

OECD QSAR Toolbox v.3.0

Step-by-step example of how to categorize an inventory by mechanistic behaviour of the chemicals which it consists

Outlook

- **Background**
- Objectives
- Specific Aims
- Trend analysis
- The exercise
- Workflow

Background

- This is a step-by-step presentation designed to take Toolbox users through the workflow of categorizing an inventory using mechanistic similarity.

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Objectives

This presentation demonstrates a number of functionalities of the Toolbox including:

- Clustering chemicals from an imported inventory (chemical list).
- Selecting a cluster and place it into separate data matrix for later analyses.
- And, apply a trend analysis for aquatic toxicity to the selected cluster.

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Specific Aims

- To examine the workflow of clustering an inventory.
- To introduce the user to new functionalities within selected modules.
- To explain the rationale behind each step of the exercise.

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Trend analysis

- For a given toxicological endpoint, the members of a category are often related by a trend (e.g. increasing, decreasing or constant). The trend could be related to structural or chemical property.
- A demonstration of consistent trends in the behavior of a group of chemicals is one of the desirable attributes of a chemical category and an indicator that there is a common mechanism of action. When a consistent trend is observed and some chemicals in the category have measured values, missing values can be estimated by simple scaling from the measured values.

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The Exercise Part I

- In this part of the exercise we will import a chemical list containing 300 substances, representing a typical inventory of chemicals used by a down stream user.
- The inventory will be loaded into the Toolbox data matrix.
- The inventory will be profiled by the "Aquatic toxicity classification by ECOSAR Classification" profiling scheme.
- This inventory will be clustered by the ECOSAR Classification grouping method.

The Exercise Part II

- In this part of the exercise an example cluster or defined category will be examined.
- Data on the chemicals which belong to selected cluster will be gathered.
- A data gap will be filled by trend analysis - In this exercise we will predict the toxicity towards mortality of the *Pimephales promelas* (LC50 for 24h).
- A report of the prediction will be generated.

The Exercise

Necessary to download the file

- The inventory is stored in the following smi file: OECD Mock Inventory.smi*
- This file contains a list of Chemical Abstract Service (CAS) numbers, which can be opened with Notepad.

*OECD Mock Inventory.smi - file is packed in the zip file with all power point tutorials.

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Workflow

- **The Toolbox has six modules which are used in a sequential workflow:**

- Chemical Input
 - Profiling
 - Endpoints
 - Category Definition
 - Filling Data Gaps
 - Report
-
- Part I
- Part II

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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 is the correct one.

Chemical Input Ways of Entering a Chemical

User Alternatives for Chemical ID:

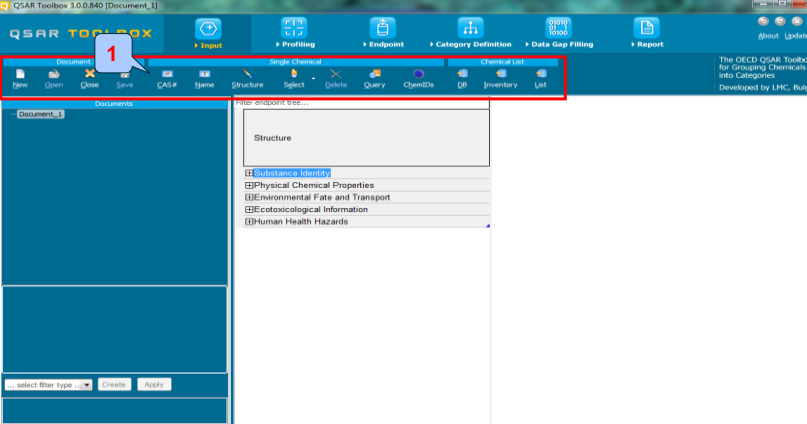
A. Single target chemical

- 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

Chemical Input Screen Input target chemical by CAS#

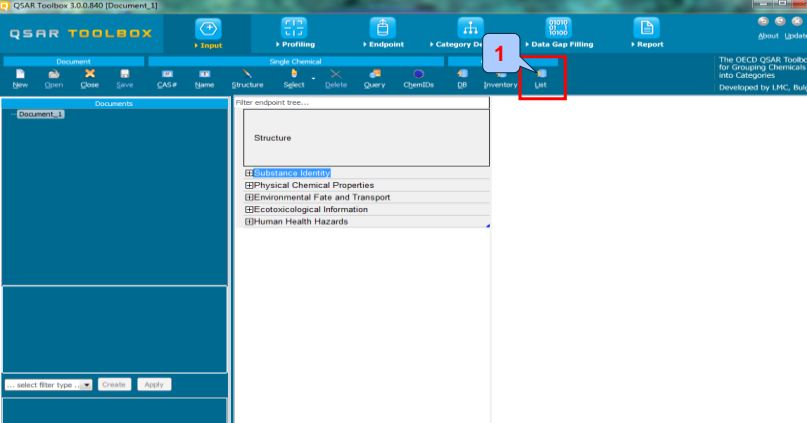


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Chemical Input Screen Input target chemical by CAS#



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1. Click on List.

Chemical Input Screen Missing SMILES

- Since in the entered list there are CAS numbers for which there are no SMILES in the Toolbox, the user will be asked if he/she wants the Toolbox to search for in the databases. In this example select **NO**.

Chemical Input Screen Missing SMILES

The screenshot shows the QSAR Toolbox software interface. A confirmation dialog box is displayed in the center, asking: "There are empty SMILES with defined CAS in the list. Would you like to search in the database with CAS?". The dialog box has two buttons: "Yes" and "No". A red "1" in a blue box is positioned over the "No" button, with an arrow pointing to it from a larger blue box below the dialog box that contains the text "1. Click NO in dropdown box.".

Chemical Input Screen Displaying structures

- The structures of the 300 chemicals are displayed with 2D image. The missing SMILES are displayed with empty window - for example chemical #110 (see next screen shot).
- These empty windows remind the user where are the gaps in the inventory.
- Remember all subsequent functions are based on chemical structure, so the chemicals with blank windows will not be placed in a cluster or category.

Chemical Input Screen Displaying structures

The screenshot shows the QSAR Toolbox interface with a table of chemical data. The table has columns for chemical IDs (108, 109, 110, 112, 113) and rows for 'Structure' and various property categories. The cell for chemical 110 in the 'Structure' row is highlighted with a red box, indicating it is empty.

Filter endpoint tree...	108 [target]	109 [target]	110 [target]	112 [target]	113 [target]
Structure					
Substance Identity					
Physical Chemical Properties					
Environmental Fate and Transport					
Ecotoxicological Information					
Human Health Hazards					

Chemical Input Chemical Identity

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

Chemical Input Chemical Identity

The screenshot shows the QSAR Toolbox interface with the 'Chemical Identity' section active. The 'Substance Identity' tab is selected, displaying a table of chemical identifiers for various targets. A red oval highlights the 'Chemical Name' row for target 109, which lists '3-aminobiphenyl', '3-aminobiphenyl (3-n-propyl methacrylate)', and '3-ylamine propyl 2-methylprop-2-yl methacrylate'.

Filter endpoint tree...	108 [target]	109 [target]	110 [target]	111 [target]	112 [target]	113 [target]
Structure						
Substance Identity	2310-98-8	2013-17-2	23058-36-2	2644-60-5	2644-60-5	2578-10-4
CAS Number	2310-98-8	2013-17-2	23058-36-2	2644-60-5	2644-60-5	2578-10-4
Chemical IDs	Enecac Number 218	NA	NA	Enecac Number 246	Enecac Number 246	Enecac Number 246
Chemical Name	2-propenoic acid, 2-methacrylic acid, propyl methacrylate	3-aminobiphenyl (3-n-propyl methacrylate)	3-aminobiphenyl (3-n-propyl methacrylate)	2,6-bis(1-methylethyl)hexan-3-one	4-hexen-3-one	pyridine
Chemical Name	propyl 2-methylprop-2-yl methacrylate	3-ylamine propyl 2-methylprop-2-yl methacrylate		2,6-diisopropylaniline	4,6-diisopropylaniline	aniline, 2,6-diisopropyl
Structural Formula	C=C(O)C(=O)CC	C1=CC=C(N)C=C1		C1=CC(=C(N)C=C1)C(C)C	C1=CC(=C(N)C=C1)C(C)C	C1=CC(=C(N)C=C1)C(C)C
Physical Chemical Properties						
Environmental Fate and Transport						
Ecotoxicological Information						
Human Health Hazards						

Chemical Input Chemical Identity

The color code indicates the reliability of the chemical identifier:

- **Green:** There is a high reliability between the identifier and the structure. This color is attributed 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 color is attributed 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 color is attributed if the identifier is allocated to different structures in different databases.
- **Black:** The quality of the structure and its identifier is unknown.

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 - Chemical Input
 - **Profiling**

Profiling Overview

- As you are aware the “profiling” refers to the electronic process of retrieving relevant information on the target compound(s), which are stored in the Toolbox other than fate and toxicity data.
- Key to this exercise is the information on likely mechanism(s) of action.

Profiling Side-Bar of Profilers

- Remember detailed explanation of the different profilers is available in the in Manual for getting started (Chapter 4). <http://www.oecd.org/dataoecd/58/56/46210452.pdf>
- Background information can be retrieved by highlighting a profiler and a click on the button “View”.
- For grouping chemicals into meaningful categories for aquatic toxicity the “Aquatic toxicity classification by ECOSAR” is one of the most adequate scheme.

Profiling Side-Bar of Profilers

The screenshot shows the QSAR Toolbox 3.0.0.855 interface. On the left, the 'Profiling Methods' sidebar is visible. A red circle highlights the 'Aquatic toxicity classification by ECOSAR' option. A red arrow points to the 'View' button next to it. The main window displays the 'ECOSAR Class Definition: Acid Halides' dialog box. The dialog box contains the following text:

ECOSAR Class Definition: Acid Halides
The Acid Halide class is identified by any of the following structures:

$$\text{C-Halogen} \quad \text{P-Halogen} \quad \text{S-Halogen}$$

The Halogens include chlorine (Cl), bromine (Br), fluorine (F) and iodine (I).
The C(-O) carbon, P(-O) phosphorus and S(-O) sulfur can have other attachments. In the current ECOSAR program, these other attachments can be anything.

SMILES String Identifications:

C(-O)C	C(-O)C	C(-O)F	C(-O)I
P(-O)C	P(-O)C	P(-O)F	P(-O)I
S(-O)C	S(-O)C	S(-O)F	S(-O)I

Associated ECOSAR Classes: None

Example Acid Halides:

CAS No.	Name	SMILES Notation
75-36-5	Acetyl chloride	CC(=O)Cl
505-96-7	Acetyl bromide	CC(=O)Br
96-88-4	Benzoyl chloride	O=C(c1ccccc1)Cl
98-09-3	Benzotrifluoride	ClC(F)(F)F(c1ccccc1)Cl
838-72-6	Phosphoric dichloride, phenyl-	O=P(Cl)(Cl)ClC(c1ccccc1)Cl

1. Highlight the "Aquatic toxicity classification by ECOSAR" profiler; 2. Click View to see the drop-down box.

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Profiling Side-Bar of Profilers

The screenshot shows the QSAR Toolbox 3.0.0.855 interface. On the left, the 'Profiling Methods' sidebar is visible. A red circle highlights the 'Aquatic toxicity classification by ECOSAR' option. A red arrow points to the 'Apply' button next to it. The main window displays a table of chemical structures and their properties.

Structure	100 [target]	109 [target]	110 [target]	111 [target]	112 [target]	113 [target]
Structure						
Substance Identity	2210-28-8	2243-47-2	23056-36-2	24544-94-5	2497-21-4	2578-
Chemical IDs	Emecsa Number 218	NA	NA	Emecsa Number 246	Emecsa Number 219	Emec
Chemical Name	2-propenoic acid, 2-(3-aminobiphenyl)methylacetyl, pr.	3-aminobiphenyl-n-propyl methacrylate	propyl methacrylate	hex-4-en-3-one	2-chloro-4-hexan-3-one	2-chloropyridine
Structural Formula	C=C(O)C=C(C)OCC	c1c(c2cc1)Nccc2	CC(C)C(=O)CC	C=C(O)C=C(C)CC	C=C(O)C=C(C)CC	c1cc(C)nc1

1. Select the ECOSAR profiler by clicking on the box next to it (a green tick mark appears); 2. Click Apply.

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Profiling

Profiling results

- The actual profiling will take several seconds depending on the number and type of selected profilers.
- The results of profiling automatically appear as a dropdown box (see next screen shot).
- Please note the specific profiling results of Aquatic toxicity classification by ECOSAR.
- These results will be used to division chemicals from the inventory into suitable clusters in the next steps of the exercise.

Profiling

Profiling results

The screenshot shows the QSAR Toolbox software interface. The main window displays the 'Profiling' results for a selected chemical. The interface includes a menu bar with options like 'Input', 'Profiling', 'Endpoint', 'Category Definition', 'Data Gap Filling', and 'Report'. Below the menu bar, there are several tabs and buttons for managing the profiling process. The main workspace is divided into a 'Filter endpoint tree' on the left and a table of results on the right. The table has columns for '1 (target)', '2 (target)', '3 (target)', '4 (target)', and '5 (target)'. The '1 (target)' column contains chemical structures. The '2 (target)' column contains a chemical structure. The '3 (target)' column contains a chemical structure. The '4 (target)' column contains a chemical structure. The '5 (target)' column contains a chemical structure. The table rows include 'Structure', 'Substance Identity', 'Physical Chemical Properties', 'Environmental Fate and Transport', 'Ecotoxicological Information', 'Human Health Hazards', and 'Profile'. The 'Profile' row is highlighted in blue, and the 'Aquatic toxicity classification by ECOSAR' entry is circled in red.

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 - Chemical Input
 - Profiling
 - **Endpoint**

Endpoints Overview

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

Endpoints Case study

- In this example, since we categorize an inventory for later analysis we do not need of data gathering.
- In this module we need only to select the Aquatic ECETOC, Aquatic OASIS and Aquatic US-EPA ECETOX databases.
- These databases contain results on aquatic toxicity for various species, and durations.
- **Click** on the "Category Definition" to move to the next module.

Endpoints Case study

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

- Callout 1:** Points to the 'Ecotoxicological Information' section in the left sidebar, which is expanded.
- Callout 2:** Points to the 'Aquatic ECETOX' and 'Aquatic OASIS' databases in the 'Database' list.
- Callout 3:** Points to the 'Gather' button in the top toolbar.
- Structure Panel:** Displays chemical structures for Phenols, Epoxides, mono, Vinyl/Allyl Sulfones, and Neutral Organics.
- Endpoint List:** A table with columns for 'Filter endpoint tree' and 'Target'. The 'Target' column contains the following entries: Phenols, Epoxides, mono, Vinyl/Allyl Sulfones, Neutral Organics, Neutral Organics, and Neutr.

1. **Expand** Ecotoxicological information section
2. Select the databases listed in the previous slide both databases mentioned in the previous slide databases
2. **Click** Gather

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 - Profiling
 - Endpoint
 - **Category definition**

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 to define a category.

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 trend-analysis.
- Detailed information about grouping chemical (Chapter 4) could be downloaded from:
<http://www.oecd.org/dataoecd/58/56/46210452.pdf>

Category Definition

Side bar to ECOSAR category

- ECOSAR has been used by the U.S. Environmental Protection Agency to predict the aquatic toxicity of new industrial chemicals in the absence of test data.
- SARs are developed for chemical classes (e.g. phenols) based on measured test data which have been submitted by industry or they were taken from other sources.
- The ECOSAR classification in the Toolbox is used for grouping chemicals by structural (and in some cases mechanistic) similarity.

Category Definition Clustering

The chemicals in the inventory can be clustered in to 55 clusters based on EcoSAR Categories.

- 72 are neutral organics.
- 30 are esters.
- 28 are phenols.
- 23 are anilines (unhindered).
- 14 are aldehydes (mono)
- 10 are aliphatic amines
- Other clusters consist of less than 10 compounds.

Category Definition Clustering

1. Highlight the "Aquatic toxicity classification by ECOSAR";

2. Click Clustering.

Category Definition

Select working cluster

1. **Highlight** specific cluster to select it as working- in this example **select "Phenols"**. 2. **Click OK** to read data for members of the cluster

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Category Definition

Read data for the members of the cluster

- The chemicals which belong to the selected cluster are immediately loaded in a separate data matrix.
- The Toolbox automatically starts the process of data gathering. The user is asked to select the endpoint that should be retrieved.
- In "Read data?", the user can either "Choose" a specific endpoint or by default retrieve data on "All endpoints" which are stored in previously selected data bases (see below).

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Category Definition

Read data for the members of the cluster

- Due to the overlap between the Toolbox databases same data for intersecting chemicals could be found simultaneously in more than one database. The data redundancy is identified and the user has the opportunity to select either a single data value or all data.

Repeated values for: 822 data-points; 325 groups; 63 chemicals

Data points...	Endpoint	CAS	Structure	Value	Age	Select one
<input checked="" type="checkbox"/>	LC50	108-95-2	<chem>c1ccccc1</chem>	4E4 micrograms per liter		1
<input checked="" type="checkbox"/>	LC50	108-95-2	<chem>c1ccccc1</chem>	4E4 micrograms per liter		Invert
<input checked="" type="checkbox"/>	LC50	108-95-2	<chem>Oc1ccccc1</chem>	24,8(23;26,9) milligram per liter	29 day(s)	Check All
<input checked="" type="checkbox"/>	LC50	108-95-2	<chem>Oc1ccccc1</chem>	2,48E4(2,3E4;2,69E4) micrograms per liter	29 day(s)	Uncheck All
<input checked="" type="checkbox"/>	LC50	108-95-2	<chem>Oc1ccccc1</chem>	6,75E4 micrograms per liter		OK
<input checked="" type="checkbox"/>	LC50	108-95-2	<chem>Oc1ccccc1</chem>	67,5 milligram per liter		Cancel
<input checked="" type="checkbox"/>	LC50	108-95-2	<chem>Oc1ccccc1</chem>	6,75E4 micrograms per liter	3-8 month(s)	

1. Click Select one and then; 2. Click OK.

Category Definition

Select working cluster

QSAR Toolbox 3.0.0.860 [oeqd_mock_inventory.txt]

Filter endpoint tree...

Structure	1 Target	2 Target	3 Target	4 Target	5 Target	
<chem>Oc1ccc(O)cc1</chem>	(27,8458)14	3.6 mg/L	M. 8.2 mg/L, 0.319	M. 46.1 mg/L, 41.1	M. 435 mg/L, 433x3	M. 18.9 mg/L
	Aquatic toxicity classification by ECD...	Phenols	Phenols	Phenols	Phenols	Phenols

Chemical statistics presents the number of chemicals and the available experimental data. This is statistics for the current row on data matrix.

Category Definition

Navigation through the endpoint tree

- The user can navigate through the data tree by closing or opening the nodes of the tree.
- In this example, the LC50-24h Mortality for *Pimephales promelas* is the target endpoint.

Category Definition

Navigation through the endpoint tree-use filter

1. Type "LC50" in the filter box; 2. By double clicking on the specific nodes open the endpoint tree go to the target endpoint- Ecotoxicological information; Aquatic toxicity; Mortality; LC50; 24h; Animalia; Chordata(Vertabrates); Actinopterygii(fish); Pimphales promelas

Structure	Target	Target	Target	Target
<chem>C1=CC=C(C=C1)O</chem>	OH	OH	OH	OH
Danio rerio	(2/3)	M	35-100 mg/L = 2	
— Ethacostoma lapidum	(1/1)			
— Ethacostoma rubrum	(1/1)			
— Gambusia affinis	(1/2)	M	73 mg/L, 61 mg/L	
— Gastromyzus aculeatus	(1/2)	M	24 mg/L, 49 mg/L	
— Gila elegans	(1/2)			
— Heteromysallus fossilis	(2/6)	M	41.9 mg/L, 15.9	
— Hyporhamphus calidus	(1/1)			
— Ictalurus punctatus	(1/1)	M	13.3 mg/L	
— Jordanella floridae	(1/1)			
— Kribia sandwicensis	(1/1)	M	14 mg/L	
— Lepomis macrochirus	(2/18)	M	25.9(2.2,38.2)	
— Mugil saliens	(1/1)	M	21.5 mg/L	
— Nolemigeus crysoleucas	(1/2)	M	120 mg/L, 35 mg/L	
— Nothobranchius guentheri	(2/2)	M	57(45.71) mg/L	
— Notropis melanopterus	(2/16)	M	14 mg/L, 3.65 m	
— Oncorhynchus kisutch	(1/1)			
— Oncorhynchus mykiss	(2/2)	M	5.6 mg/L, 11 mg	
— Oncorhynchus tshawytscha	(3/3)			
— Oryzias latipes	(2/5)	M	150 mg/L, 40 m	
— Pimephales promelas	(1/5)	M	100-500 mg/L, 1	
— Pimephales promelas	(2/3)	M	40 (30, 6.5) m	
— Phacelgara occidentalis	(4/10)	M	49.9(39.5,87.8)	
— Phacelgara occidentalis	(1/1)			

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 - **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
- Select the most relevant data gap method:
 - Read-across is the appropriate data-gap filling method for "qualitative" endpoints where possible results are positive, negative or equivocal. Read-across is also recommended for "quantitative endpoints" (e.g., 96h-LC50 for fish) when there are few analogues with experimental results.
 - Trend analysis is the appropriate data-gap filling method for "quantitative endpoints" (e.g., 96h-LC50 for fish) when a high number of analogues with experimental results.
 - "(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 will use trend analysis.

Data gap filling Apply Trend analysis

1. Highlight the data endpoint box corresponding to the target endpoint under 4-bromo-2,6-dimethylphenol; 2. Select Trend analysis; 3. Click Apply.

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Data gap filling Trend analysis

Trend analysis prediction of Ecotoxicological Information@Aquatic Toxicity making a linear approximation, based on 6 values from 6 analogs.
Observed target value: N/A, Predicted target value: 3.28 mg/L.

Model equation: Ecotoxicological Information@Aquatic Toxicity = +1.81 + 0.851 * log Kow

Descriptor X: log Kow

Data gap filling 0/100

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Data gap filling

Interpreting Trend analysis

- The resulting plot outlines the experimental LC50 results of all analogues (Y axis) according to a descriptor (X axis) with Log Kow being the default descriptor.
- The **RED** dot represents the estimated result for the target chemical.
- The **BLUE** dots represent the experimental results available for the analogues.

Data gap filling

Analysis of the results

- The resulting trend analysis reveals a consistent trend in results with toxicity increase linearly with log Kow.
- It can be used to fill the data gap.
- By extension it can be used to fill data gaps for this endpoint for all chemicals in this cluster (i.e., category).
- See also the presentation "How to build user defined QSAR model" available at the OECD website.
- Accept the prediction (see next screen shot).

Data gap filling

Accepting the prediction result

The screenshot shows the QSAR Toolbox interface during the 'Data Gap Filling' process. The 'Target Endpoint' is set to 'Ecotoxicological Information#Aquatic Toxicity Mortality (LC50 24h, Phenols (Chemicals(Overlaid))#ActiveComp ppb(h))'. The graph displays a scatter plot of log Kow values versus aquatic toxicity mortality, with a red regression line. A table at the top right shows chemical structures and their predicted values. A blue callout box with '1.' points to the 'Accept prediction' button, and another with '2.' points to the 'Return to data matrix' button.

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Data gap filling

Accepting the prediction result

The screenshot shows the QSAR Toolbox interface displaying a list of chemical structures and their predicted values. A red circle highlights the predicted value '3.21(0.55-19.2)' for the compound 'Phenol'.

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Filled data gap

- By accepting the prediction the data gap was filled (see next screen shot).
- You are now ready to complete the final module and to download the report.
- **Click** on "Report" to proceed to next module.

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- **Report**

QSAR TOOLBOX

Report Overview

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

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QSAR TOOLBOX

Report Generate report.

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

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Congratulation

- You have used the Toolbox to categorize an inventory by mechanistic behavior.
- You now know another useful tool in the Toolbox.
- Continue to practice with this and other tool and soon you will be comfortable dealing with many situations where the Toolbox is useful.