

## OECD (Q)SAR Toolbox v.4.4.1

Tutorial on using the PBT prioritization scheme

# Outlook

- **Aim**
- Keywords
- PBT scheme
- Workflow of the prediction
- Export of the results

# Aim

This is a step-by-step presentation designed to take the user of Toolbox through the PBT prioritization scheme implemented in the software.

# Outlook

- **Aim**
- Keywords
- PBT scheme
- Workflow of the prediction
- Export of the results

# Keywords

**TARGET CHEMICAL** - chemical of interest

**MODULE** – a Toolbox module is a section dedicated to specific actions and options (e.g. Profiling)

**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)

**EXPORT** – Toolbox allows to export data and predictions for chemicals in an Excel format

**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

**PBT SCHEME** – PBT prioritization scheme based on experimental data and (Q)SAR models for assessing persistency, bioaccumulation and toxicity of substances

# Outlook

- Aim
- Keywords
- **PBT scheme**
  - **Background**
- Workflow of the prediction
- Export of the results

# Background:

## PBT prioritization scheme

- The PBT prioritization scheme is based on experimental data and (Q)SAR models.
- A substance is classified based on thresholds for persistence, bioaccumulation and toxicity, and the following classifications could be assigned:
  - very persistent (**vP**),
  - persistent (**P**),
  - very bioaccumulative (**vB**),
  - bioaccumulative (**B**),
  - very toxic (**vT**),
  - toxic (**T**).
- The thresholds are illustrated in the table on the next slide.

# Background:

## PBT assessment criteria

Classification	Criteria	Guidance	Data and models
vP	$BOD \leq 30\%$	REACH Annex XIII [1]	Experimental data only
P	$30\% < BOD \leq 40\%$ or biodegradation probability $< 0.5$	REACH Annex XIII [1]	Experimental data and BIOWIN 5 and 6 models
vB	$BCF \geq 3.699 \log(L/kg \text{ wet})$	REACH Annex XIII [1]	Experimental data and BCFWIN model
B	$3.301 \leq BCF < 3.699 \log(L/kg \text{ wet})$ or $\log Kow > 4.5$	REACH Annex XIII [1]	Experimental data and BCFWIN and KOWWIN models
vT	$LC50 \leq 1 \text{ mg/l}$	GHS classification [2]	Experimental data only
T	$1 \text{ mg/l} < LC50 \leq 10 \text{ mg/l}$	GHS classification [2]	Experimental data only

[1] [https://echa.europa.eu/documents/10162/13632/information\\_requirements\\_r11\\_en.pdf](https://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf)

[2] [https://www.unece.org/fileadmin/DAM/trans/danger/publi/ghs/ghs\\_rev04/English/ST-SG-AC10-30-Rev4e.pdf](https://www.unece.org/fileadmin/DAM/trans/danger/publi/ghs/ghs_rev04/English/ST-SG-AC10-30-Rev4e.pdf)



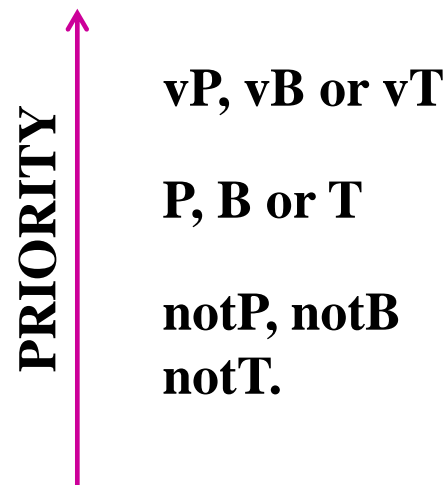
# Background:

## PBT assessment criteria

### PBT priority grouping:

Based on the collected experimental data and results provided by (Q)SAR models, the system applies the worst case scenario to categorize chemicals using the following priority:

- With the **highest priority** are chemicals **with available experimental data** for P, B or T assessment.
- In case of unavailable experimental data for P, B or T, (Q)SAR models are applied for making predictions.

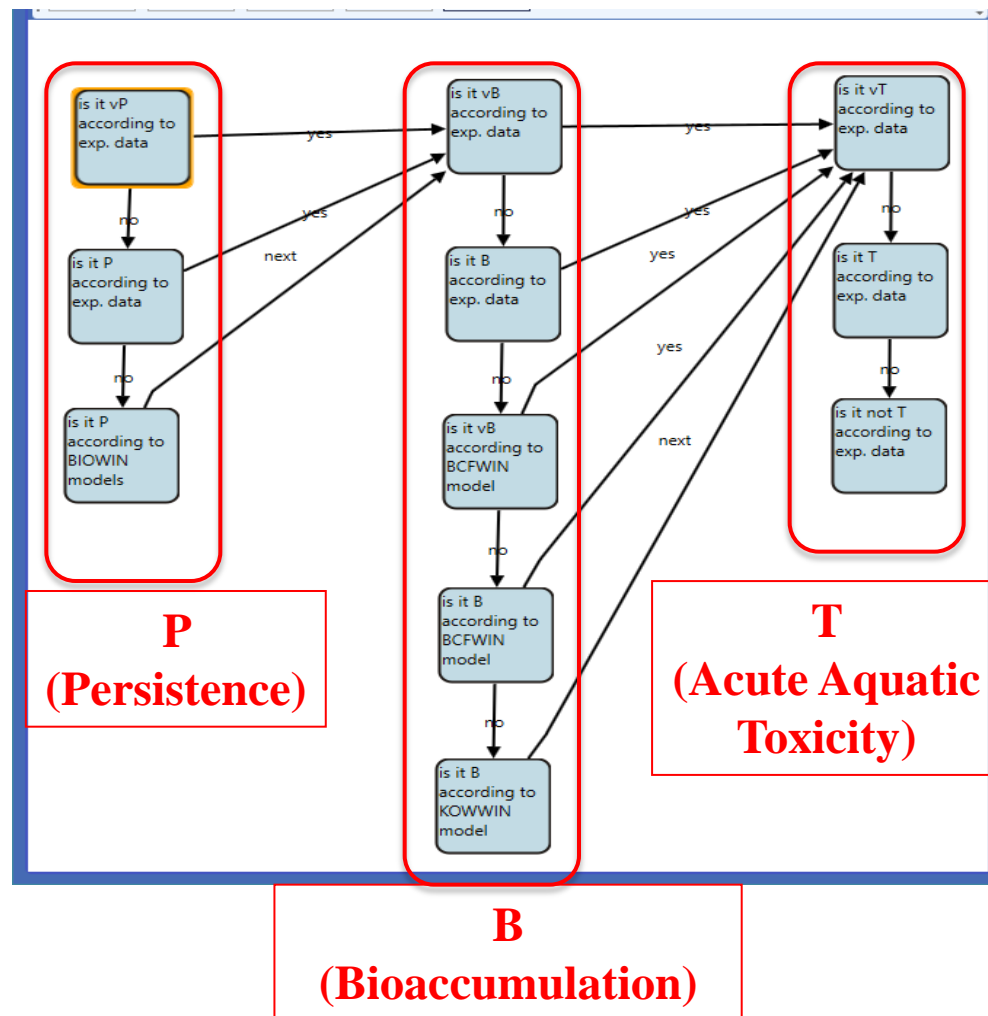


# Outlook

- Aim
- Keywords
- **PBT scheme**
  - Background
  - **Implementation**
- Workflow of the prediction
- Export of the results

# Implementation of PBT prioritization scheme

- The PBT prioritization scheme is a graph of logically connected nodes.
- The nodes are divided into three groups based on the P, B or T classification for hazard assessment.



# Implementation of PBT prioritization scheme

- Each node (1) contains a data or parametric (model) boundary (2) where the criteria for PBT assessment are set.
- Data query is depicted here.

Category tree

ADD  
DEL  
AND

is it vP according to exp. data

Data query

1

2

Query details

[1] Data Query Metab...

Save

Endpoint definition

Filter: [ ] Close

- ☐ % degradation (test mat. analysis)
- ☐ % degradation (CH4 evolution)
- ☐ % degradation (CO2 evolution)
- ☐ % degradation (DOC removal)
- ☐ % degradation (inorg. C analysis)
- ☐ % degradation (O2 consumption)
- ☐ % degradation (radiochem. meas.)
- ☐ % degradation (TOC removal)
- ☒ BOD
  - ☒ Biodegradation NITE
  - ☐ calculated rating of total degradation time (QSAR/QSPR)
  - ☐ half-life in days (QSAR/QSPR)
  - ☐ not specified
  - ☐ Other
  - ☐ Other Endpoint
- ☐ Photodegradation
- ☐ ...

1373

Metadata

Descriptors (numerical metadata)

Data

	All	Any	Min	Max	Average	...
Mean value:	≤				30	
Min value:	none					
Max value:	none					
Unit	Biodegr...	%				

BOD≤30%

# Outlook

- Aim
- Keywords
- PBT scheme
  - Background
  - Implementation
- **Workflow of the prediction**
- Export of the results

# Workflow of the prediction: Steps

- Input of target chemical(s)
- Profiling: Example prioritization scheme (PBT)
- Report

# Outlook

- Aim
- Keywords
- PBT scheme
  - Background
  - Implementation
- **Workflow of the prediction**
  - **Chemical input**
- Export of the results

# Chemical Input

- 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

### I. Single target chemical:

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

### II. Group of chemicals:

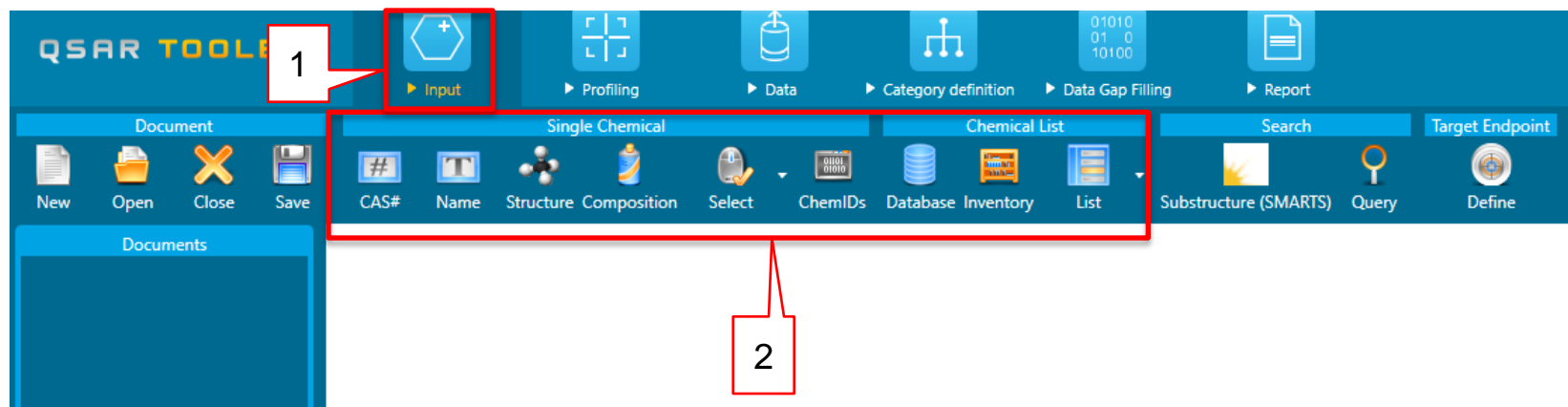
- User's List
- Inventory/Database

## Chemical Input: Single chemical

- Open the Toolbox.
- Click on “Input” (see next screen shot).

# Chemical Input

## Single chemical



1. Click **Input** (1) to display the main Input section (2).

# Chemical Input

## Single chemical: CAS RN

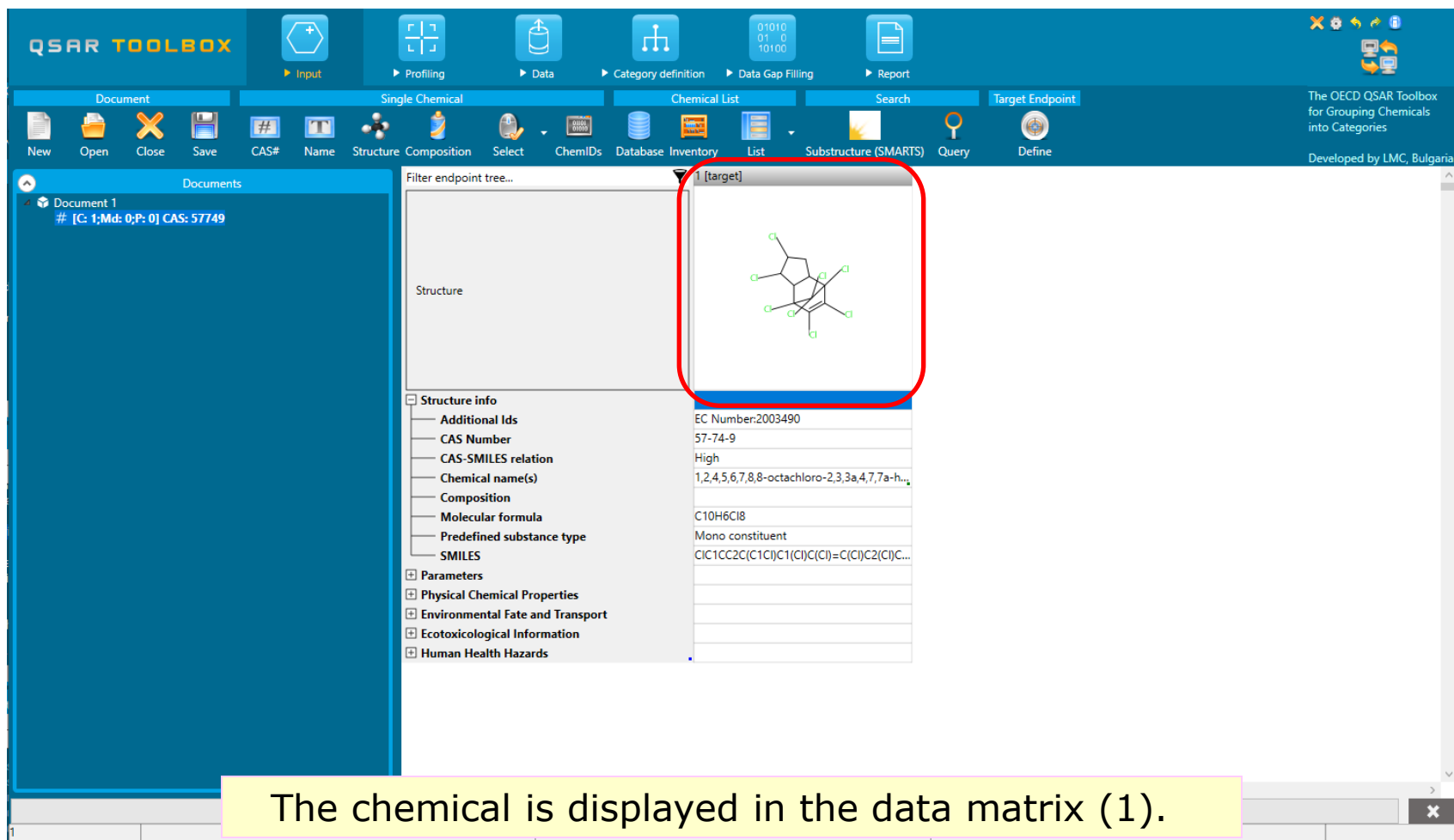
The screenshot shows the QSAR Toolbox software interface. The main menu is on the left, and the search window is on the right. The search window is titled 'Search by CAS #' and contains a search bar with the text '57749' and a 'Search' button. The search results are displayed in a table with columns for CAS, SMILES, CS Relation, Substance, Composition, Name, and Sources. The first result is highlighted with a red box and a checkmark, indicating it is the selected chemical.

CAS	SMILES	CS Relation	Substance	Composition	Name	Sources
57-74-9	<chem>C1C1CC2C(C1C1)C(C)C(C1)-C...</chem>	High	Mono constituent		1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7...	NICNAS COSING
57-74-9	<chem>C1C1CC2C(C1C1)[C@H]1(C)C(C...</chem>	Low	Mono constituent		Chlordane	Carcinogenicity&mutagenicity IS! Riocides and plant protection TSSF
57-74-9	<chem>Cl[C@H]1C[C@@H]2[C@H]C@...</chem>	Low	Mono constituent		Chlordane Analytical	

1. Click **CAS#** (1);
2. Type in the **CAS # 57-74-9** (the target chemical) (2) ;
3. Click on **Search** (3);
4. Select the first chemical with High relation CAS-SMILES (4);
5. Click **OK** (5).

# Chemical Input

## Single chemical: CAS RN



The screenshot shows the QSAR Toolbox software interface. The 'Single Chemical' tab is selected. The 'Structure' panel displays a chemical structure, which is highlighted with a red box. The 'Structure info' panel shows the following details:

- EC Number: 2003490
- CAS Number: 57-74-9
- CAS-SMILES relation: High
- Chemical name(s): 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-h...
- Composition: C10H6Cl8
- Molecular formula: C10H6Cl8
- Predefined substance type: Mono constituent
- SMILES: ClC1CC2C(C1Cl)C1(Cl)C(Cl)=C(Cl)C2(Cl)C...

The chemical is displayed in the data matrix (1).

# Outlook

- Aim
- Keywords
- PBT scheme
  - Background
  - Implementation
- **Workflow of the prediction**
  - Chemical input
  - **Profiling**
- Export of the results

## Profiling Overview

- “Profiling” refers to the electronic process of retrieving relevant information on a compound which is stored in the Toolbox, other than its fate and (eco)toxicity data.
- Toolbox has many predefined profilers but it also allows the user to develop new profilers.

# Profiling

1. Select **Profiling tab** (1);
2. Click **Unselect All** (2);
3. Tick **Example prioritization Scheme (PBT)** (3);
4. Click on **Apply** (4).
5. Expand the cell to see the results: P, vB, vT.
6. Double-click on the profiling results cell (5)
7. The results are explained in the next slides.

QSAR Toolbox 4.4 [Document 1]

QSAR TOOLBOX

Input Profiling Category definition Data Gap Filling Report

Apply View New Delete

Document 1  
# [C: 1;Md: 0;P: 0] CAS: 57749

Filter endpoint tree... 1 [target]

Structure

Structure info  
Parameters  
Physical Chemical Properties  
Environmental Fate and Transport  
Ecotoxicological Information  
Human Health Hazards  
Profiling  
Custom

Example Prioritization Scheme (PBT)

P  
vB  
vT

Profiling methods

Options Select All Unselect All Invert

☐ Skin irritation/corrosion  
☐ Empiric  
☐ Chemical elements  
☐ Groups of elements  
☐ Lipinski Rule Oasis  
☐ Organic functional groups  
☐ Organic functional groups (nested)  
☐ Organic functional groups (US EPA)  
☐ Organic functional groups, Norbert Haider (check)  
☐ Structure similarity  
☐ Tautomers unstable  
☐ Toxicological  
☐ Repeated dose (HESS)  
☒ Custom  
☒ Example Prioritization Scheme (PBT)  
☐ Skin sensitisation (US EPA)

Metabolism/Transformations

Profiling results

P  
vB  
vT

Details Close



# Profiling: explanation of "P" prediction

1. Double left-click on the cell with profiling results (1)
2. The **Profiling results** window is displayed (2)
3. Select "P" (4)
4. Click **Details** (5)
5. The PBT scheme is displayed and the query, which gives the prediction is marked (see next slide)

The screenshot displays the QSAR Toolbox interface. On the left, the 'Structure' panel shows a chemical structure and its properties. The 'Profiling' section is expanded, and the 'Custom' sub-section is selected. The 'Example Prioritization Scheme (PBT)' is highlighted. A red box labeled '1' points to the 'P' prediction in the 'Profiling results' window. The 'Profiling results' window is shown in the foreground, with a red box labeled '2' pointing to the 'P' prediction. The 'Details' button is highlighted with a red box labeled '4'. The 'PBT' scheme is shown in the background, with a red box labeled '3' pointing to the 'P' prediction. The 'PBT' scheme is also shown in the background, with a red box labeled '5' pointing to the 'P' prediction.

**Structure**

Filter endpoint tree... 1 [target]

Structure

Structure info

- Additional Ids
- CAS Number
- CAS-SMILES relation
- Chemical name(s)
- Composition
- Molecular formula
- Predefined substance type
- SMILES

Parameters

- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards

Profiling

- Custom
- Example Prioritization Scheme (PBT)

EC Number: 2003490

57-74-9

High

1,2,4,5,6,7,8,8-octachloro-2,...

C10H6Cl8

Mono constituent

C1C1CC2C(C1C)C1(C)C(C)...

Calculated value: -0.267

**Explanation for Example Prioritization Scheme (PBT) -> P**

Categories

Explanation

MetaInfo Table

Definition	Properties	Training Set	Literature
The system collects persistent (P) experimental data in the Toolbox databases and applies BOWIN 5 and BOWIN 6 models using the following criteria for assessment:			
P classification criteria according to the REACH Annex XIII [1]			
Very Persistent (vP): T1/2 > 60 days in marine, fresh or estuarine water (BOD < 30%)			
P: T1/2 > 40 days in fresh or estuarine water (BOD < 40%) or predicted biodegradation probability less than 0.5 (considered as "does not biodegrade fast")			
1. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.11: PBT/vPvB assessment. 2014. <a href="https://echa.europa.eu/documents/10162/13632/inform">https://echa.europa.eu/documents/10162/13632/inform</a>			

Generated from: C:\Program Files (x86)\Common

Profiling results

P

vB

vT

Details

Close

# Profiling: explanation of “P” prediction

Explanation for: Example Prioritization Scheme (PBT) -> P
— □ ×

**Categories**

3 → is it P according to exp. data (no)

→ next → is it B according to exp. data

→ 1 → is it P according to BOWIN models (yes)

**Explanation**

probability=

Calculated value: -0.267

Definition	Properties	Training Set	Literature	MetalInfo Table	Custom Captions	Scheme
The system collects persistent (P) experimental data in the Toolbox databases and applies BIOWIN 5 and BIOWIN 6 models using the following criteria for assessment:						
P classification criteria according to the REACH Annex XIII [1]						
Very Persistent (vP): T <sub>1/2</sub> > 60 days in marine, fresh or estuarine water (BOD < 30%)						
P: T <sub>1/2</sub> > 40 days in fresh or estuarine water (BOD < 40%) or predicted biodegradation probability less than 0.5 (considered as "does not biodegrade fast")						
1. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.11: PBT/vPvB assessment. 2014. <a href="https://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf">https://echa.europa.eu/documents/10162/13632/information_requirements_r11_en.pdf</a>						

Generated from: C:\Program Files (x86)\Common Files\QSAR Toolbox 4.4  
 \Config\AddIns\LMC.Toolbox.Server.Profiling.References\PBT prioritization\persistent.htm

1. The "P" node (1), which criteria are fulfilled, is coloured in green and has a check mark. A yellow border around the node indicates that it is selected and its explanation is displayed in the Literature panel (2).
2. The nodes, which criteria are not fulfilled are colored in red and marked with "X" sign (3).

# Profiling: explanation of "P" prediction

1. Click **Definition** tab (1).
2. A red circle around the query indicates that it is selected (2).
3. The selected query is a parametric query, which content is shown in the **Parameter query** tab (3).
4. Biodegradation probability (Biowin 5) model is incorporated in that query (4). The predicted outcome has to be below 0.5 (5) in order for the requirements to be fulfilled. Once finish with examination of the boundary the window could be closed (6)

The screenshot displays the QSAR Toolbox interface for explaining a prediction. The 'Definition' tab is selected (1). The 'Categories' panel shows a tree structure where the query 'is it P according to exp. data' is highlighted with a red circle (2). The 'Category tree' panel shows the selected query 'is it P according to BIOWIN models' (3). The 'Parameter query' tab is active, showing the 'Biodegradation probability (Biowin 5)' model (4). The 'Expression' field is set to '< 0.5' (5). The 'Calculated value' is -0.267 (6).

# Profiling: explanation of "vB" prediction

1. Select "vB" from the opened **Profiling results** window
2. (4).
3. Click **Details** (5).
6. The PBT scheme is displayed and the query, which gives the prediction is shown (see next slide)

The screenshot displays the QSAR Toolbox Profiling window. On the left, a tree view shows the 'Profiling' section expanded, with 'Custom' selected. The 'Example Prioritization Scheme (PBT)' is visible. The main panel shows the chemical structure of 1,2,4,5,6,7,8,8-octachloro-2,3-dibenzodioxin (EC Number: 2003490) and its properties. The 'Profiling results' window is open, showing a list of predictions: 'p', 'vB', and 'vT'. The 'vB' prediction is highlighted. A red box labeled '1' points to the 'vB' prediction. A red box labeled '2' points to the 'Details' button at the bottom of the 'Profiling results' window. A red arrow points from the 'vB' prediction to the 'Details' button.

Filter endpoint tree... 1 [target]

Structure

Structure info

- Additional Ids
- CAS Number
- CAS-SMILES relation
- Chemical name(s)
- Composition
- Molecular formula
- Predefined substance type
- SMILES

Parameters

- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards

Profiling

- Custom

Example Prioritization Scheme (PBT)

EC Number: 2003490

57-74-9

High

1,2,4,5,6,7,8,8-octachloro-2,3-dibenzodioxin

C10H6Cl8

Mono constituent

C1C1CC2C(C1Cl)C1(Cl)C(Cl)C(Cl)C(Cl)C(Cl)C1

Profiling results

- p
- vB**
- vT

Details

Close

# Profiling: explanation of "vB" prediction

1. The node, which criteria are fulfilled is green colored and marked with "✓" sign (1).
2. Here it is a node containing experimental data. The logic implemented in the PBT scheme implies that if the target chemical has experimental data (in this case vB) then the consecutive nodes from the bioaccumulation assessment are not run. Hence they are colored in grey (2).
3. All experimental data available for the target chemical is listed in the **Explanation** panel(3). The unit is L/kg.

Explanation for: Example Prioritization Scheme (PBT) -> vB

**Categories**

is it vB according to exp. data (1) ✓

is it B according to exp. data (2)

is it vT according to exp. data (3) ✓

**Explanation**

Result  
Evaluation result: True

All values

Details	Mean value	Min value	Max value	Unit (Scale)
970				L/kg
12				L/kg
10.8				L/kg
0.351				L/kg
8.01				L/kg
21				L/kg
16				L/kg
13				L/kg
31				L/kg

**MetalInfo Table**

Definition Properties Training Set Literature

The system collects bioaccumulation (B) experimental data in the Toolbox databases and applies BCFWIN and KOWIN models using the following criteria for assessment:

B classification criteria according to the REACH Annex XIII [1]

- Very Bioaccumulative (vB): BCF > 5000 L/kg (logBCF > 3.699 log (L/kg wet))
- B: BCF > 2000 L/kg (i.e. logBCF > 3.301 in log unit) or log Kow > 4.5

1. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.11: PBT/vPvB assessment. 2014. [https://echa.europa.eu/documents/10162/13632/information\\_requirement](https://echa.europa.eu/documents/10162/13632/information_requirement)

Generated from: C:\Program Files (x86)\Common Files\QSAR Toolbox 4.4\Config\AddIns\LMC.Toolbox.Server.Profiling\References\PBT prioritization\bioaccumulation.htm

# Profiling: explanation of "vB" prediction

Explanation

Result  
Evaluation result: True

All values

Details	Mean value	Min value	Max value	Unit (Scale)
2.44				
4.16				
448				
559				
2.61E+04				

Complete data

Endpoint path	Assigned SMILES	Database	Duration	Mean	70	Endpo
Environmental Fate and Transport Bioaccumulation: aquatic	True	Bioconcentration NITE	Min			BCF
			Max			

2.79E+04

3.78E+04

3

Temperature						
Mean	25	Test organisms (species)	Test specificity	Tissue analyzed	Water type	Year
Min		Cyprinus carpio	wet weight	Whole body	freshwater	1986
Max						

1. Expand the experimental result from the arrow next to the digits (1).
2. By moving the scroll bar (2), you can see all the details of the measured data (3).

# Profiling: explanation of "vT" prediction

1. Double click on the profiling result cell (1).
2. The **Profiling results** window is displayed (2).
3. Select "vT" (3).
4. Click **Details** (4).

The PBT scheme is displayed and the query, which gives the prediction is shown (see next slide).

The screenshot displays the QSAR Toolbox interface. The main panel on the right shows 'Structure info' for a chemical with EC Number 2003490, CAS Number 57-74-9, and Molecular Formula C10H6Cl8. The 'Profiling results' window is open, showing a list of results with 'vT' selected. The 'Details' button is visible at the bottom of the window. Red callout boxes with numbers 1 through 4 indicate the steps described in the text: 1 points to the 'vT' result in the Profiling results window; 2 points to the Profiling results window itself; 3 points to the 'vT' result; and 4 points to the 'Details' button.

# Profiling: explanation of "vT" prediction

1. The node, which criteria are fulfilled is colored green and marked with "✓" sign (1).
2. Here it is a node with experimental data. The logic implemented in the PBT scheme implies that if the target chemical has experimental data (in this case vT) then the consecutive nodes from the toxicity assessment are not run. Hence they are colored in grey (2).
3. All experimental data available for the target chemical is listed in the **Explanation** panel(3). The unit is mg/L or ppb. However only mg/L is considered (see slide 8).

The screenshot displays the 'Explanation for: Example Prioritization Scheme (PBT) -> vT' window. The interface includes a 'Categories' panel with a decision tree, an 'Explanation' panel with a table of values, and a 'Literature' tab with classification criteria.

**Categories Panel:** A decision tree diagram. The root node is 'is it vB according to exp. data' (green, marked with a checkmark). It branches to 'is it B according to exp. data' (grey) if 'no', and to 'is it vT according to exp. data' (green, marked with a checkmark) if 'yes'. The 'is it vT' node branches to 'is it T according to exp. data' (grey) if 'no', and to 'next' (red arrow) if 'yes'. Red callout boxes 1 and 2 point to the green nodes.

**Explanation Panel:** A table titled 'All values' showing experimental data for various parameters. Red callout box 3 points to this table.

Details	Mean value	Min value	Max value	Unit (Scale)
0.115				mg/L
0.0078				mg/L
0.0082	0.0061		0.011	mg/L
0.041	0.035		0.049	mg/L
0.0293				mg/L
0.0249	0.0161		0.0385	mg/L
0.045	0.041		0.049	mg/L
0.016				mg/L

**Literature Tab:** Shows classification criteria according to the GHS [1]. Red callout box 4 points to this tab.

T classification criteria according to the GHS [1]

- Very Toxic (vT):  $LC50 \leq 1 \text{ mg/L}$
- T:  $LC50 > 1 \text{ mg/L} < \text{and} LC50 \leq 10 \text{ mg/L}$

1. Globally Harmonized System of Classification and Labelling of Chemicals (GHS). 2011. [https://www.unece.org/fileadmin/DAM/trans/danger/publi/ghs/ghs\\_rev04/English/ST-SG-AC10-30-Rev4e.pdf](https://www.unece.org/fileadmin/DAM/trans/danger/publi/ghs/ghs_rev04/English/ST-SG-AC10-30-Rev4e.pdf)

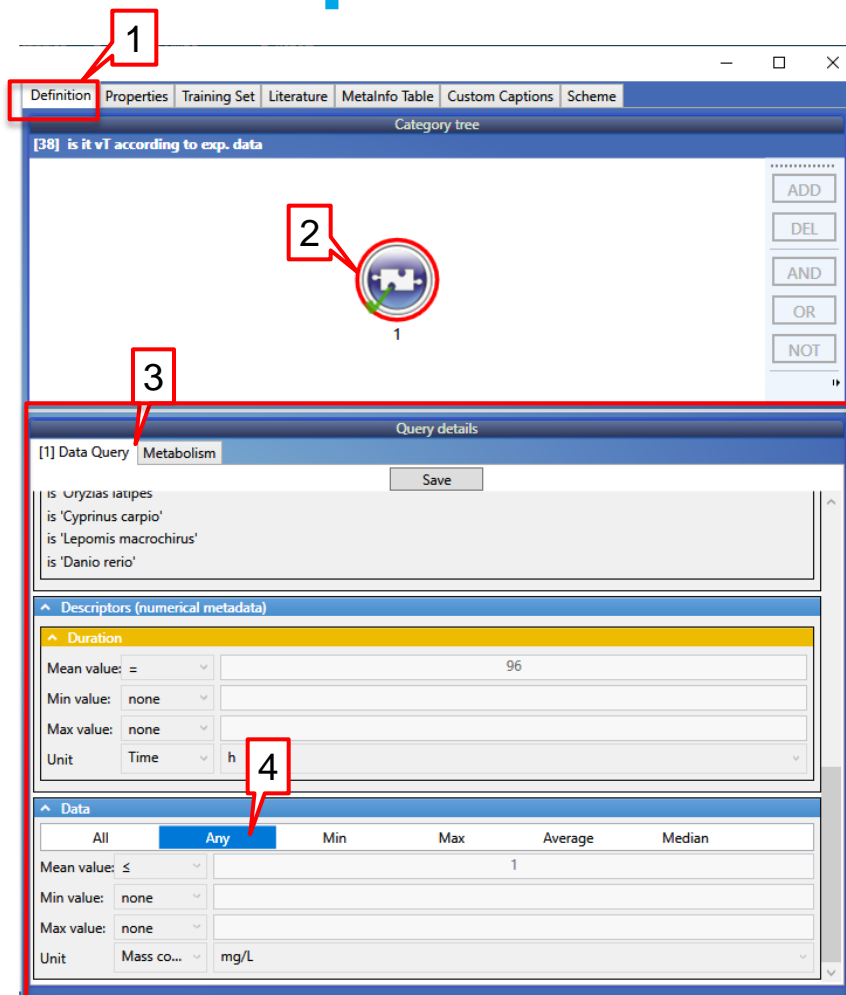
Generated from: C:\Program Files (x86)\Common Files\QSAR Toolbox 4.4\Config\AddIns\LMC.Toolbox.Server.Profiling\References\PBT prioritization\toxic.htm

4. The rules by which experimental data is collected were shown in the *Literature* tab (4).



# Profiling: explanation of “vT” prediction

1. Select **Definition** tab (1).
2. The details of the **Data query** (2), are shown in the Query details panel (3).
3. By moving the scrollbar, you can see the type of metadata included in the query.
4. In this example, the type of experimental data is **Any** (4) meaning that all available data is checked, but only data in mg/L and mean value  $\leq 1$  mg/L is considered.



# Profiling: explanation of "vT" prediction

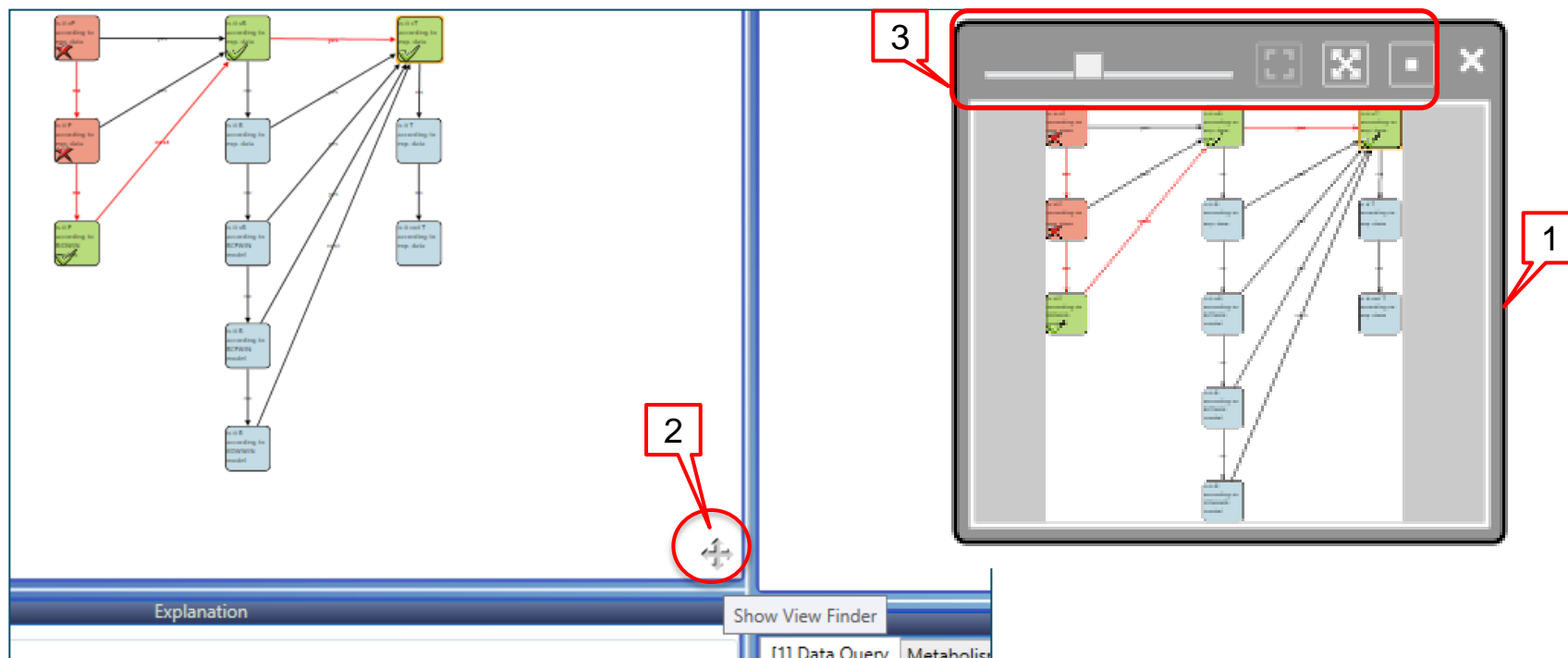
1. Expand the experimental data from the arrow next to the digits (1)
2. By moving the scroll bar (2), you can see all details of the measured data

The screenshot shows the 'Explanation' window in the QSAR Toolbox. It displays the 'All values' section with a table of experimental data. The table has columns for 'Details', 'Mean value', 'Min value', 'Max value', and 'Unit (Scale)'. The 'Details' column contains a list of values, each preceded by a dropdown arrow. The value '0.0029' is highlighted with a red box and labeled with a red '1'. Below this, the 'Complete data' section is visible, showing a table with columns for 'Endpoint path', 'Application freq', 'Assigned SMILES', 'Author', and 'Conc'. The 'Endpoint path' column contains the text 'Ecotoxicological Information Aquatic Toxicity'. The 'Application freq' column contains the value '1'. The 'Assigned SMILES' column contains the value 'True'. The 'Author' column contains the text 'Mayer,F.L.,Jr., and M.R. Ellersieck'. The 'Conc' column contains the value 'Activ'. The 'Complete data' section is also highlighted with a red box and labeled with a red '2'.

Details	Mean value	Min value	Max value	Unit (Scale)
0.077				
0.031				
0.128				
0.0248				
0.062				
0.0234				
0.0029				

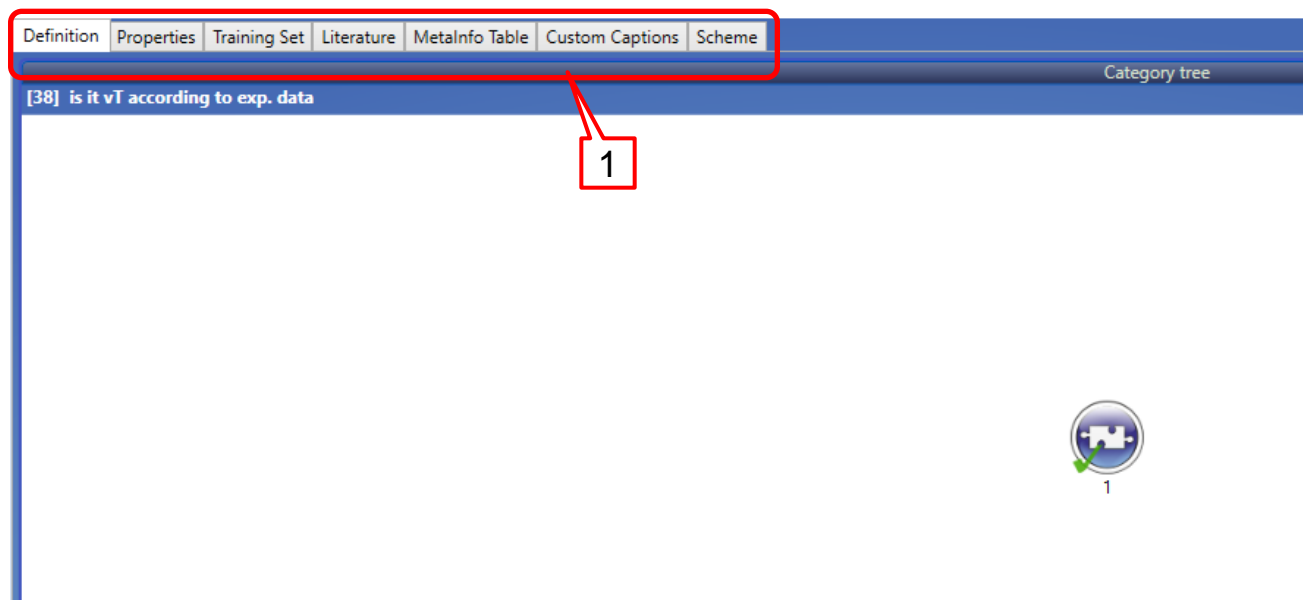
Endpoint path	Application freq	Assigned SMILES	Author	Conc
Ecotoxicological Information Aquatic Toxicity	1	True	Mayer,F.L.,Jr., and M.R. Ellersieck	Activ

# Profiling: common features of PBT interface



1. A **Viewfinder** (1) is displayed by clicking on the cross sign (2).
2. It contains navigation options for viewing the PBT scheme (3).

# Profiling: common features of PBT interface



**Properties**, **Literature** and **Scheme** tabs gives more information about the query (properties), the node(literature) and the developer (scheme) (1).

# Outlook

- Aim
- Keywords
- PBT scheme
  - Background
  - Implementation
- Workflow of the prediction
  - Chemical input
  - Profiling
- **Export of the results**

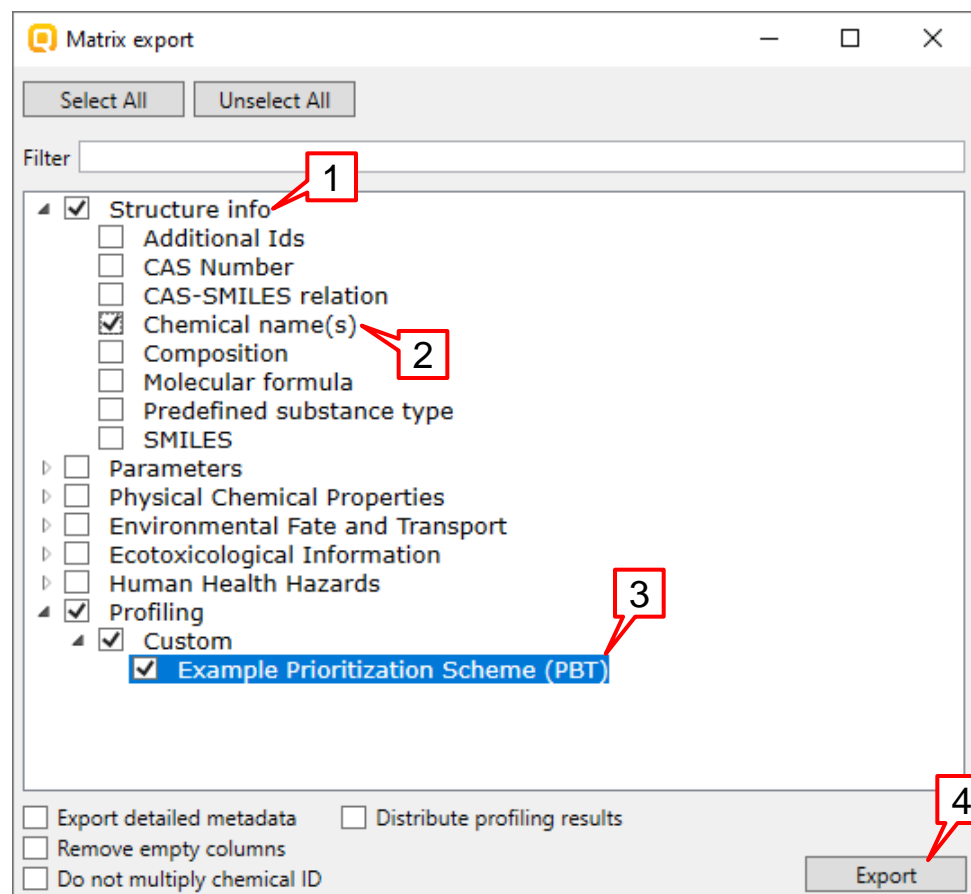
# Export of the results

1. Right click next to the name of the scheme (1)
2. Select **Export Data matrix**

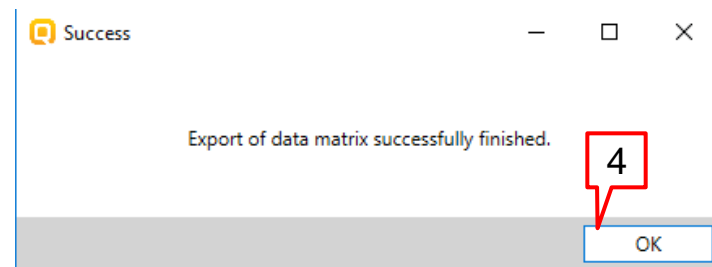
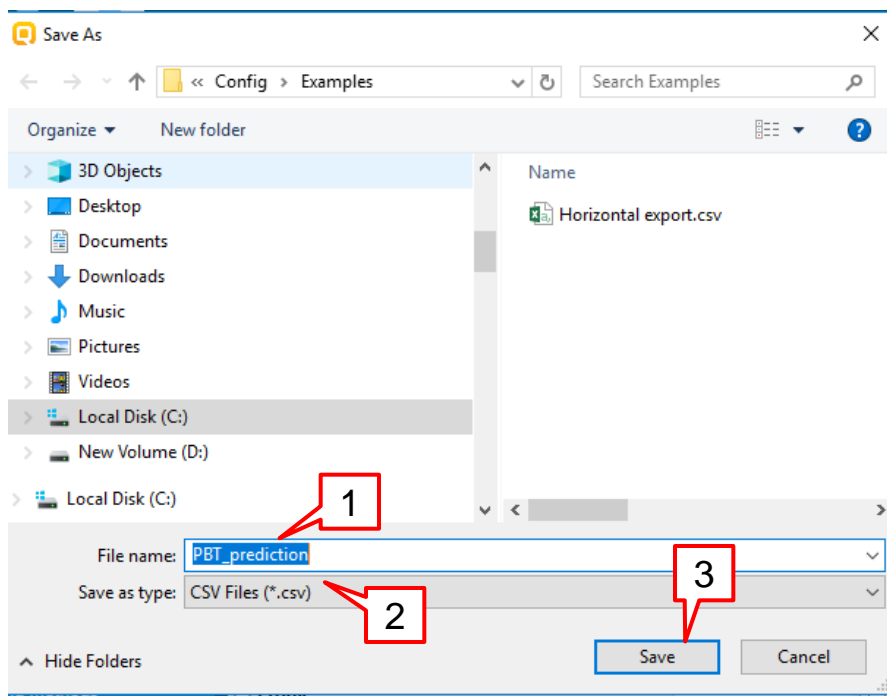
The screenshot displays the QSAR Toolbox software interface. The top navigation bar includes icons for Input, Profiling, Data, Category definition, Data Gap Filling, and Report. Below this, the 'Profiling' and 'Custom profile' tabs are active. The 'Documents' panel on the left lists 'Document 1' and 'Document 2', with 'Document 2' selected. The 'Profiling methods' panel shows a list of methods, with 'Example Prioritization Scheme (PBT)' selected under the 'Custom' category. The 'Metabolism/Transformations' panel is also visible. The main workspace shows a 'Filter endpoint tree...' and a 'Structure' panel. A right-click context menu is open over the 'Example Prioritization Scheme (PBT)' entry, with the 'Export Data matrix' option highlighted. Red callout boxes with numbers 1 and 2 point to the 'Example Prioritization Scheme (PBT)' entry and the 'Export Data matrix' option, respectively.

# Export of the results

1. Expand structure info (1) and check **Chemical name(s)** (2).
2. **Example Prioritization Scheme (PBT)** is selected by default (3).
3. Click **Export** (4).



# Export of the results



1. Type in the name of the file (1).
2. The files are only saved in .csv format(2).
3. Click **Save** (3).
4. Click **OK** in the confirmation message (4).



## Export of the results

6					
A	B	C	D	E	F
#	CAS Number	Chemical name(s)	SMILES	Example Prioritization Scheme (PBT)	
1	57-74-9	1,2,4,5,6,7,8,8-oct	<chem>ClC1CC2C(C1Cl)C1(Cl)C(Cl)=</chem>	P;vB;vT	
0 chemical(s) were marked private and not exported.					

The file can be open as an Excel sheet.