

OECD QSAR Toolbox v.3.0

Step-by-step example on how to predict the skin sensitisation potential approach of a chemical by read-across based on an analogue approach

Outlook

- **Background**
- Objectives
- Specific Aims
- Read across and analogue approach
- The exercise
- Workflow

Background

- This is a step-by-step presentation designed to take the first time user of the Toolbox through the workflow of a data filling exercise by read-across based on an analogue approach.

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Objectives

This presentation demonstrates a number of functionalities of the Toolbox:

- Identify analogues for a target chemical.
- Retrieve experimental results available for those analogues.
- Fill data gaps by read across.

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Specific Aims

- To introduce to the first time user the workflow of the Toolbox.
- To familiarize the first time user with the six modules of the Toolbox.
- To familiarize the first time user with the basic functionalities within each module.
- To explain to the first time user the rationale behind each step of the exercise.

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- Workflow

Read-across and Analogue Approach Overview

- Read-across can be used to estimate missing data from a single or limited number of chemicals using an analogue approach. It is especially appropriate for “qualitative” endpoints for which a limited number of results are possible (e.g. positive, negative, equivocal).
- In the analogue approach, endpoint information for a single or small number of tested chemicals is used to predict the same endpoint for an untested chemical that is considered to be “similar”.
- Analogous sets of chemicals are often selected based on the hypothesis that the toxicological effects of each member of the category will show a common behaviour.

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The Exercise

- In this exercise we will predict the skin sensitization potential for an untested compound, (4-nitrobenzoyl chloride) [CAS # 122-04-3], which will be the "target" chemical.
- This prediction will be accomplished by collecting a small set of test data for chemicals considered to be in the same category as the target molecule.
- The category will be defined by the mechanism of protein binding common to all the chemicals in the category.
- The prediction itself will be made by "read-across".

The Exercise Side-Bar On Sensitization

- Allergic contact dermatitis that results from skin sensitization is a significant health concern.
- Skin sensitization is a toxicological endpoint that is complex and conceptually difficult.
- However, there is growing agreement that most organic chemicals must react covalently with skin proteins in order to behave as skin sensitizers.
- Therefore, mechanisms by which organic chemicals bind with proteins are relevant to grouping chemicals that may be skin sensitizing agents.

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- **Workflow**

Workflow

- **The Toolbox has six modules which are used in a sequential workflow:**
 - Chemical Input
 - Profiling
 - Endpoints
 - Category Definition
 - Filling Data Gaps
 - Report

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 - **Chemical Input**

Chemical Input Overview

- This module provides the user with several means of entering the chemical of interest or the target chemical.
- Since all subsequent functions are based on chemical structure, the goal here is to make sure the molecular structure assigned to the target chemical is the correct one.

Chemical Input

Ways of Entering a Chemical

User Alternatives for Chemical ID:

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
- Chemical IDs such as EC number, EINECS number

B. Group of chemicals

- User List/Inventory
- Specialized Databases

Getting Started

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

Chemical Input Screen

Input screen

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05.10.2012

19

Chemical Input Screen

Input target chemical by CAS#

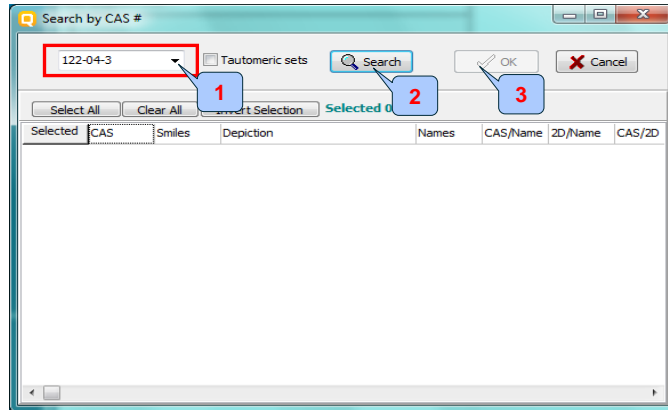
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05.10.2012

20

Chemical Input Screen

Enter CAS# of 4-nitrobenzoyl chloride

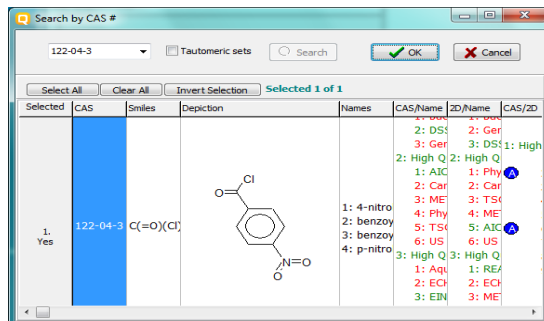


1. Enter the CAS# In the field; 2. Click Search button; 3. Press OK

Chemical Input

Target chemical identity

The Toolbox now searches the databases to find out if the CAS# you entered is linked to a molecular structure stored in the Toolbox. It is displayed as a 2-dimensional depiction.



In case a structure has several CAS numbers or a structure could be related to more than one substance, more than one chemical identity could be retrieved. In this case the user can decide which substance is to be retained for the subsequent workflow.

Chemical Input

Target chemical identity

- **Double click** "Substance Identity"; this displays the chemical identification information.
- Note that existing in the Toolbox name of target chemical are in different colours (see next screen shot).
- The workflow on the first module is now complete, and the user can proceed to the next module.

Chemical Input

Target chemical identity

The screenshot shows the QSAR Toolbox software interface. The main window is titled "QSAR Toolbox 3.0.0.840 [Document_1]". The interface is divided into several sections:

- Menu Bar:** Includes options like Document, Single Chemical, Endpoints, Category Definition, Data Gap Filling, and Report.
- Toolbar:** Contains icons for various functions such as Open, Save, Print, and Structure.
- Document Panel:** Shows the current document name and a chemical structure.
- Main Workspace:** Displays the "Substance Identity" section, which includes:
 - Structure:** A chemical structure diagram.
 - Substance Identity:** A list of identifiers including CAS Number, Chemical IDs, Chemical Name, and Structural Formula.
 - Physical Chemical Properties:** A section for environmental and toxicological data.

In the "Chemical Name" field, a list of names is shown, with "4-nitrobenzyl chloride" highlighted in red. The list includes: "4-nitrobenzyl chloride", "benzyl chloride", "4-benzyl chloride", "p-nitrobenzyl chloride", and "C1=CC=C(C=C1)COC(=O)C".

Chemical Input

Chemical identity

The colour code indicates the reliability of the chemical identifier:

- **Green:** There is a high reliability between the identifier and the structure. This colour is applied if the identifier is the same in several quality assured databases.
- **Yellow:** There is only a moderate reliability between the identifier and the structure. The colour is applied if the identifier is the same in several databases for which the quality assurance could not be established.
- **Red:** There is a poor reliability between the identifier and the structure. The colour is applied if the identifier is allocated to different structures in different databases.

Outlook

- Background
- Objectives
- Specific Aims
- Read across and analogue approach
- The exercise
- **Workflow**
 - Chemical Input
 - **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

Summary information of the different profilers are provided in the “About”

The screenshot shows the QSAR Toolbox 3.0.0.0 GUI. In the left sidebar, under 'Protein binding', the 'Protein binding by OASIS' option is highlighted. A red callout box '1' points to this option. A right-click context menu is visible over it, with a red callout box '2' pointing to the 'About' option. The 'About' dialog box is open, showing details for the 'Protein binding by OASIS' profiler. A red callout box '3' points to the 'Close' button at the bottom of the dialog box.

1. Select the name of the profiler, perform **right click** on it and then
2. Select **About**
3. **Close** before proceeding

Profiling Side-Bar to Profiling

- For most of the profilers, background information can be retrieved by highlighting one of the profilers (for example, Protein binding by OASIS) and clicking on "View" (see next screen shot).

Profiling Side-Bar to Profiling

1. Highlight the profiler

2. Click View

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05.10.2012

30

Profiling

Profiling the target chemical

- The outcome of the profiling determines the most appropriate way to search for analogues (detailed information in Manual for getting started (Chapter 4). <http://www.oecd.org/dataoecd/58/56/46210452.pdf>)
- Table 4 - 1 in chapter 4 (Manual for getting started) lists a selection of profilers and their relevance for different endpoints of regulatory relevance.
- For example the following mechanistic profiling schemes are relevant to the Skin sensitization:
 - Protein binding by OASIS v.1.1 – mechanistic grouping
 - Protein binding by OECD – mechanistic grouping
 - Protein Binding Potency – mechanistic grouping

Profiling

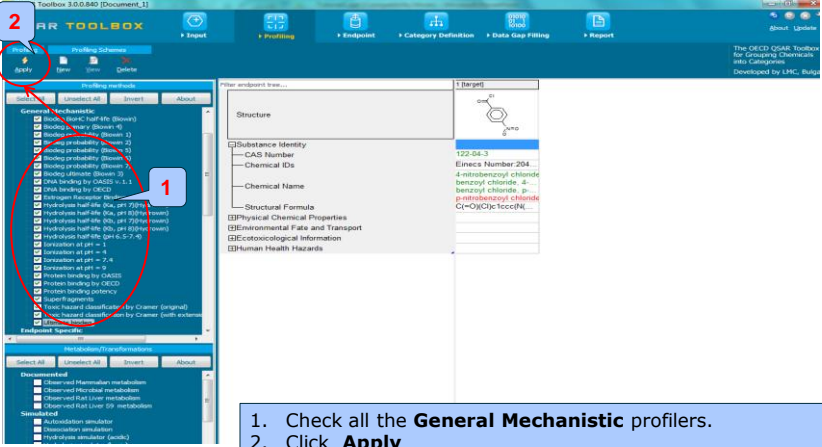
Profiling the target chemical

- **Click** in the box next to the name of the profiling methods related to the target endpoint.
- This selects (a **green** check mark appears) or deselects (**green** check mark disappears) profilers.
- For this example, **check** all the general mechanistic profilers and **click** on apply (see next screen shot).

QSAR TOOLBOX

Profiling

Profiling the target chemical



The screenshot shows the QSAR Toolbox software interface. The 'Profiling' step is active. The 'General Mechanistic' section is expanded, and the 'Apply' button is highlighted with a red circle and the number '2'. A blue box with the number '1' points to the list of profilers. The 'Target' section shows the chemical structure and properties of 4-mitrobenzoyl chloride.

1. Check all the **General Mechanistic** profilers.
2. Click **Apply**

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QSAR TOOLBOX

Profiling

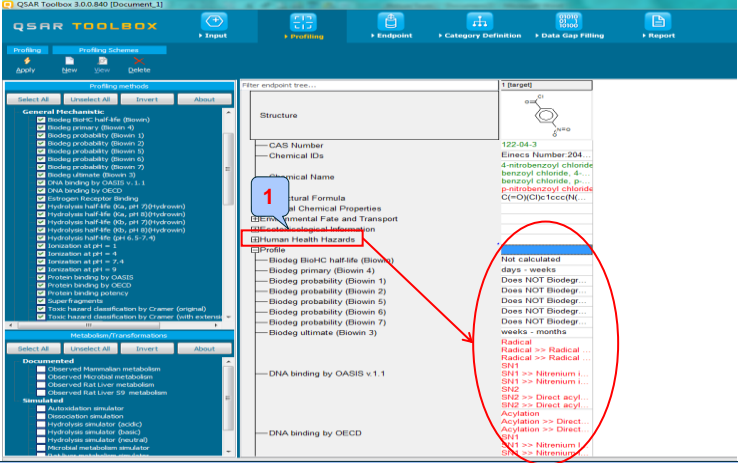
Profiling the target chemical

- 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 specific protein-binding profiler – Protein binding by OASIS (see side-bar on sensitisation above).
- This result will be used to search for suitable analogues in the next steps of the exercise.

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Profiling

Profiling the target chemical



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

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Outlook

- Background
- Objectives
- Specific Aims
- Read across and analogue approach
- The exercise
- **Workflow**
 - Chemical Input
 - Profiling
 - **Endpoint**

The OECD QSAR Toolbox for Grouping Chemicals into Categories 05.10.2012 36

Endpoint Overview

- “Endpoint” 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).

Endpoint Case study

- In this example, we limit our data gathering to a single toxicity endpoint (skin sensitization).
- In this example, we collect data from the databases containing experimental results for Skin sensitisation (Skin sensitisation and Skin sensitisation ECETOC).
- **Click** on “Endpoint” in the Toolbox workflow.
- **Expand the** “Human Health Hazards” section
- **Click** on the box to select that database.
- **Click** on “Gather data” (see next screen shot).

Endpoint Gather data

1. Expand the Human Health Hazards section
2. Select databases related to the target endpoint
3. Click Gather

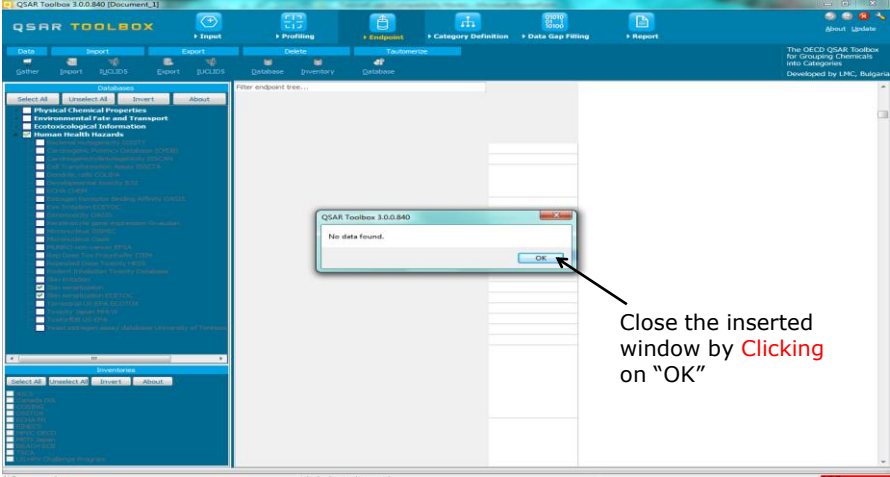
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Endpoint Gather data

- 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 Skin sensitization and Skin sensitization ECETOC .
- In this example, an insert window appears stating there was "no data found" for the target chemical (see next screen shot).

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Endpoint Gather data



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05.10.2012

41

Outlook

- Background
- Objectives
- Specific Aims
- Read across and analogue approach
- The exercise
- **Workflow**
 - Chemical Input
 - Profiling
 - Endpoint
 - **Category definition**

The OECD QSAR Toolbox for Grouping Chemicals into Categories

05.10.2012

42

Recap

- In module one, you have entered the target chemical being sure of the correct structure.
- In the second module, you have profiled the target chemical.
- In the third module, you have found that no experimental data is currently available in the Toolbox for this structure.
- In other words, you have identified a data gap which you would like to fill.
- **Click** on "Category Definition" to move to the next module.

Category Definition Overview

- This module provides the user with several means of grouping chemicals into a toxicologically meaningful category that includes the target molecule.
- This is the critical step in the workflow.
- Several options are available in the Toolbox to assist the user in refining the category definition.

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.
- Detailed information about grouping chemicals on the following link (Chapter 4).
<http://www.oecd.org/dataoecd/58/56/46210452.pdf>
- For example, starting from a target chemical for which a specific protein binding mechanism is identified, analogues can be found which can bind by the same mechanism and for which experimental results are available.

Category Definition

Protein binding by OASIS v.1.1 grouping method

- This is one of the best grouping methods in the Toolbox. It is built on conventional organic chemical reactions and as such is qualitative in character.
- This method is particularly relevant for respiratory and skin sensitization and acute aquatic toxicity, but also for chromosomal aberration and acute inhalation toxicity.

Category Definition

Side bar to Protein binding by OASIS v.1.1 categorization

- This scheme includes 130 categories organized in three level of information:
 - ✓ Level I: Mechanistic Domains (11 categories)
 - ✓ Level II: Mechanistic alerts associated to each mechanistic domain are created on the basis of a common reactive centre being activated by a number of substituents (35 categories)
 - ✓ Level III: A number of structural alerts specifying the substituents to a common reactive centre are made up each mechanistic alert (85 categories)

Category Definition

Side bar to Protein binding by OASIS categorization

- Each category from level III is presented by defined 2-dimensional structural alerts that is responsible for the eliciting toxic effects, such as skin sensitization which are a result of protein binding.
- The associated chemical reactions are in accordance with existing knowledge on electrophilic interaction mechanisms of various structural functionalities.

Category Definition

Side bar to Protein binding by OASIS categorization

- There is an agreement that most organic chemicals must react covalently with skin proteins in order to behave as skin sensitizers.
- Therefore, chemical reactions by which organic chemicals bind with proteins are relevant to grouping chemicals that may be skin sensitizing agents. So you have mechanistic plausibility for defining your category based on similar protein-binding mechanism.

Category Definition

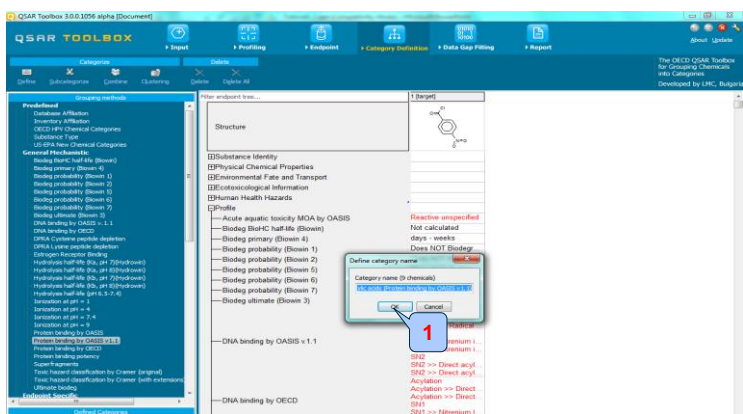
Defining Protein binding by OASIS v.1.1

The screenshot shows the QSAR Toolbox software interface. The 'Category Definition' dialog box is open, displaying a list of chemical categories. A red circle highlights the 'Define' button in the top-left corner of the dialog box. Another red circle highlights the 'OK' button in the bottom-right corner of the dialog box. A third red circle highlights the 'Protein binding by OASIS v.1.1' category in the list. The background shows the main QSAR Toolbox interface with a sidebar on the left and a main window on the right.

1. Highlight the "Protein binding by OASIS v.1.1"; 2. Click Define; 3. Click OK to confirm the defined categories for the target chemical

Category Definition

Defining Protein binding by OASIS



1. Click OK to confirm the name of the category

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05.10.2012

Category Definition

Analouges

- The data is automatically collated.
- Based on the defined category (Acylation<AND>Acylation<<Direct acylation involving a leaving group<AND>Acylation<<Direct acylation involving a leaving group<<Acyl halides of carboxylic acids) 8 analogues have been identified

Document_1

Defined Categories

[8] Acyl halide of carboxylic acids<AND>MA: Direct acylation involving a leaving group<AND>Media

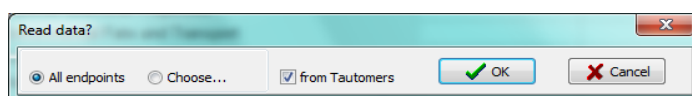
- The name of the category appear in the "Defined Categories" window, indicating the number of substances belonging to the category.
- In other words, these 9 compounds along with the target chemical form a category, which can be used for data filling. (see next slide)

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05.10.2012

Category Definition

Read data for Analogues

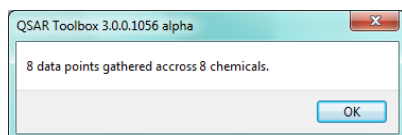
- The Toolbox automatically requests the user to select the endpoint that should be retrieved.
- The user can either select the specific endpoint or by default choose to retrieve data on all endpoints (see below).



Category Definition

Read data for Analogues

- The Toolbox automatically informs the user for the number of gathered data points across the chemicals in the category



- Click OK to confirm the appeared message

Category Definition

Summary information for Analogues

- The experimental results for the analogues are inserted into the matrix

Chemical statistics presenting the number of chemicals and the available experimental data.

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05.10.2012

Category Definition

Side bar of experimental data

- Double-click on the cell with measured data to see detailed information;
- Click on the X to close the dropdown box.

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05.10.2012

Category Definition

Navigation through the endpoint tree

- The user can navigate through the data tree by closing or opening the nodes of the endpoint tree.
- Double-click** on the node next to **Human Health Hazards** then **Sensitisation**, followed by **Skin**, **In Vivo** and **LLNA** and finally **EC3**.
- Local lymph node assay is in vivo method for assessment of relative skin sensitization potential of chemicals. The potential is expressed as EC3 values.
- In this example, results from skin sensitisation testing for chemicals reacting via nucleophilic substitution of acyl halides are available (see next screen shot).

Category Definition

Navigation through the endpoint tree

The screenshot shows the QSAR Toolbox interface with the following components:

- Left Panel:** A list of grouping methods including Predicted, Delivered Affinity, OECD HHV Chemical Categories, and General Relationships.
- Endpoint Tree:** A hierarchical tree structure where 'Human Health Hazards' is expanded to 'Sensitisation', which is further expanded to 'Skin', 'In Vivo', and 'LLNA'. The 'EC3' node is highlighted with a red box and a blue callout box containing the number '1'.
- Main Window:** Displays chemical structures and their corresponding data points in a table. The table has columns for 'Structure', 'EC3', and 'M-Positive'. The 'EC3' column shows values like 'M-Positive', 'M-Positive', 'M-Positive', and 'M-Positive'.

1. This is the target endpoint

Outlook

- Background
- Objectives
- Specific Aims
- Read across and analogue approach
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- **Workflow**
 - Chemical Input
 - Profiling
 - Endpoint
 - Category definition
 - **Data Gap Filling**

Recap

- You have identified a mechanistic category (Acylation<AND>Acylation<<Direct acylation involving a leaving group<AND>Acylation<<Direct acylation involving a leaving group<<Acyl halides of carboxylic acids) for the target chemical (4-nitrobenzoyl chloride).
- You have now retrieved in the available experimental results on skin sensitisation (EC3) values for eight chemicals with the same mechanism of protein binding as the target compound, which were found in the "Skin Sensitisation" databases.
- The user can now proceed to the next module; click on "Data Gap Filling".

Data Gap Filling Overview

- “Data Gap Filling” module give access to three different data gap filling tools:
 - Read-across
 - Trend analysis
 - Q)SAR models
- Depending on the situation, the most relevant data gap mechanism should be chosen, taking into account the following considerations:
 - Read-across is the appropriate data-gap filling method for “qualitative” endpoints like skin sensitisation or mutagenicity for which a limited number of results are possible (e.g. positive, negative, equivocal). Furthermore read-across is recommended for “quantitative endpoints” (e.g., 96h-LC50 for fish) if only a low number of analogues with experimental results are identified.
 - Trend analysis is the appropriate data-gap filling method for “quantitative endpoints” (e.g., 96h-LC50 for fish) if a high number of analogues with experimental results are identified.
 - “(Q)SAR models” can be used to fill a data gap if no adequate analogues are found for a target chemical.
- In this example, we use read-across.

The OECD QSAR Toolbox for Grouping Chemicals into Categories

05.10.2012

61

Data Gap Filling Apply Read across

Target	1	2	3	4	5
Structure					
Substance Identity					
— CAS Number	122-04-3	98-88-4	625-36-5	764-65-2	3282-30-2
— Chemical IDs	Einecs Number 204	EC Number 202-710-8	Einecs Number 202	Einecs Number 210	Einecs Number 212
— Chemical Name	4-nitrobenzoyl chloride	benzoyl chloride	3-chloropropionyl c...	nonanoyl chloride	EC Number 2
— Structural Formula	benzoyl chloride, 4-nitro	benzoyl chloride, p...	3-chloropropionyl c...	propionyl chloride	2,2-dimethylp...
— Physical Chemical Properties	benzoyl chloride, p...	benzoyl chloride, p...	propionyl chloride	propionyl chloride	propionyl chl...
— Environmental Fate and Transport	<chem>C1=O(C)C=C(Cl)C=C1</chem>	<chem>C1=O(C)C=C(Cl)C=C1</chem>	<chem>C1=O(C)C=C(Cl)C=C1</chem>	<chem>C1=O(C)C=C(Cl)C=C1</chem>	<chem>C1=O(C)C=C(Cl)C=C1</chem>
— Ecotoxicological Information					
— Human Health Hazards					
— Acute Toxicity					
— Carcinogenicity					
— Developmental Toxicity / Teratogenicity					
— Genetic Toxicity					
— Immunotoxicity					
— Irritation / Corrosion					
— Neurotoxicity					
— Repeated Dose Toxicity					
— Sensitisation					
— Skin					
— In Chemico					
— In Vitro					
— In Vivo					
— BOP/MT					
— LLNA					
— EC3	M Positive	M Positive	M Positive	M Positive	M Positive
— Toxicity to Reproduction					
— Toxicokinetics, Metabolism and Distribution					

1. Click on the cell corresponding to “EC3” for the target chemical.
2. Select Read-across
3. Click Apply

The OECD QSAR Toolbox for Grouping Chemicals into Categories

05.10.2012

62

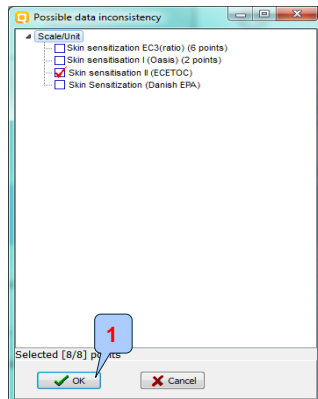
Data Gap Filling Scale definition

- Skin sensitisation is “qualitative” endpoint for which the results are presented with categorical data (for example: positive; negative; weak sensitizer; strong sensitizer ,etc).
- Skin sensitisation potential of the chemicals came from different authors coded with different names (for example: data from John Moores University of Liverpool are: *Strongly sensitizing, Moderately sensitizing etc.*; data from European centre for Ecotoxicology and Toxicology of chemicals are: *Positive, Negative, and Equivocal*).
- The main purpose of the scales is to unify all data available in the Toolbox databases for a certain endpoint.
- The default scale for Skin Sensitisation is “Skin Sensitisation ECETOC”. It converts all skin data into: Positive, Negative, and Equivocal.

The OECD QSAR Toolbox for Grouping Chemicals into Categories

63

Data Gap Filling Scale definition



1. Click **OK**

The OECD QSAR Toolbox for Grouping Chemicals into Categories

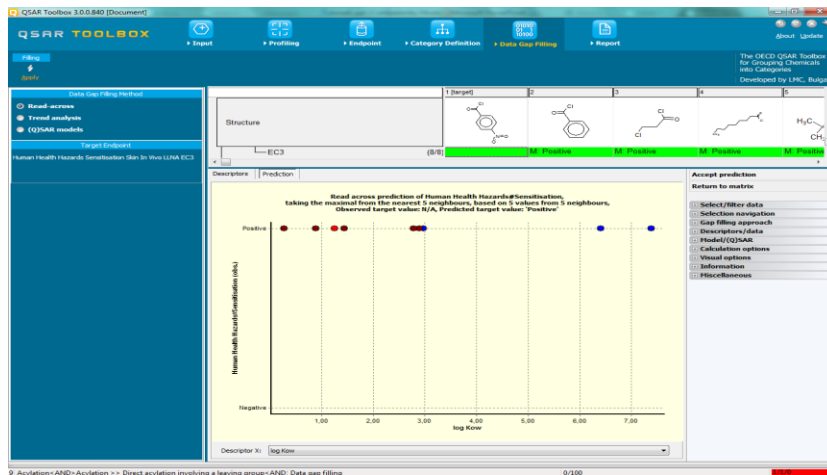
05.10.2012

64

Data Gap Filling Read-across

- The resulting plot is experimental results of all analogues (Y axis) according to a descriptor (X axis) with the default descriptor of log Kow (see next screen shot).
- The **RED** dot represents predicted results for the target chemical .
- The **BROWN** dots represent the experimental results available for the analogues that are used for the read-across.
- The **BLUE** dot represent the experimental results available for the analogues but not used for read-across.

Data Gap Filling Read-across



Data Gap Filling Interpreting Read-across

- In this example, all results of the analogues are consistent; all the analogues are Skin sensitizers.
- The same positive sensitising potential is therefore predicted for the target chemical.
- Accept the prediction by **clicking** "Accept prediction" (see next screen shot).

Data Gap Filling Accepting the predicted result

The screenshot shows the QSAR Toolbox interface. At the top, the 'Data Gap Filling' menu is active. The main window displays a 'Read across prediction of human health hazard (sensitization)' for a target chemical (EC3) based on 5 neighbors. A graph shows 'Human Health Hazard (Sensitization)' on the y-axis and 'log Kow' on the x-axis. A 'Confirm' dialog box is overlaid on the graph, asking 'The current model is still not saved. Do you want to save it now?' with 'Yes' and 'No' buttons. A red circle highlights the 'Yes' button. A red circle with the number '1' highlights the 'Accept prediction' button in the top right corner of the software window.

1. Select **Accept prediction**
2. Click **Yes** if you want to save the QSAR model based on the results from trend analysis, otherwise click **NO**

Q SAR TOOLBOX

Data Gap Filling Accepting the predicted result

The screenshot shows the Q SAR Toolbox interface with the 'Data Gap Filling' method selected. The main plot area displays a scatter plot with 'log Row' on the x-axis (ranging from 1.00 to 7.00) and 'Human Health Hazard(log10(1+EC50))' on the y-axis (ranging from Negative to Positive). A 'Confirm' dialog box is open, asking: 'Do you want to collect additional data for chemicals from data matrix for reporting purposes? (this data will be provided in data matrix tables)'. The dialog has 'Yes' and 'No' buttons. A red circle labeled '1' points to the 'Accept prediction' button in the top right corner of the software window. Another red circle labeled '2' points to the 'Yes' button in the 'Confirm' dialog.

1. **Click** Yes if you want additional data for the analogues to be presented in the report, otherwise **click** NO
2. **Click** Return to matrix

The OECD QSAR Toolbox for Grouping Chemicals into Categories 05.10.2012 69

Q SAR TOOLBOX

Outlook

- Background
- Objectives
- Specific Aims
- Read across and analogue approach
- The exercise
- **Workflow**
 - Chemical Input
 - Profiling
 - Endpoint
 - Category definition
 - Data Gap Filling
 - **Report**

The OECD QSAR Toolbox for Grouping Chemicals into Categories 05.10.2012 70

Recap

- Read-across is the appropriate data-gap filling method for “qualitative” endpoints like skin sensitisation. Since all the tested chemicals in the category were positive, it was easy to accepting the prediction of positive for the target chemical.
- You are now ready to complete the final module and to download the report.
- **Click** on “Report” to proceed to the last module.

Report Overview

- Report module could generate report on any of predictions performed with the Toolbox.
- Report module contains predefined report templates as well as a template editor with which users can develop a user defined templates.
- The report can then be printed or saved in different formats.

Report Generation report

1. **Expand** Prediction in the "Available data to report" window; 2. **Select** the prediction for the target chemical; 3. **Click** Create

The OECD QSAR Toolbox for Grouping Chemicals into Categories 05.10.2012 73

Congratulation

- You have now been introduced to the work flow of the Toolbox and completed the tutorial on data gap filling by read-across based on an analogue approach.
- You have been introduced to the six modules of the Toolbox, the basic functionalities within each module and the rationale behind each module.
- Note proficiency comes with practice.

The OECD QSAR Toolbox for Grouping Chemicals into Categories 05.10.2012 74