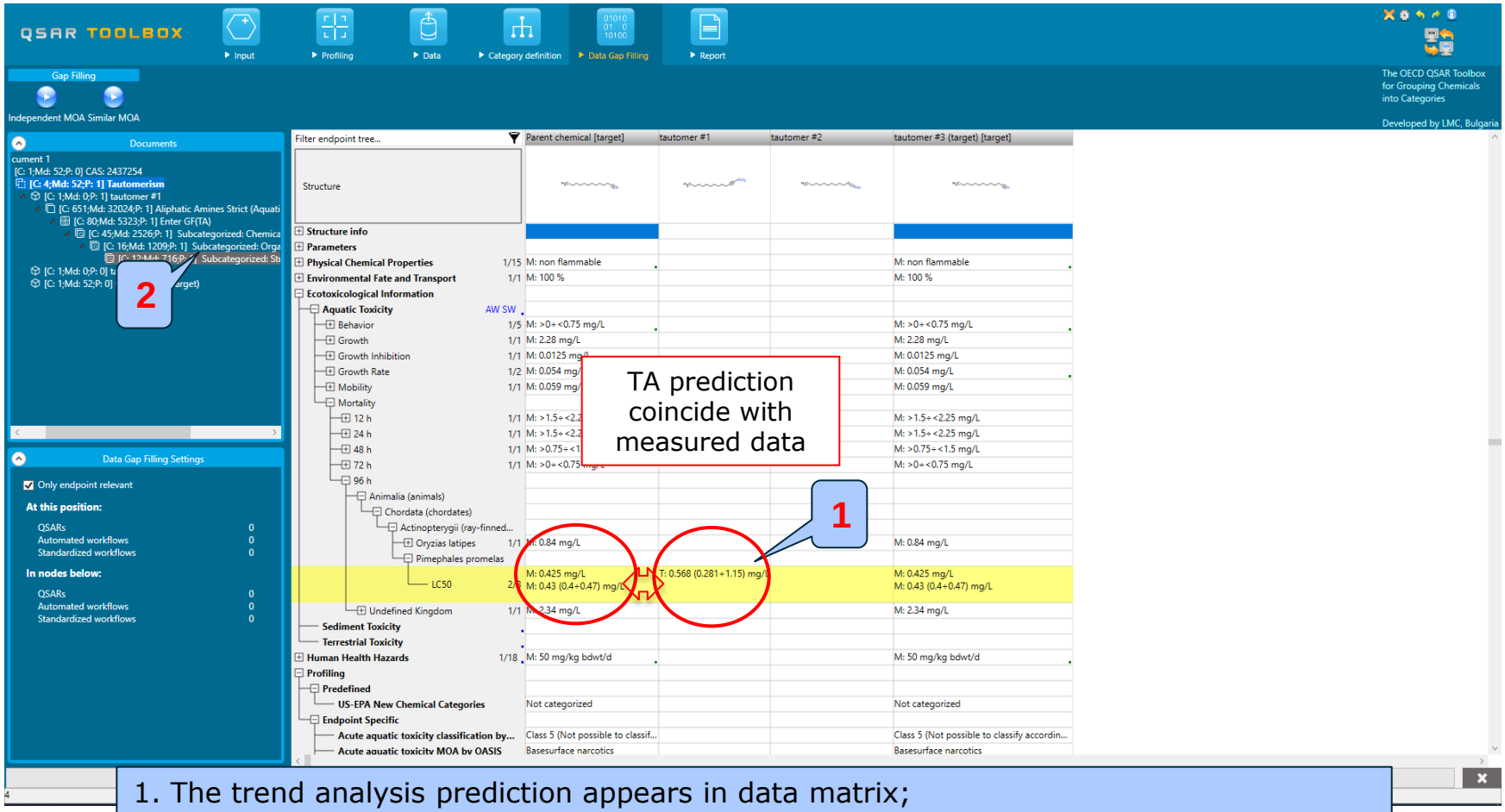
- In this example, all analogues are aliphatic amines
- All analogues exhibit toxic effect to fish (*P.promelas*)
- The same toxic effect is therefore predicted for the target (i.e. focused tautomer).
- The prediction of tautomer is further transferred to the parent chemical using "**Transfer to target"** (see next screen shots)

Outlook

- Background
- Keywords
- Objectives
- The exercise
- **Workflow**
  - Input
  - Profiling
  - Data
  - Handling of tautomerism of target chemical
    - Profiling set of tautomers
    - Focus active tautomer
    - Defining category for active tautomer
    - Trend analysis of the focused tautomer
  - **Assigning prediction of tautomer to parent**

Handling tautomerism of target chemical

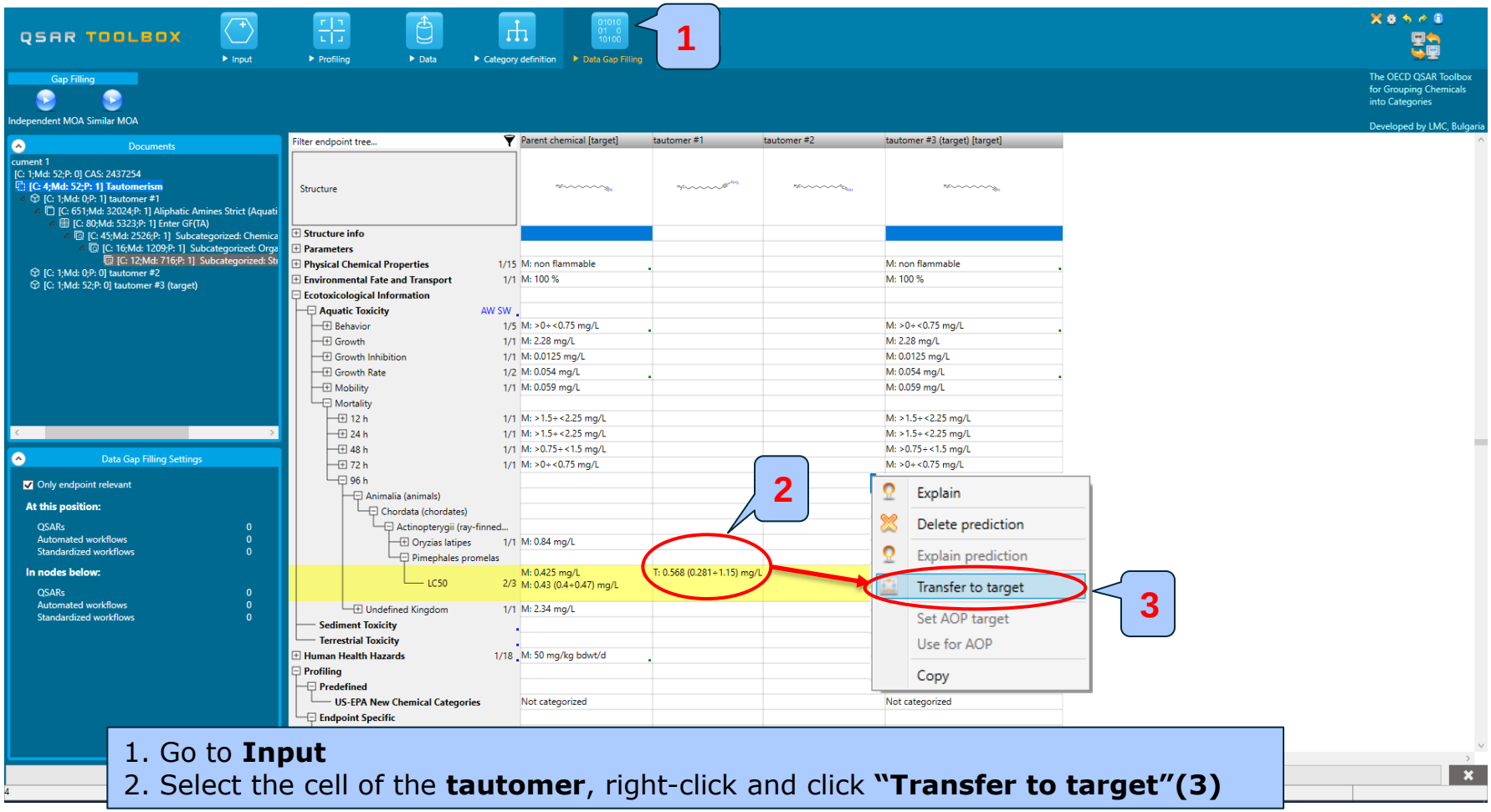
Assigning data to parent chemical



1. The trend analysis prediction appears in data matrix;
2. The prediction of the tautomeric form is assigned to the last SMILES within the set;

Handling tautomerism of target chemical

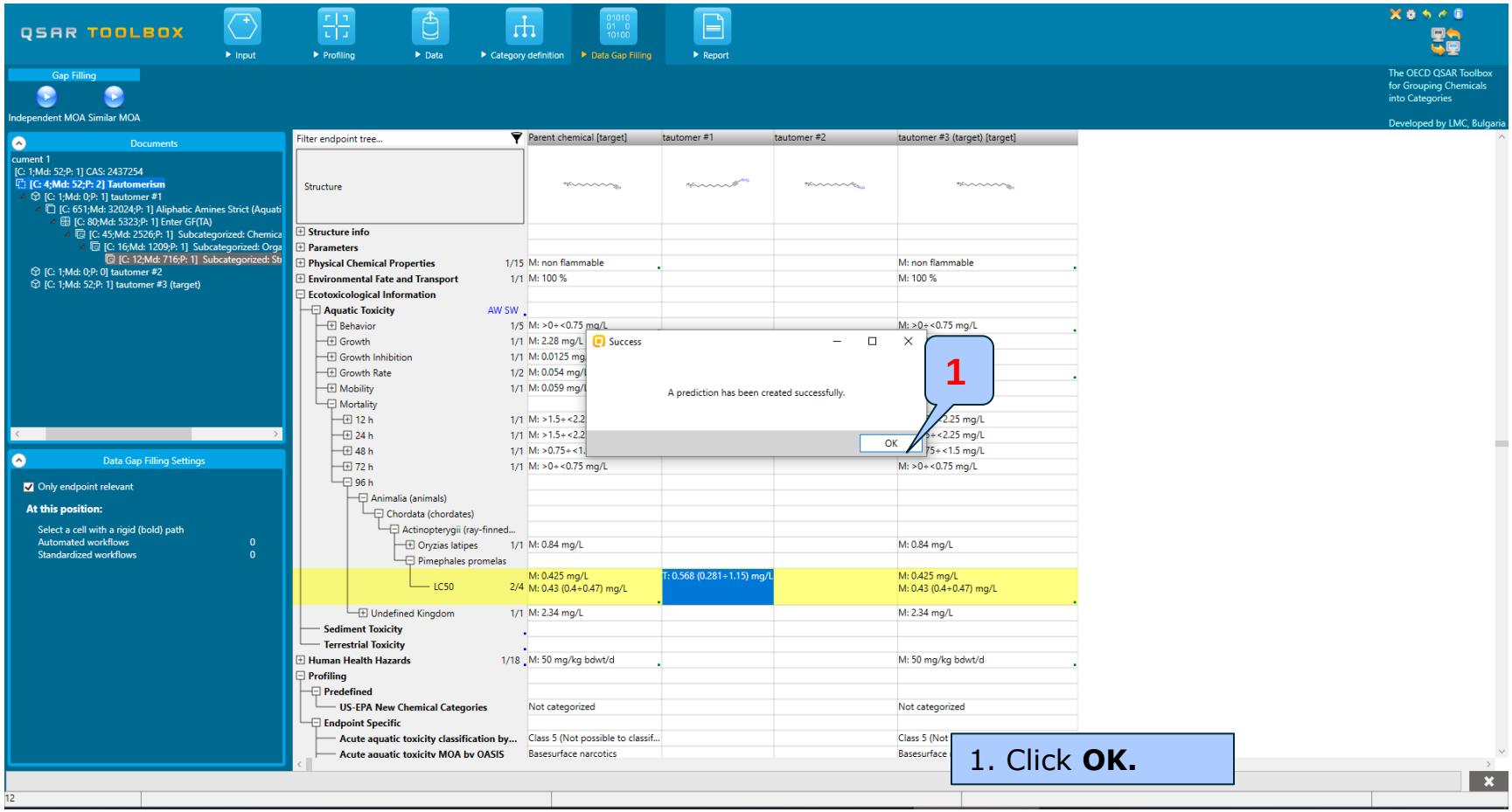
Assigning data to parent chemical



1. Go to **Input**
2. Select the cell of the **tautomer**, right-click and click **"Transfer to target"(3)**

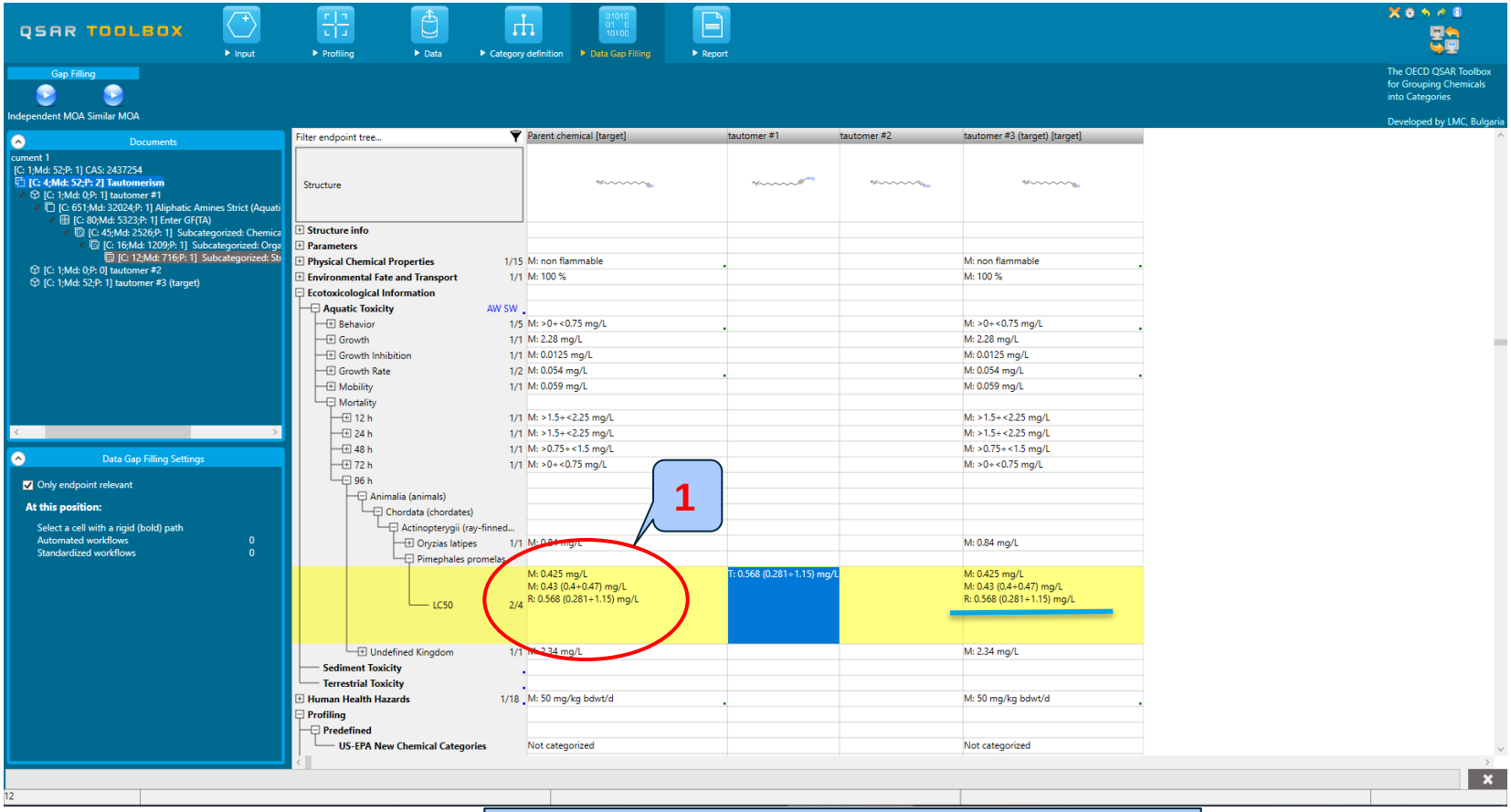
Handling tautomersim of target chemical

Assigning data to parent chemical



Handling tautomersim of target chemical

Assigning data to parent chemical



1. The Prediction is transferred to the target.

Outlook

- Background
- Keywords
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- The exercise
- **Workflow**
  - Input
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    - Defining category for active tautomer
    - Trend analysis of the focused tautomer
  - Assigning prediction of tautomer to parent
  - **Report**

Report

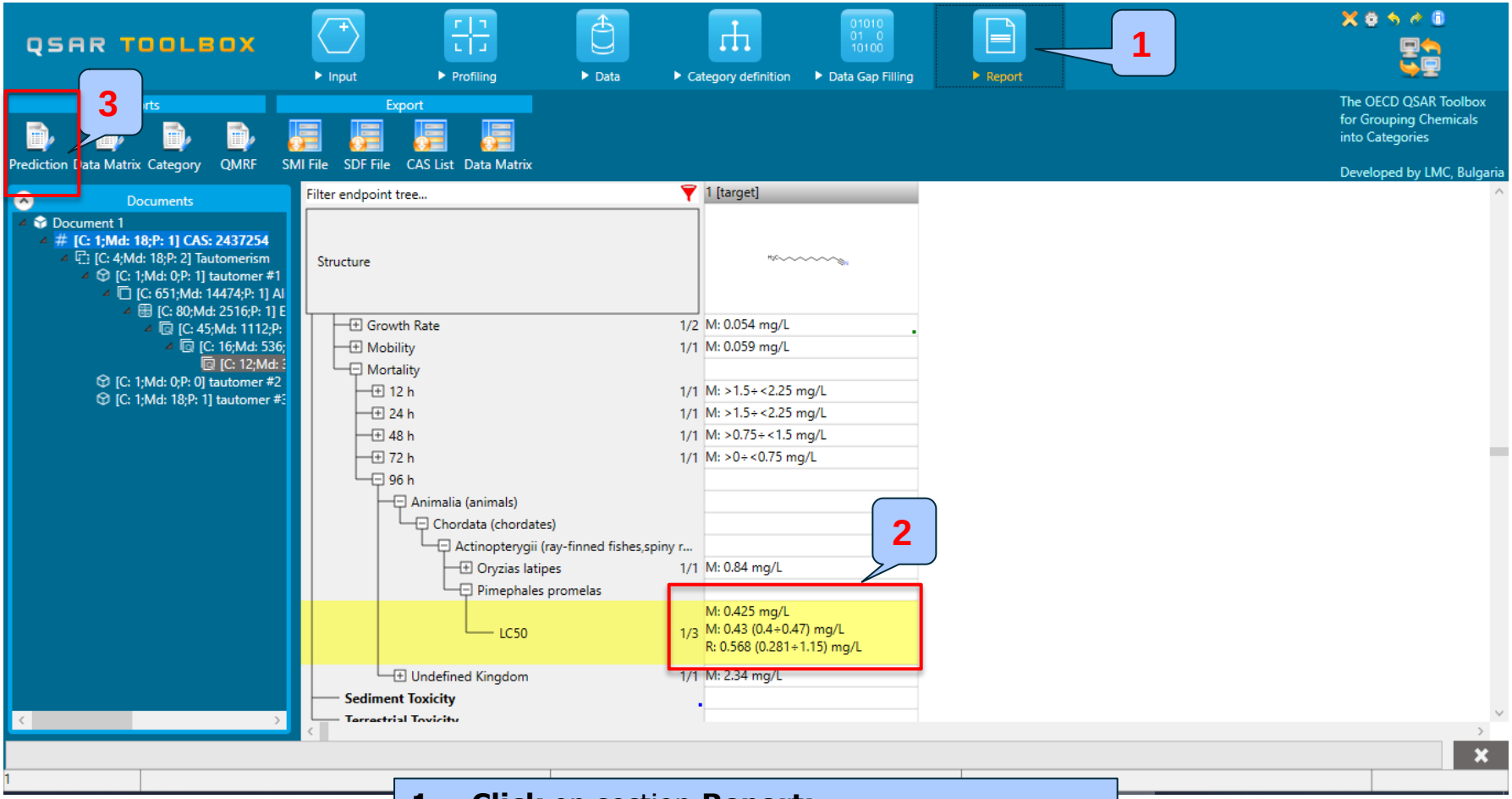
- Remember the report module allows you to generate a report on the predictions performed with the Toolbox. This module contains predefined report templates as well as a template editor with which users can define their own user defined templates. The report can then be printed or saved in different formats.

- The report consist of two sections:

  - Summary report for the whole tautomeric set
  - Report for the individual prediction obtained for the active tautomeric form

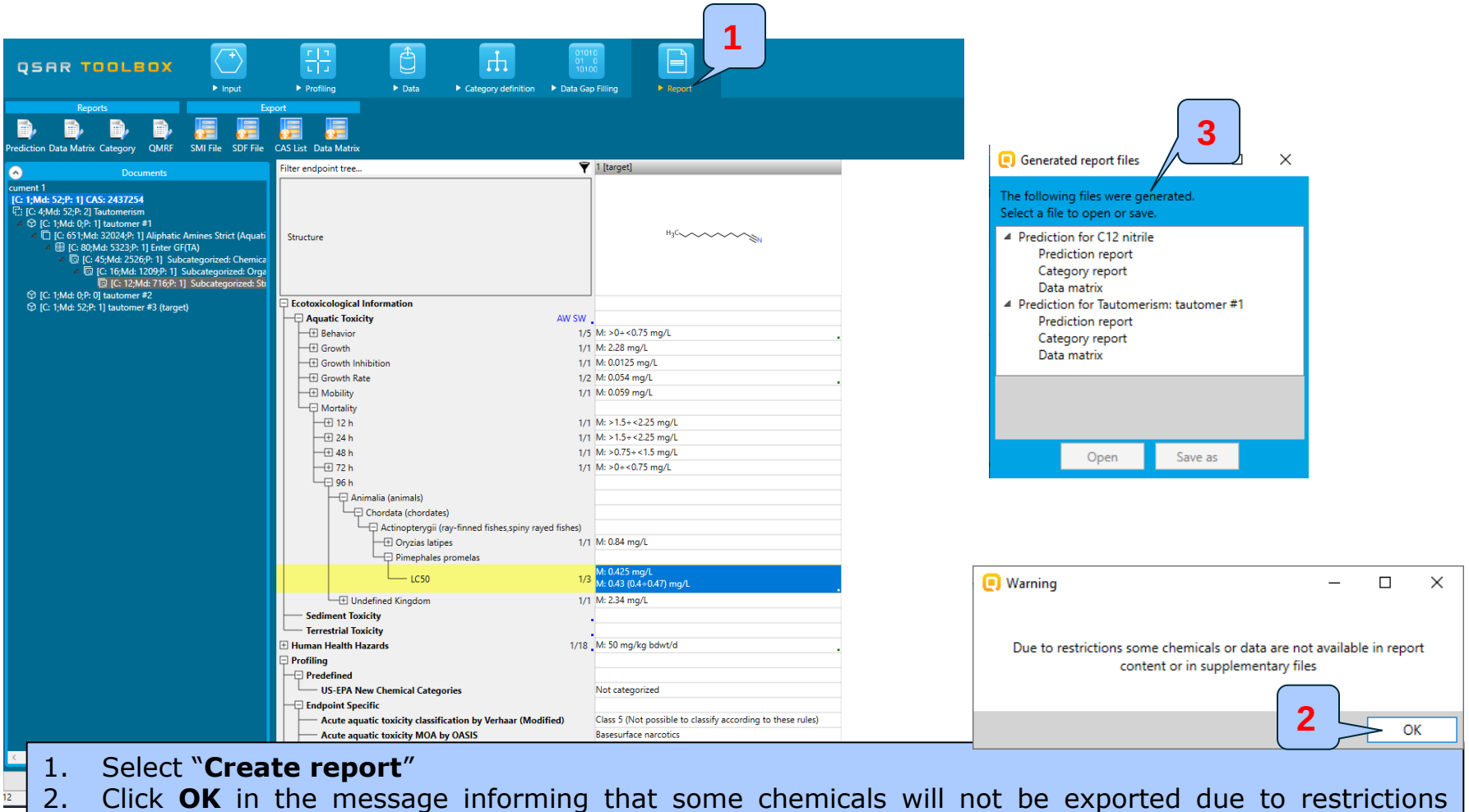
- Generating the report is shown on next screenshots

Report



1. **Click** on section **Report;**
2. Select the **Prediction (marked with "R");**
3. Click **Prediction.**

Report



1. Select "**Create report**"
2. Click **OK** in the message informing that some chemicals will not be exported due to restrictions associated with the ECHA CHEM database.
3. Select the prediction report of the target.

Report

QSAR Toolbox prediction for single chemical

Date: 14 Apr 2020
Author(s):
Contact details:

Target information		
Structural information SMILES: CCCCCCCCCCCC#N Structure 	**Numerical identifiers** CAS#: 2437-25-4 Other: EC Number:2194401	**Chemical names** 1S/C12H23N/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-11H2,1H3 C(CCCCCC)CCCCC#N C12 nitrile

1

Prediction summary
~~Predicted endpoint:~~ LC50; Mortality; ~~Pimephales~~ promelas; 96 h; No guideline specified
Predicted value: 0.568 (from 0.281 to 1.15)
Unit/scale: mg/L
Data gap filling method: Read-across analysis
Summary: *manually editable field*
Not provided by the user

1. Predicted value

Outlook

- Background
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- The exercise
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  - Input
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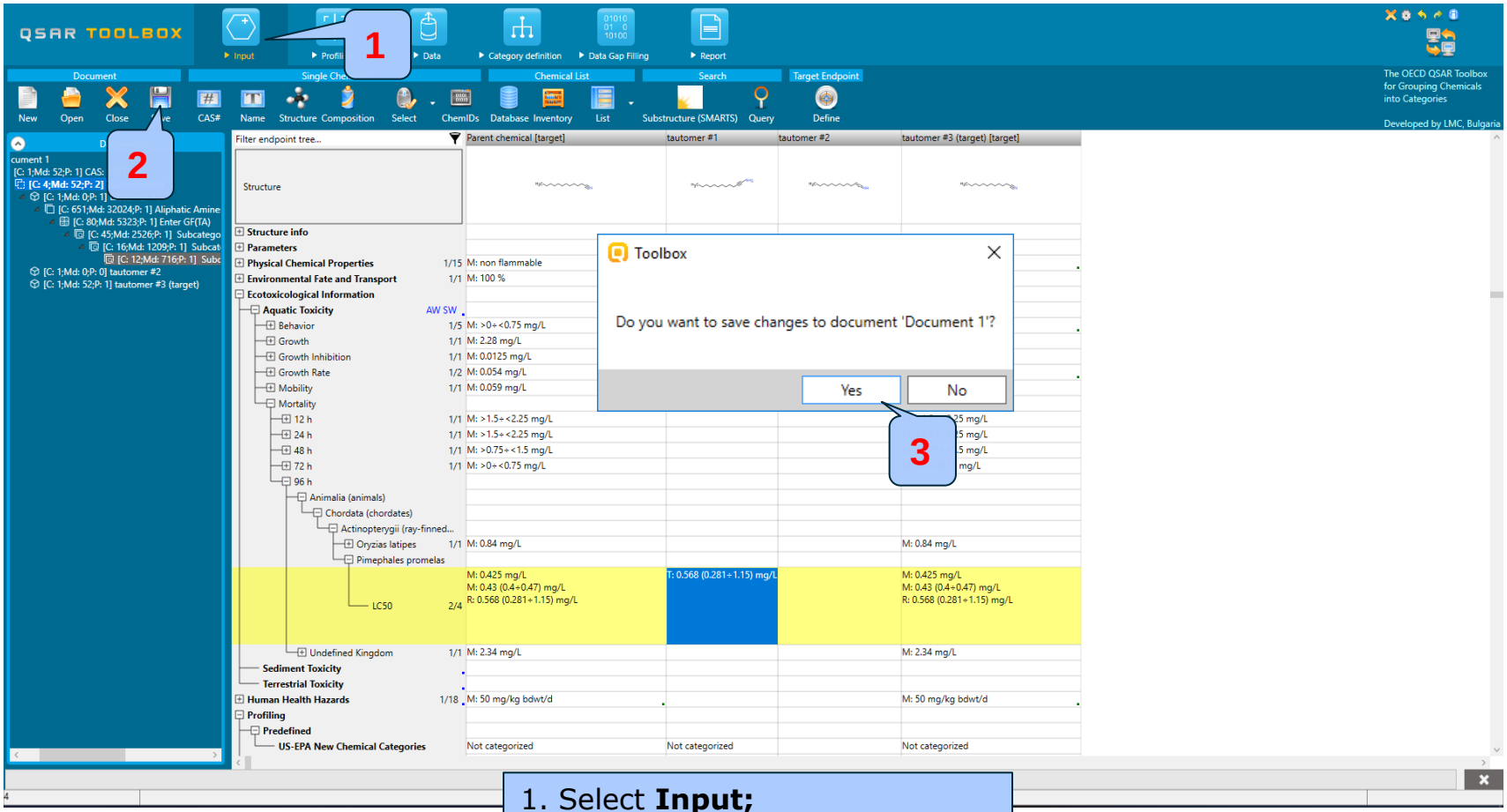
  - Data
  - Handling of tautomerism of target chemical
  - Assigning prediction of tautomer to parent
  - Report
- **Save prediction**

Saving the prediction result

- This functionality allow storing/restoring the current state of Toolbox documents including loaded chemicals, experimental data, profiles, predictions etc, on the same computer. The functionality is implemented based on saving the sequence of actions that led to the current state of the Toolbox document and later executing these actions in the same sequence in order to get the same result(s).

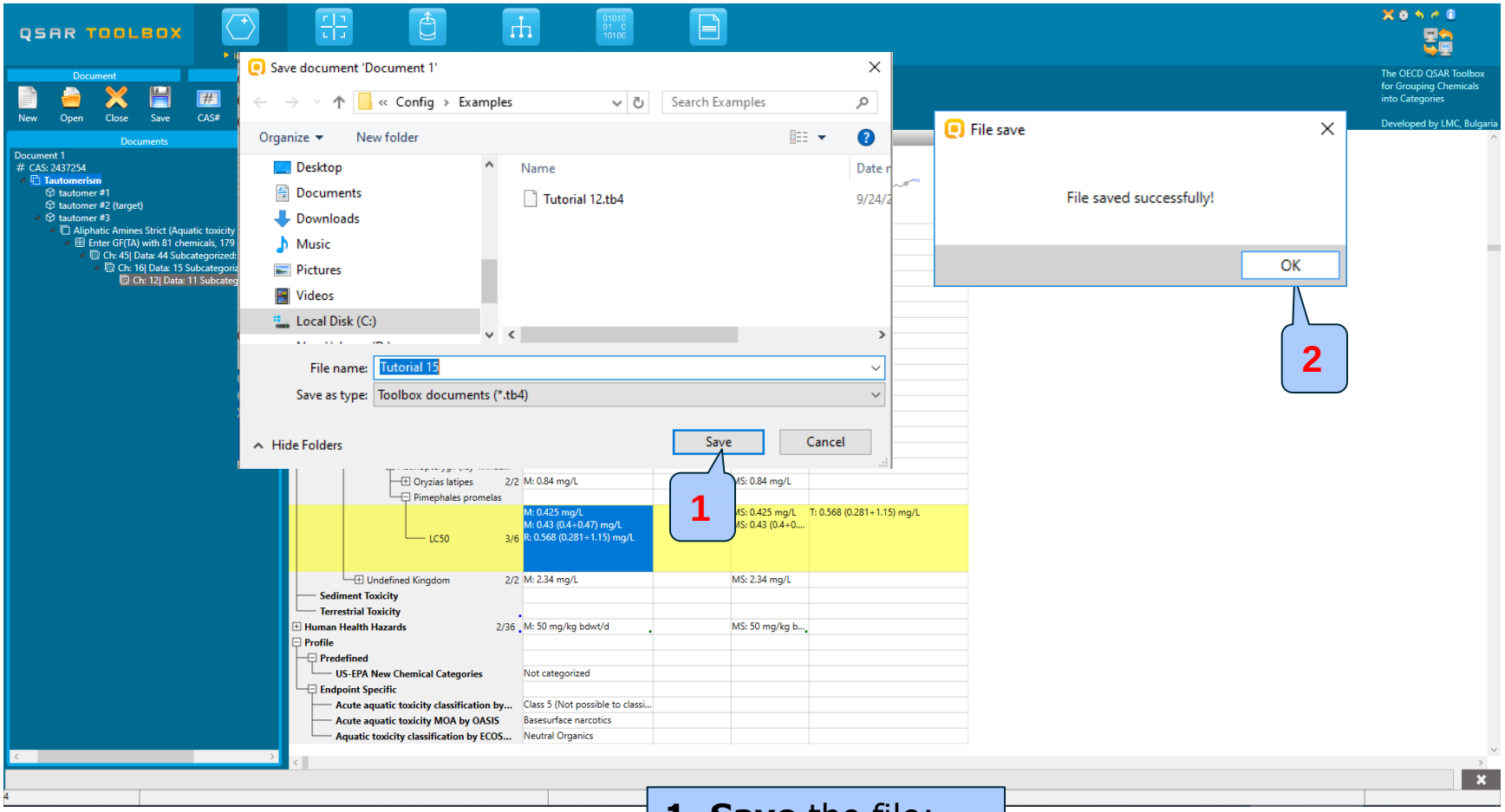
- Saving/Loading the file with TB prediction is shown on next screenshots

Saving the prediction



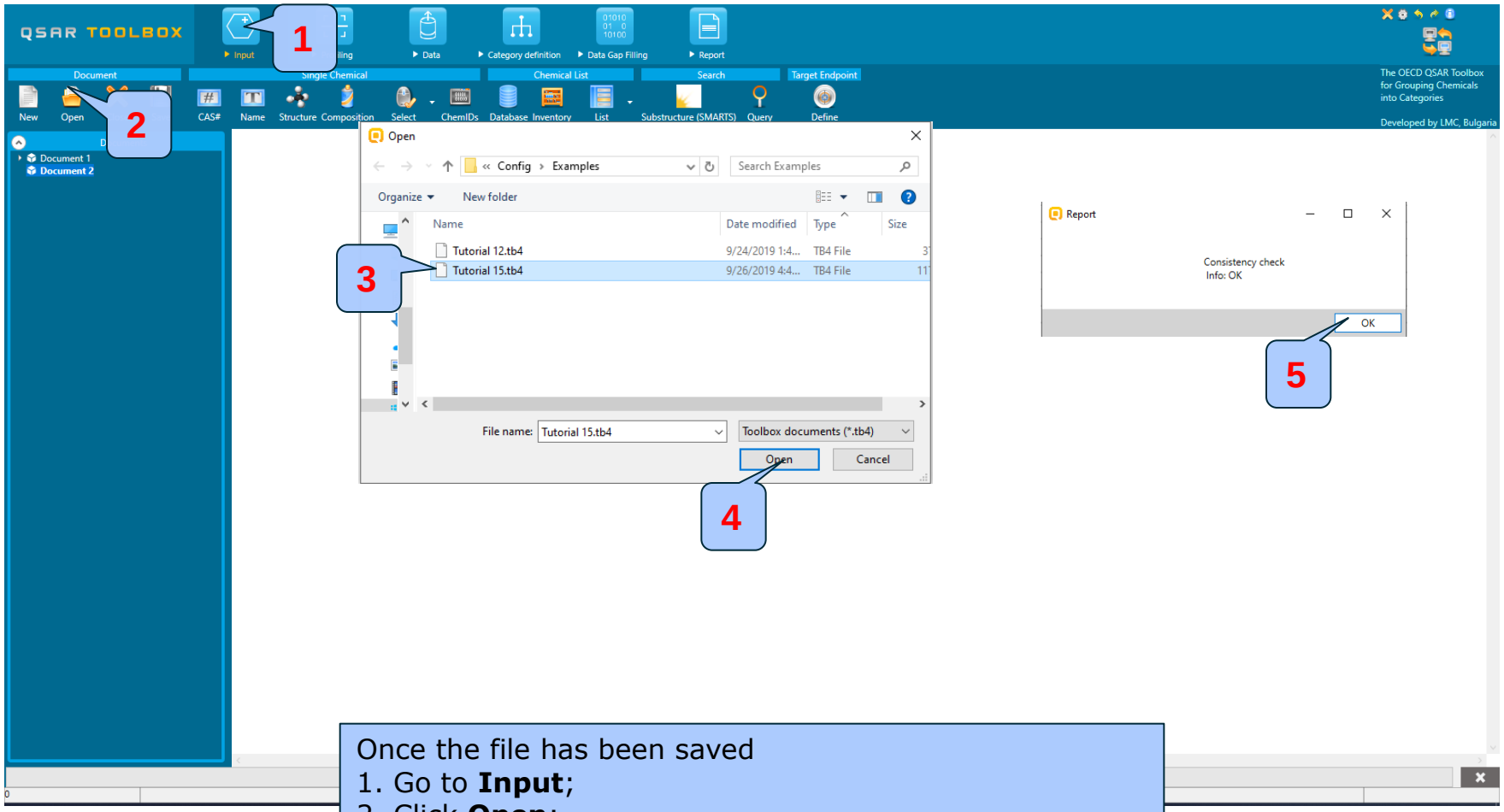
1. Select **Input;**
2. Click on **Save** button;
3. Click **Yes.**

Saving the prediction



1. Save the file;
2. Click **OK**.

Open saved file



Once the file has been saved
1. Go to **Input**;
2. Click **Open**;
3. Find and **select file**; 4. Click **Open** 5. Click **OK.**