QSAR TOOLBOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

User manual

Database Import Wizard

Document history

Version	Comment
Version 1.0	Database Import Wizard for version 2.1 of the QSAR Toolbox

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Language: English

If you have questions or comments that relate to this document, please send them to ehscont@oecd.org or visit the QSAR Toolbox discussion forum at https://community.oecd.org/community/toolbox_forum

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1 Executive summary

The QSAR Toolbox Database Import Wizard, together with the IUCLID 5 import wizard (see guidance document "IUCLID 5 Import/Export via Webservices"), is the entry point for importing custom user data to the QSAR Toolbox database. It can import XLS files (Excel 97-2003 version) as well as TXT (UNICODE) plain text files. Both file types pertain to how the data is read by QSAR Toolbox, but not how the data is parsed afterwards.

2 QSAR Toolbox data model

The QSAR Toolbox operates with the following data model:

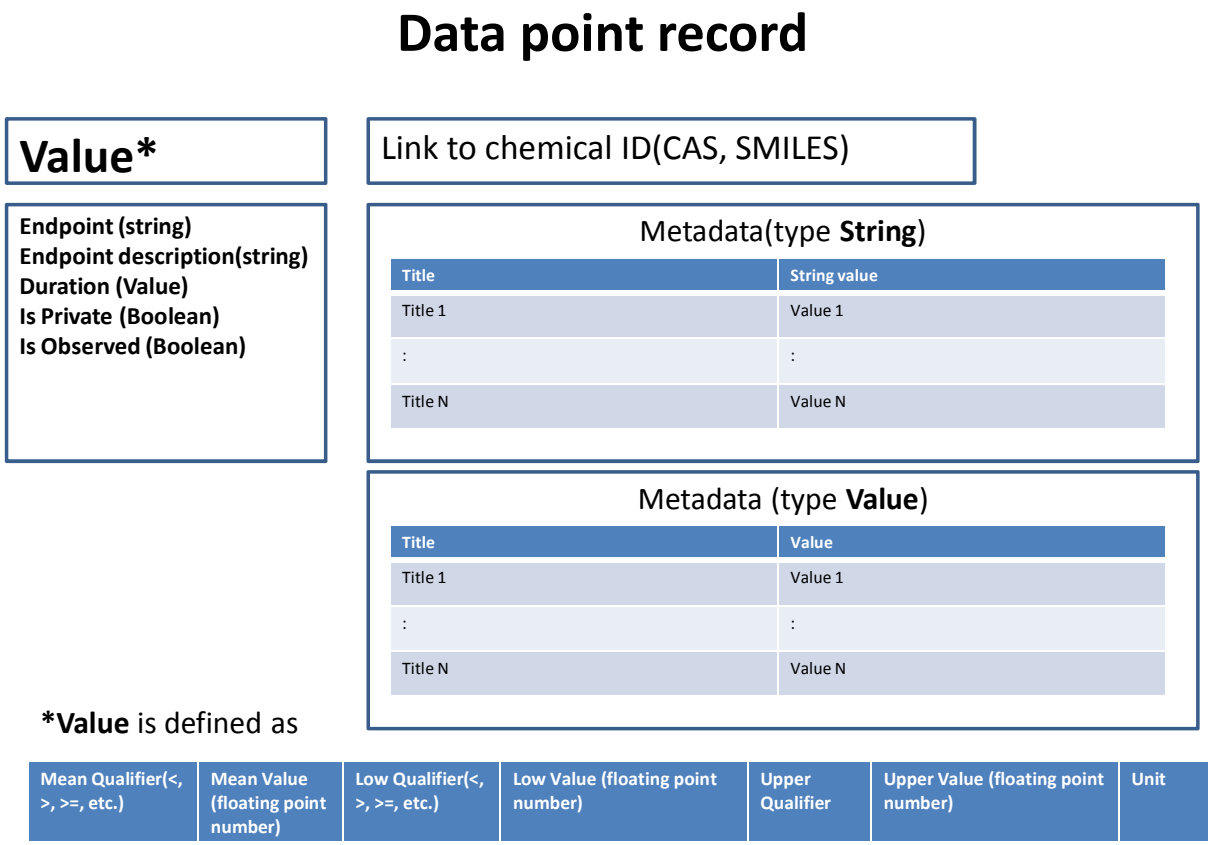


Figure 1: Database structure of the QSAR Toolbox

The Import's function is to translate the information in a file (be it XLS or TXT), separate it in different chunks (see the figure above) and write them into the database. The information consists of the chemical connected with numerical and meta-data. In other words the point of the import is to define a list of data points (the number that the user sees in the data-matrix and uses for gap-filling) with its corresponding metadata, namely the additional information on duration, test organisms, endpoint etc. In order to properly parse the information the import expects one of two file layouts as outlined below.

3 Import layouts

The two layouts the QSAR Toolbox can parse are the so called Vertical layout and the Horizontal layout. The Horizontal layout has each data point, with its corresponding **chemical** and **metadata**, defined in a single row. In a way each **row is a single record** (hence "horizontal"). The Vertical layout on the other hand can have **multiple records on each row** with the metadata for each record defined on a **column by column basis** (hence "vertical").

3.1 Vertical layout

This layout is used where there is a list of chemicals and a result for each chemical, but all results have the same metadata. So the chemical is defined in the first columns, and the next columns are used for the data points. For each data column there is one set of metadata. This means the vertical layout can import multiple values for a chemical.

	A	B	C	D	E
1	**CAS**	**NAME**	**SMILES**	**Experiment 1**	**Experiment**
2	CAS# 1	NAME 1	SMILES 1	Value 1	Value 1
3	CAS# 2	NAME 2	SMILES 2	Value 2	Value 2
4					
5					
6	CAS# K	NAME K	SMILES K	Value K	Value K

Figure 2: Vertical layout

Figure 2 illustrates the format of an XLS file for import. The first three columns represent the chemical identity information and column D and E represent results from two different "experiments" (a package of metadata such as Organ, Duration, Temperature, Dose, Species, Endpoint etc.).

3.2 Horizontal layout

This layout is used when each data point is defined in a row. Here the user specifies in which column is the data, the metadata and the type of metadata.

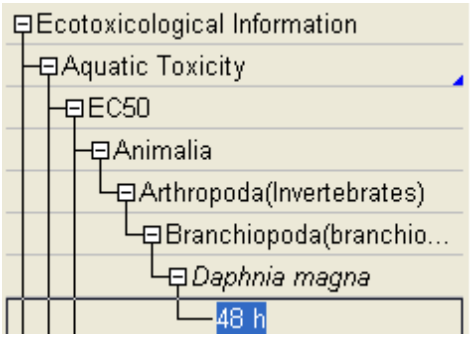
	A	B	C	D	E	F	G	H
1	**CAS**	**NAME**	**SMILES**	**Param descriptor 1**	**Param descriptor 2**		**Param descriptor N**	**VALUE**
2	CAS# 1	NAME 1	SMILES 1	Param descriptor value [1,1]	Param descriptor value [2,1]		Param descriptor value [1,1]	Value 1
3	CAS# 2	NAME 2	SMILES 2	Param descriptor value [1,2]	Param descriptor value [2,2]		Param descriptor value [1,2]	Value 2
4								
5								
6	CAS# K	NAME K	SMILES K	Param descriptor value [1,K]	Param descriptor value [2,K]		Param descriptor value [2,K]	Value K

Figure 3: Horizontal layout

Figure 3 shows how an XLS file could look like for horizontal import. Each row defines a record in its entirety. At import time the user specifies which columns contain chemical identity data (CAS, Name, SMILES), which columns contain the Value (the result that is seen in the Data-matrix and used for Data-gap filling) and which columns contain the metadata (e.g. Organ, Duration, Temperature, Dose, Species, Endpoint etc.).

4 Endpoint tree path

When a data point is imported into the QSAR Toolbox, the database engine needs to assign it to a leaf node in the endpoint tree. However, the way the endpoint tree is constructed differs significantly from version 1.1 of the QSAR Toolbox. For the user the tree looks similar in both versions, but the underlying logic has changed.



In Toolbox 1.1

This would be a **predefined** endpoint tree to the leaves of which the data is assigned.

In Toolbox 2.0

This has two components. **Predefined** part (Ecotoxicological Information#Aquatic Toxicity). **Dynamic** part (EC50#Animalia#Arthropoda(Invertebrates)#Branchiopoda(branchiopods)#Daphnia magna#48 h)

Figure 4: Endpoint tree in Toolbox version 1.1 vs. Endpoint tree in QSAR Toolbox version 2.0

In Toolbox 1.1 the tree displayed in the data-matrix was predefined and data could be imported to any of its leaves. In the QSAR Toolbox 2.0 however the data-matrix displays not only the **predefined** part of the endpoint tree but also builds a dynamic part based on the metadata of the currently displayed data points and/or QSARs.

To check which part is predefined and which part is dynamic press the Ctrl key and the predefined part of the tree will be underscored.

5 Building the dynamic tree

The dynamic tree is a feature of the QSAR Toolbox where the endpoint tree is expanded with nodes that organize the data point's metadata. In essence it is a way to visualize the data the user has gathered from the database. The data is assigned to a path (what we call **predefined** path). The **dynamic** part of the tree is a function of the data point's metadata. It is an instruction that the user has given to the QSAR Toolbox software requiring that the data point's metadata are connected with metadata fields in a specific order. The metadata fields and their hierarchy are called the **Set tree hierarchy** feature.

It is important to make the distinction between what is the data point's **endpoint tree path** and on what node the data point is displayed on the data-matrix. The first one is an immutable attribute of the data point, and the latter is an undefined path that is build at runtime based on the **endpoint tree path**, the loaded data point's metadata and the current settings of the **Set tree hierarchy** feature.

How does the above pertain to the import?

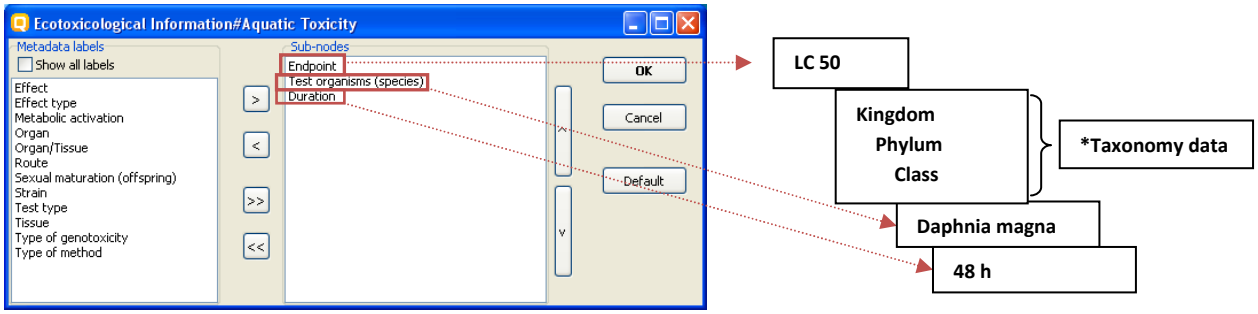
All the **Aquatic Toxicity** data in the QSAR Toolbox is assigned to the **Ecotoxicological Information#Aquatic Toxicity** path. However, when the user installs the QSAR Toolbox and loads data for aquatic toxicity, the entire tree path is shown, for example: **Ecotoxicological Information#Aquatic Toxicity#LC50#Animalia#Arthropoda(Invertebrates)#Branchiopoda(branchiopods)#Daphnia magna#48 h**

Where do the other fields come from?

The other fields come from the data point's metadata. The metadata fields build the dynamic part of the endpoint tree - **LC50#Animalia#Arthropoda(Invertebrates)#Branchiopoda(branchiopods)#Daphnia magna#48 h**.The data point itself is associated to the shallow (**predefined** part) of the tree - **Ecotoxicological Information#Aquatic Toxicity**.

Ecotoxicological Information — **Predefined part**
Aquatic Toxicity
LC50
Animalia
Arthropoda(Invertebrates) — **Dynamic part**
Branchiopoda(branchiopods)
Daphnia magna
48 h

When a data point is read from the database and needs to be displayed to the data-matrix, the tree is expanded to display the metadata of the data points (**Set tree hierarchy** feature):



***Taxonomy data – A large diversity of species has been stored and organized in Toolbox Taxonomy library including more than 12,295 biological species. Species have been distributed in five kingdoms: Animalia, Plantae, Fungi, Protozoa and Monera. Biological information is organized in the following taxa: Kingdom/Phylum/Class. Scientific information is associated automatically to each of the biological species.**

Figure 5: Endpoint tree hierarchy

The QSAR Toolbox has default settings regarding which metadata is displayed. The default fields used are Endpoint, Duration, Test organisms (species), Effect, Effect type, Metabolic activation, Sexual maturation (offspring), Strain, Test type, Type of genotoxicity, Type of method, Tissue, Organ, Route. The list with default fields pertains to the whole endpoint tree. For **Ecotoxicological Information#Aquatic Toxicity** the default hierarchy is **Effect#Endpoint#Duration#Test organisms (species).**

Table 1: Examples of metadata field values

Metadata field	Examples of metadata field values
Endpoint	LC 50,EC10, EC 50, LOEL, NOEL, Skin sensitisation, Carcinogenicity, Ames, Chromosomal aberration, Estrogen receptor binding….
Duration	years, months, days, hours, minutes, seconds…
Test organisms (species)	Daphnia magna, Lepomis symnetricus, Oncorhynchus mykiss, Poecilia reticulata, Tetrahymena pyriformis….
Effect	Immobilization, Mortality, Reproduction….
Effect type	Maternal toxicity, Developmental toxicity, Fetotoxicity, Embryotoxicity
Metabolic activation	with S9, without S9, no S9 info, with and without
Sexual maturation (offspring)	Male, Female, Male/Female…
Strain	TA 98, TA 100, TA 104, New Zealand White, Swiss, Fischer 344/DuCrj
Test type	bacterial reverse mutation assay (e.g. Ames test), in vitro mammalian cell micronucleus test, bacterial gene mutation assay, acute, subacute, chronic, developmental, static, semi-static, flow-through
Type of genotoxicity	Gene mutaion, Chromosomal aberration, DNA damage and/or repair, genome mutation
Type of method	in vivo, in vitro, other
Organ	Lung, Liver
Route	oral, inhalation, dermal, implantation, intramuscular, intraperitoneal

This means that if a user wants to have a consistent display of the endpoint tree, he/she must import the metadata to the aforementioned fields before defining additional fields. For instance the above long path has two components – predefined and dynamic:

- Predefined: **Ecotoxicological Information#Aquatic Toxicity**
- Dynamic:**LC50#Animalia#Arthropoda(Invertebrates)#Branchiopoda(branchiopods)#Daphnia magna#48 h**

In the Import wizard these two translate to **Endpoint tree path** (Figure 5) and metadata (Figure 6). The **Animalia#Arthropoda(Invertebrates)#Branchiopoda(branchiopods)** part is a separate feature in which Kingdom#Phylum#Class information is inserted before the field **Test organisms (species)**. In this respect the user should take extra caution to import species information to the **Test organisms (species)** metadata field.

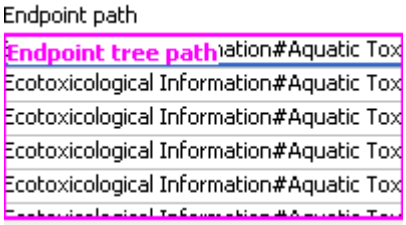


Figure 5: Endpoint tree path

Endpoint	Duration.Mean value/Scale value	Duration.Unit	Test organisms (species)
LC50	48	h	Daphnia magna
LC50	48	h	Daphnia magna
LC50	48	h	Daphnia magna
LC50	48	h	Daphnia magna
LC50	48	h	Daphnia magna
LC50	48	h	Daphnia magna
LC50	48	h	Daphnia magna
LC50	48	h	Daphnia magna
LC50	48	h	Daphnia magna

Figure 6: Metadata

⚠ Metadata information should always be provided for the fields **Test organisms (species), Duration** and **Endpoint**.

6 Running the import wizard

The import wizard is organised in a three step process:

First step (Figure 7**)**: The first window of the import wizard outlines the open file control [1], the file review pane [2], database name edit box[3], the used decimal and thousands separators and the import as inventory check box. It is very important that the thousands and decimal separators are properly set while importing. Especially with TXT file this could lead to erroneous parsing of results.

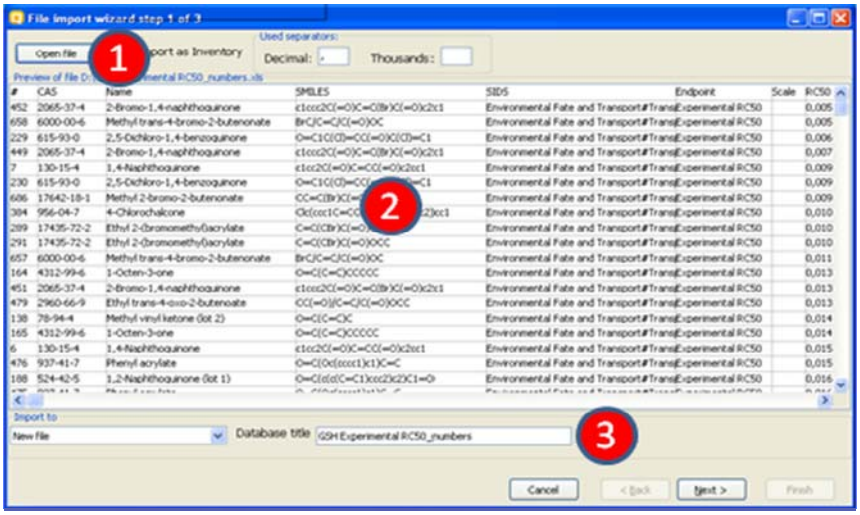


Figure 7: Import wizard step one

Second step: During the second step, the file's layout is selected which leads to two separate code paths, vertical or horizontal.

6.1 Vertical

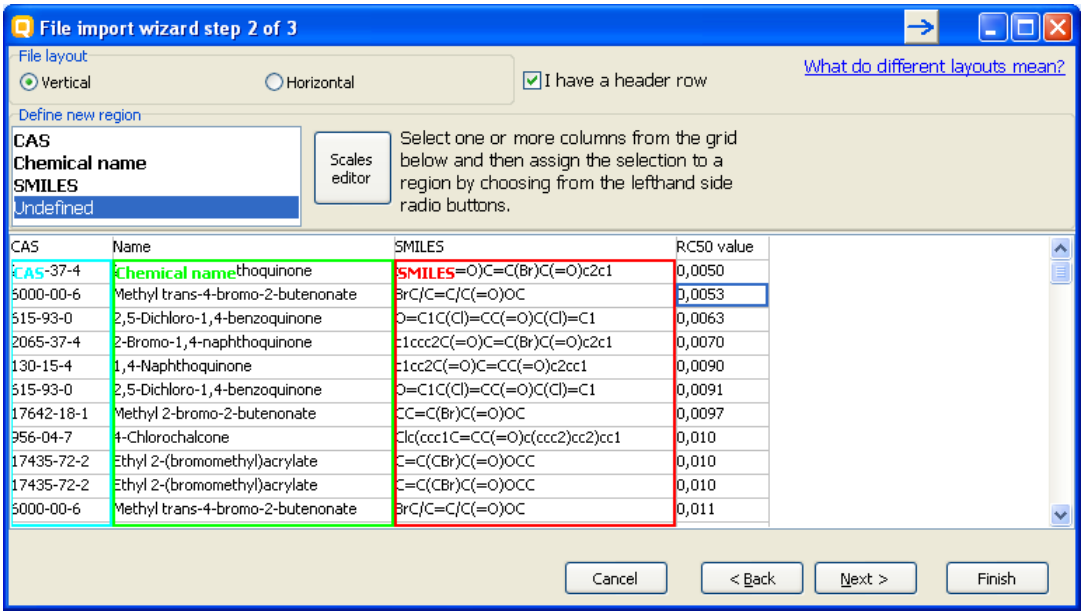


Figure 8: Import wizard step 2 (vertical import)

The second step window (Figure 8) contains the **CAS**, **Chemical name** and **SMILES** columns. Here is also a button that invokes the Scales definitions editor in case the user wants to import categorical data that has no available scale.

⚠ The type of the column is specified by clicking on the column and then selecting its type (CAS/Chemical name/SMILES) from the list box above. To remove designations click a column and then click on **Undefined** from the list box.

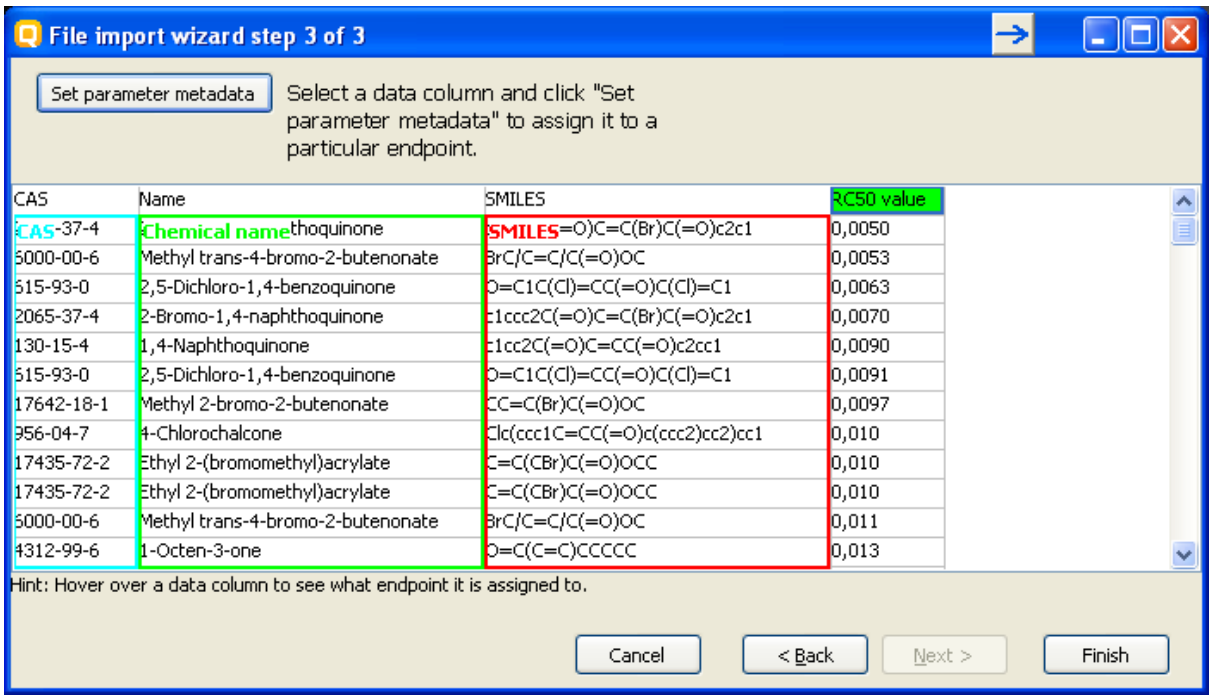


Figure 9: Import wizard step 3 (vertical import)

The third step of the vertical import (Figure 9) is where the user specifies the meaning of the different results columns. In the example above it is only one (RC50 value), but the import can handle multiple columns at once. To set the column metadata double-click on the column or click on the column and press "**Set parameter metadata**". This will bring up the metadata editor (Figure 10).

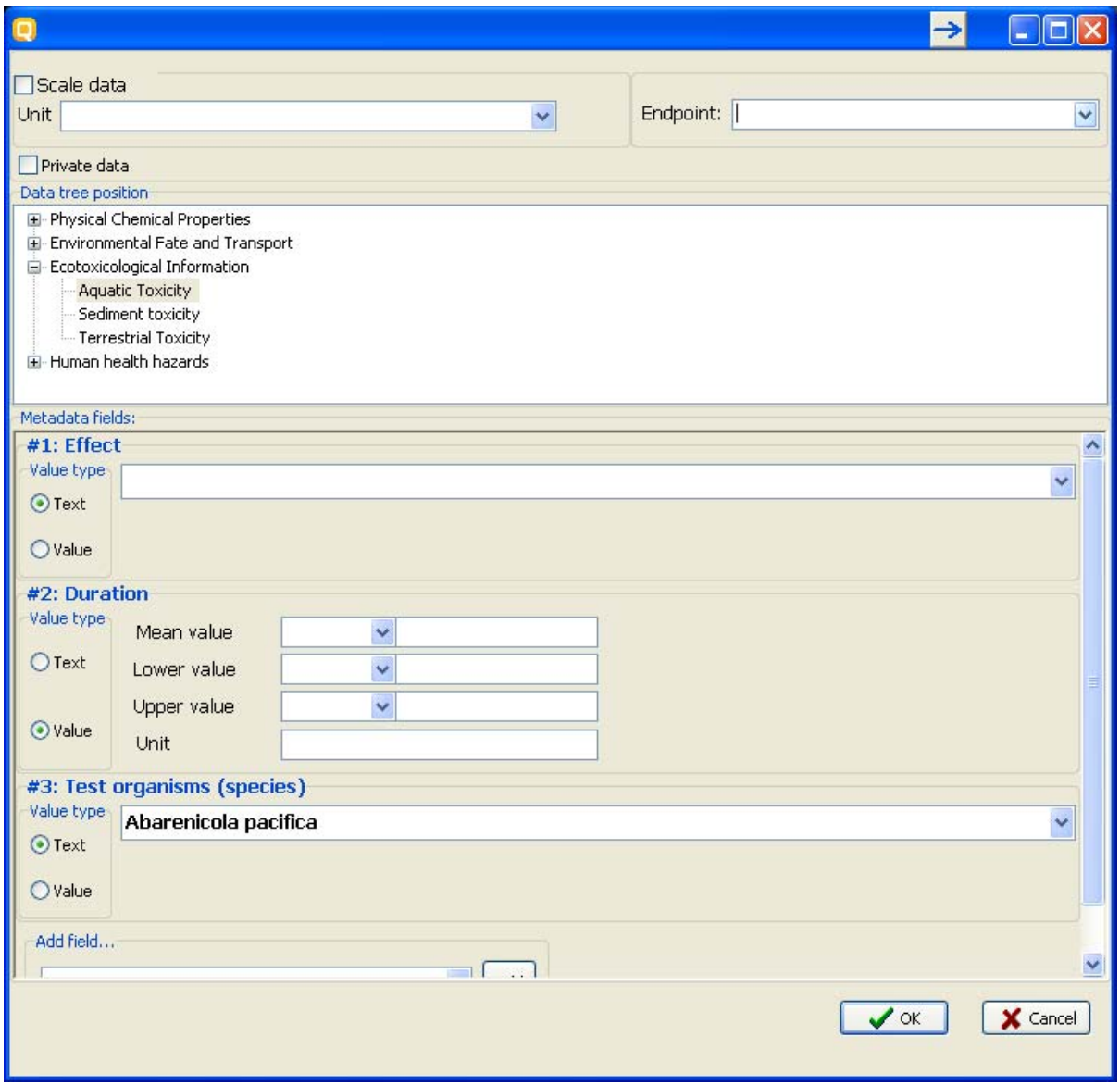


Figure 10: Metadata editor

The most important part of the metadata setup is setting the "**Data tree position**" it should be a leaf from the displayed endpoint tree. If the column contains categorical data the user should check the "**Scale data**" checkbox and specify the Scale for the values in the column.

In the "**Metadata fields**" panel the user can enter a list of the metadata for the data point. There are two types of metadata "**Text**" and "**Value**". The first is a

simple string while the latter is a **Mean/Lower value/Upper value** combination.

⚠ The Vertical import imports the data column without qualifiers and only to the **Mean** part of the data point record. If the user wants to enter qualified numbers or Mean/Low/Max combinations it is recommended to use the **Horizontal layout**.

After all metadata is set for all columns the user should press **Finish**. After the process is finished, an "**Import successful**" message will be displayed and the wizard will close.

6.2 Horizontal

The **Horizontal** layout is selected from a radio-button group in the second step of the import. There are basically two things the user can define, marked (1) and (2) in figure 11 below.

First, in the "**Define new region**" panel are the **CAS**, **NAME**, **SMILES**, **Endpoint tree path** and **Data** items. When they are defined the minimum is met.

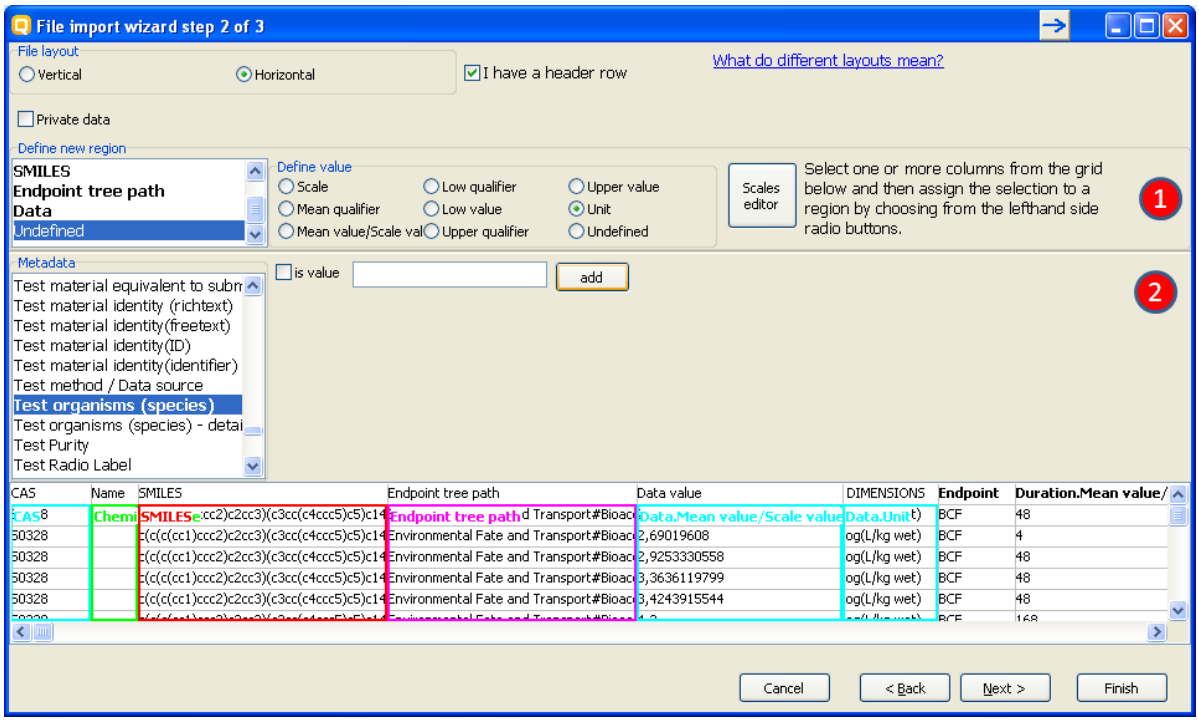


Figure 11: Import wizard step 2 (horizontal import)

⚠ The type of the column is specified by clicking on the column and then clicking its type (CAS/Chemical name/SMILES) from the list box in the **Define new region** panel or selecting a metadata field label from the list box in the **Metadata** panel. To remove designations click a column and then click on **Undefined** from the list box.

The definition of the **Data** region has its particularities. The data-record can contain categorical data - which would require two columns, one for the Scale, and one for the Value of the record. On the other hand the data-record can contain a value – which in the QSAR Toolbox is a packet of Mean/Min/Max value plus corresponding qualifiers and a Unit. These two are combined in the **Define value** panel, part of the **Define new region** panel.

⚠ When defining the data record the user should define:

I. **For categorical data** – **Scale** column for the scale name. This should contain a name of a scale **exactly** as defined in the scales list in the QSAR Toolbox database. The **Mean value/Scale value** column should contain a value that is **exactly** one of the scale's members

II. **For value data –** At least one column for the **Mean/Min/Max** values. Qualifiers and Unit are optional

Second is the "**Metadata**" panel. The data there is not mandatory for the import but can be used to import additional data to the data value. Defining numerical metadata is just like the data-record value definition process.

The third stage of the horizontal import is for review purposes. It is recommended that the user should look again at each column that is to be imported. The data record regions will be marked with color and text. The metadata fields are marked with a bold text over the first row for each column. The metadata of type value will be marked with <name of metadata>.<data_subtype> (for example "**Duration.Units**").

Where all columns are set and double-checked, the user should press **Finish**. After the process is finished, an "**Import successful**" message will be displayed and the wizard will close.

Appendix I: Preparing a file for horizontal import

File layout

A file prepared for import should follow the layout as shown in chapter 3.

Horizontal layout - this layout is used when the file is in the form where a row defines a single data point. Here the user specifies which column is the data, which column is metadata and the type of metadata.

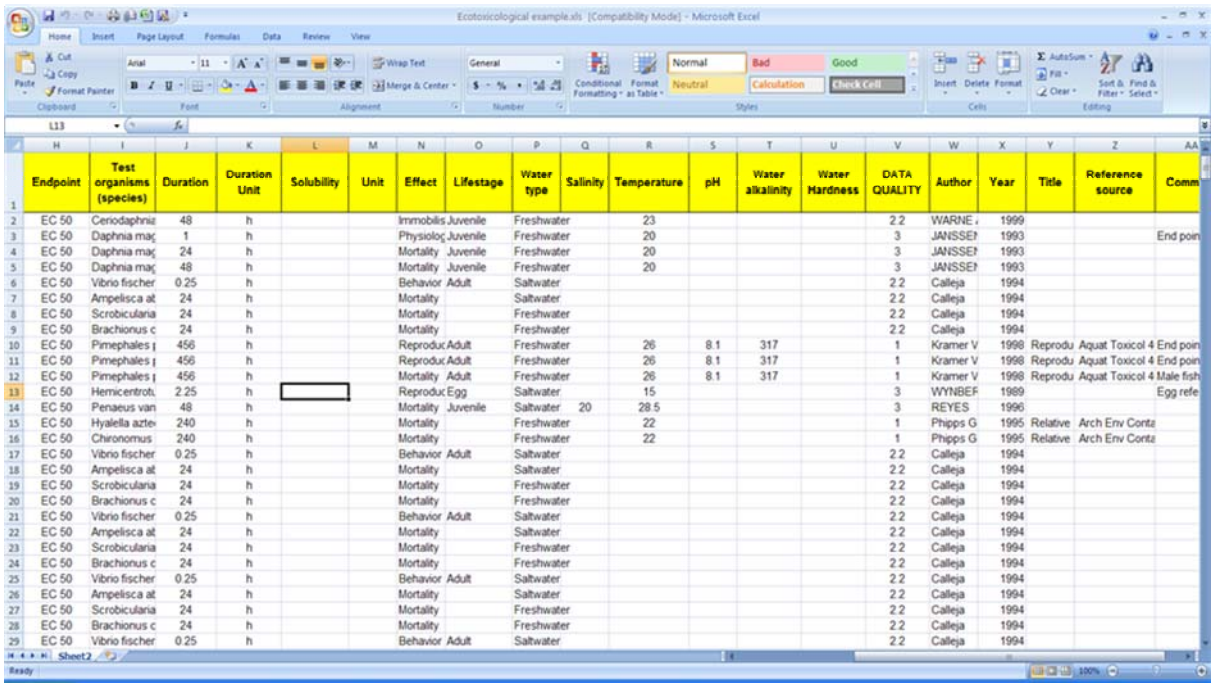
	A	B	C	D	E	F	G	H
1	**CAS**	**NAME**	**SMILES**	**Param descriptor 1**	**Param descriptor 2**		**Param descriptor N**	**VALUE**
2	CAS# 1	NAME 1	SMILES 1	Param descriptor value [1,1]	Param descriptor value [2,1]		Param descriptor value [1,1]	Value 1
3	CAS# 2	NAME 2	SMILES 2	Param descriptor value [1,2]	Param descriptor value [2,2]		Param descriptor value [1,2]	Value 2
4								
5								
6	CAS# K	NAME K	SMILES K	Param descriptor value [1,K]	Param descriptor value [2,K]		Param descriptor value [2,K]	Value K

Figure 1. File layout for horizontal import

Figure 1 illustrates the format of an XLS file for horizontal import. Each row defines a record in its entirety. At import time the user specifies which columns has chemical identity information (CAS, Name, SMILES), which columns contain the values (what is seen in the Data-matrix and used in Data-gap filling) and which columns contain the metadata (Organ, Duration, Temperature, Dose, Species, Endpoint etc.).

Horizontal example – compact view

Ecotoxicological example



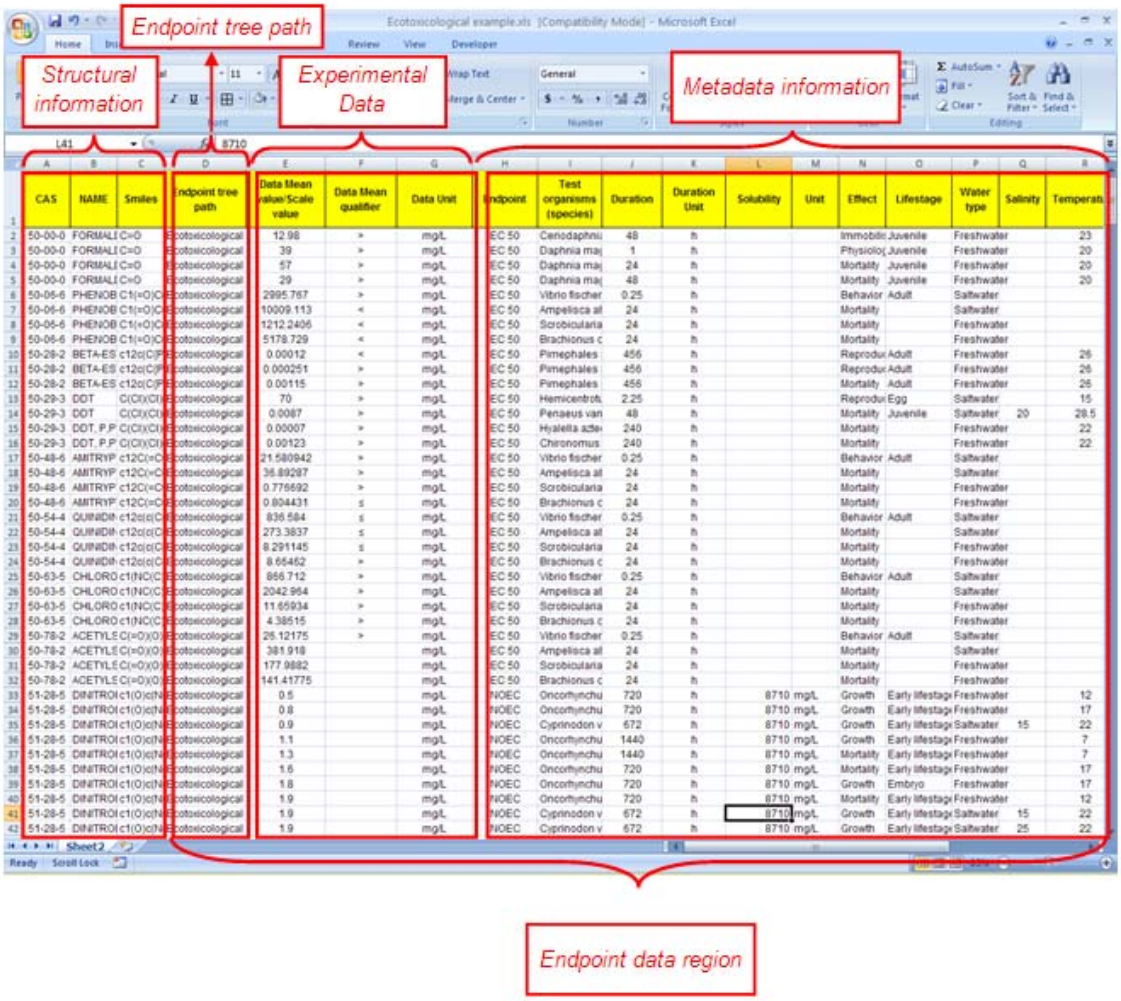
	Endpoint	Test organisms (species)	Duration	Duration Unit	Solubility	Unit	Effect	Lifestage	Water type	Salinity	Temperature	pH	Water alkalinity	Water Hardness	DATA QUALITY	Author	Year	Title	Reference source	Comm
2	EC 50	Ceriodaphnia	48	h			Immobilis	Juvenile	Freshwater		23				2 2	WARNE	1999			
3	EC 50	Daphnia mag	1	h			Physiolog	Juvenile	Freshwater		20				3	JANSSEN	1993			End poin
4	EC 50	Daphnia mag	24	h			Mortality	Juvenile	Freshwater		20				3	JANSSEN	1993			
5	EC 50	Daphnia mag	48	h			Mortality	Juvenile	Freshwater		20				3	JANSSEN	1993			
6	EC 50	Vibrio fischer	0.25	h			Behavior	Adult	Saltwater						2 2	Calleja	1994			
7	EC 50	Ampelisca at	24	h			Mortality		Saltwater						2 2	Calleja	1994			
8	EC 50	Scrobicularia	24	h			Mortality		Freshwater						2 2	Calleja	1994			
9	EC 50	Brachionus c	24	h			Mortality		Freshwater						2 2	Calleja	1994			
10	EC 50	Pimephales p	456	h			Reproduc	Adult	Freshwater		26	8.1	317		1	Kramer V	1998	Reprodu	Aquat Toxicol 4	End poin
11	EC 50	Pimephales p	456	h			Reproduc	Adult	Freshwater		26	8.1	317		1	Kramer V	1998	Reprodu	Aquat Toxicol 4	End poin
12	EC 50	Pimephales p	456	h			Mortality	Adult	Freshwater		26	8.1	317		1	Kramer V	1998	Reprodu	Aquat Toxicol 4	Male fish
13	EC 50	Hemicentrotu	2.25	h			Reproduc	Egg	Saltwater		15				3	WYNBEF	1989			Egg refe
14	EC 50	Penaeus van	48	h			Mortality	Juvenile	Saltwater	20	28.5				3	REYES	1996			
15	EC 50	Hyalella azte	240	h			Mortality		Freshwater		22				1	Phipps G	1995	Relative	Arch Env Conta	
16	EC 50	Chironomus	240	h			Mortality		Freshwater		22				1	Phipps G	1995	Relative	Arch Env Conta	
17	EC 50	Vibrio fischer	0.25	h			Behavior	Adult	Saltwater						2 2	Calleja	1994			
18	EC 50	Ampelisca at	24	h			Mortality		Saltwater						2 2	Calleja	1994			
19	EC 50	Scrobicularia	24	h			Mortality		Freshwater						2 2	Calleja	1994			
20	EC 50	Brachionus c	24	h			Mortality		Freshwater						2 2	Calleja	1994			
21	EC 50	Vibrio fischer	0.25	h			Behavior	Adult	Saltwater						2 2	Calleja	1994			
22	EC 50	Ampelisca at	24	h			Mortality		Saltwater						2 2	Calleja	1994			
23	EC 50	Scrobicularia	24	h			Mortality		Freshwater						2 2	Calleja	1994			
24	EC 50	Brachionus c	24	h			Mortality		Freshwater						2 2	Calleja	1994			
25	EC 50	Vibrio fischer	0.25	h			Behavior	Adult	Saltwater						2 2	Calleja	1994			
26	EC 50	Ampelisca at	24	h			Mortality		Saltwater						2 2	Calleja	1994			
27	EC 50	Scrobicularia	24	h			Mortality		Freshwater						2 2	Calleja	1994			
28	EC 50	Brachionus c	24	h			Mortality		Freshwater						2 2	Calleja	1994			
29	EC 50	Vibrio fischer	0.25	h			Behavior	Adult	Saltwater						2 2	Calleja	1994			

Content of file for import:

Any file to be imported should contain:

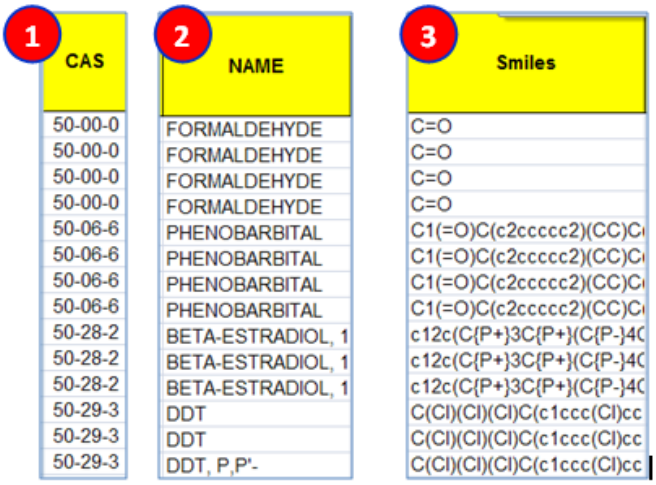
- fields with structural information (chemical identity)
- a field with the Endpoint tree path
- fields with endpoint data information (experimental results and metadata)

⚠ The endpoint tree path should point to a leaf of the **predefined** endpoint tree. For more information check chapter 4: **Endpoint tree path** of this document.



Structural information (chemical identity)

1. CAS field – Column with CAS Registry numbers
2. Name field – Column with Chemical Name(s)
3. SMILES field – Column with SMILES string



1 CAS	2 NAME	3 Smiles
50-00-0	FORMALDEHYDE	C=O
50-00-0	FORMALDEHYDE	C=O
50-00-0	FORMALDEHYDE	C=O
50-00-0	FORMALDEHYDE	C=O
50-06-6	PHENOBARBITAL	C1(=O)C(c2ccccc2)(CC)C(
50-06-6	PHENOBARBITAL	C1(=O)C(c2ccccc2)(CC)C(
50-06-6	PHENOBARBITAL	C1(=O)C(c2ccccc2)(CC)C(
50-06-6	PHENOBARBITAL	C1(=O)C(c2ccccc2)(CC)C(
50-28-2	BETA-ESTRADIOL, 1	c12c(C{P+}3C{P+}(C{P-}4(
50-28-2	BETA-ESTRADIOL, 1	c12c(C{P+}3C{P+}(C{P-}4(
50-28-2	BETA-ESTRADIOL, 1	c12c(C{P+}3C{P+}(C{P-}4(
50-29-3	DDT	C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc
50-29-3	DDT	C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc
50-29-3	DDT, P,P'-	C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc

- Field with Endpoint tree path (*Predefined path*)

Endpoint tree path
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity
Ecotoxicological Information#Aquatic Toxicity

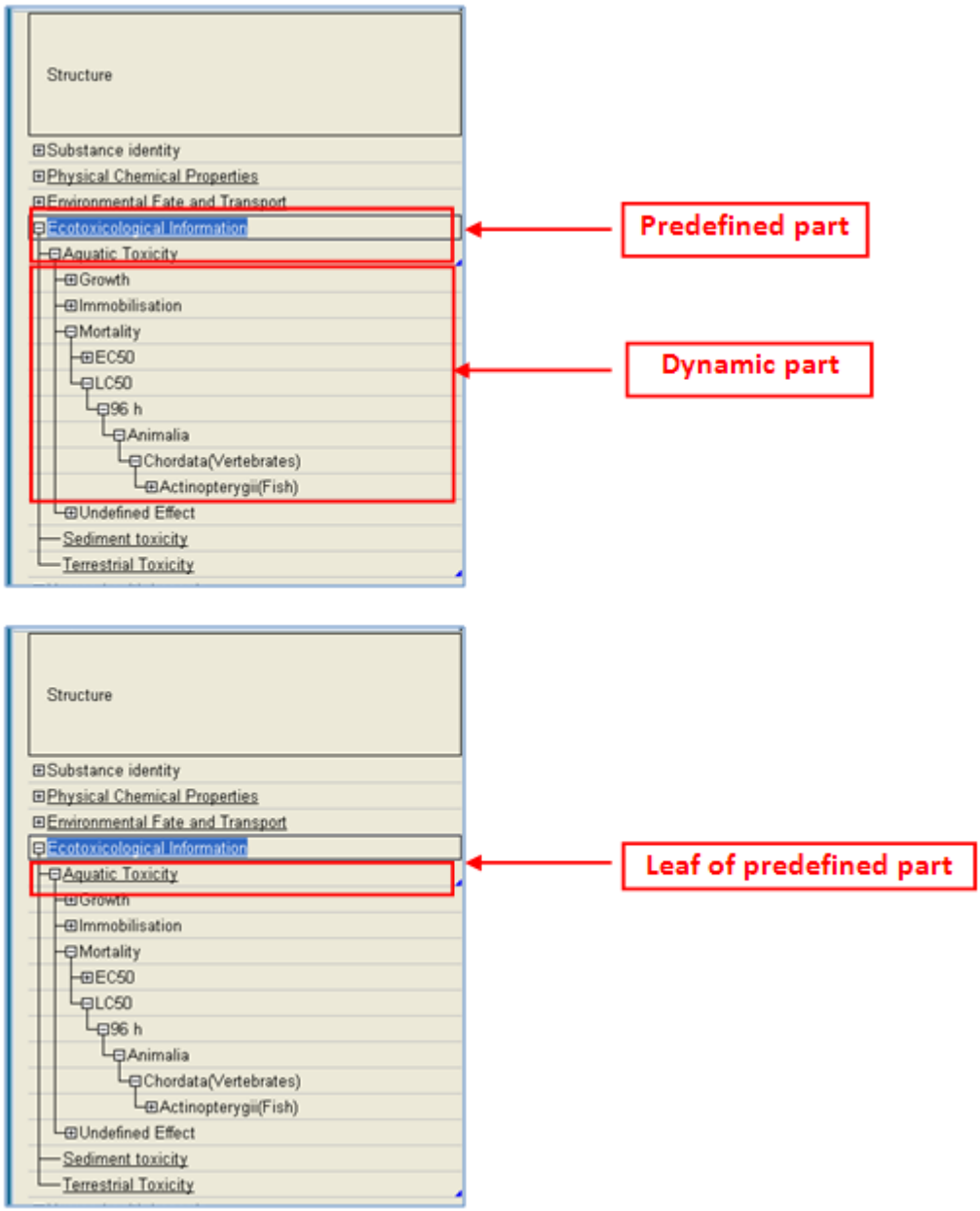
Important: The endpoint tree path should point to a leaf of the **predefined** endpoint tree. For more information check chapter 4 **Endpoint tree path** of this document.

Endpoint tree path

This is a field containing the endpoint tree path related to the endpoint for which experimental data is to be imported. The endpoint tree is separated in a predefined and a dynamic part:

- The predefined part determines the basic structure of the endpoint tree, e.g. substance identity, physical chemical properties, environmental fate and transport, ecotoxicological information, human health hazard.*(ordinary endpoint data is related to this predefined part)*
- The dynamic part of the endpoint tree builds additional layers of the tree depending on the data implemented in the databases. *(ordinary metadata is related to dynamic part)*

Enpoint data is assigned to a predefined part of the endpoint tree, i.e. it is assigned to **a leaf** of the endpoint tree:



The predefined part can be visualized by holding the Ctrl button and clicking on the Endpoint tree. The predefined part of the tree is underlined.

Endpoint data information

The QSAR Toolbox oparates with the following data structure:

Data point record

Value*

Link to chemical ID(CAS, SMILES)

Endpoint (string)
Endpoint description(string)
Duration (Value)
Is Private (Boolean)
Is Observed (Boolean)

Metadata(type **String**)

Title	String value
Title 1	Value 1
:	:
Title N	Value N

Metadata (type **Value**)

Title	Value
Title 1	Value 1
:	:
Title N	Value N

***Value** is defined as

Mean Qualifier(<, >, >=, etc.)	Mean Value (floating point number)	Low Qualifier(<, >, >=, etc.)	Low Value (floating point number)	Upper Qualifier	Upper Value (floating point number)	Unit

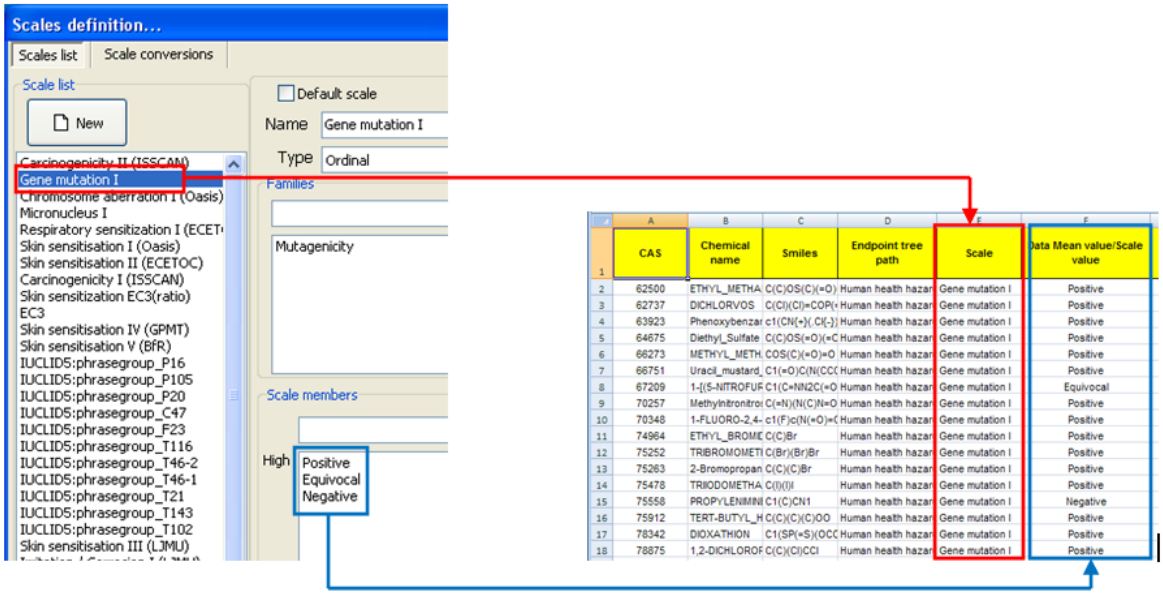
The user should therefore organize his/her data as follows:

Mean Qualifier(<, >, >=, etc.)	Mean Value (floating point number)	Low Qualifier(<, >, >=, etc.)	Low Value (floating point number)	Upper Qualifier	Upper Value (floating point number)	Unit

Data Mean value/Scale value	Data Mean qualifier	Data Unit
12.98	>	mg/L
39	>	mg/L
57	>	mg/L
29	>	mg/L
2995.767	>	mg/L
10009.113	<	mg/L
1212.2406	<	mg/L
5178.729	<	mg/L
0.00012	<	mg/L
0.000251	>	mg/L
0.00115	>	mg/L
70	>	mg/L
0.0087	>	mg/L
0.00007	>	mg/L

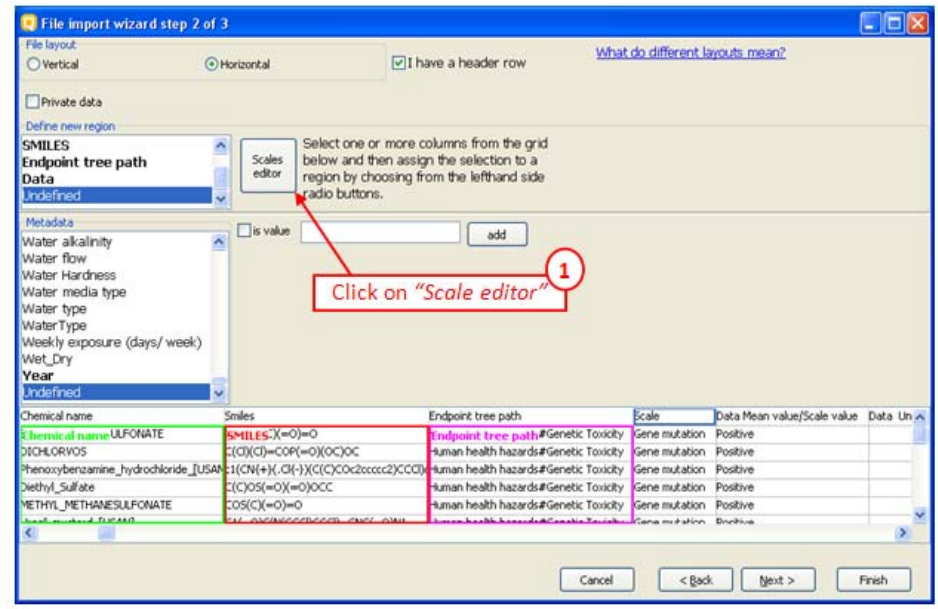
When the user defines data of a **Categorical type** (e.g. positive/negative) s/he should follow a scale definition:

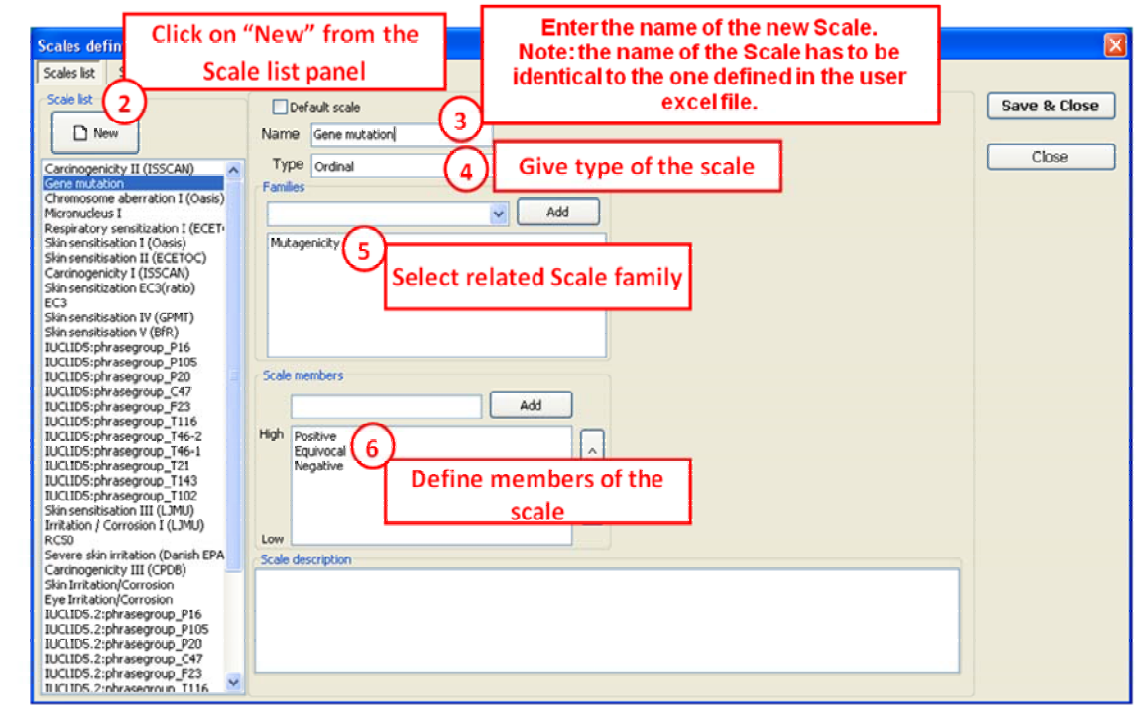
1. The file for import should have a **Scale** column for the scale name. This should contain a name of a scale **exactly** as defined in the scales list in the QSAR Toolbox database for example "Gene mutation I" is a scale from the QSAR Toolbox database scale list *(red colored fields)*:



2. The **Mean value/Scale value** column should contain only values that scale members *(blue colored fields)*

3. A new scale could be defined during the process of import:





⚠ When defining the data record the user should define:

I. **For categorical data** – **Scale** column for the scale name. This should contain a name of a scale **exactly** as defined in the scales list in the QSAR Toolbox database or as defined by the user. The **Mean value/Scale value** column should contain only values

that scale members

II. **For value data –** At least one column for the **Mean/Min/Max** values. Qualifiers and Unit are optional

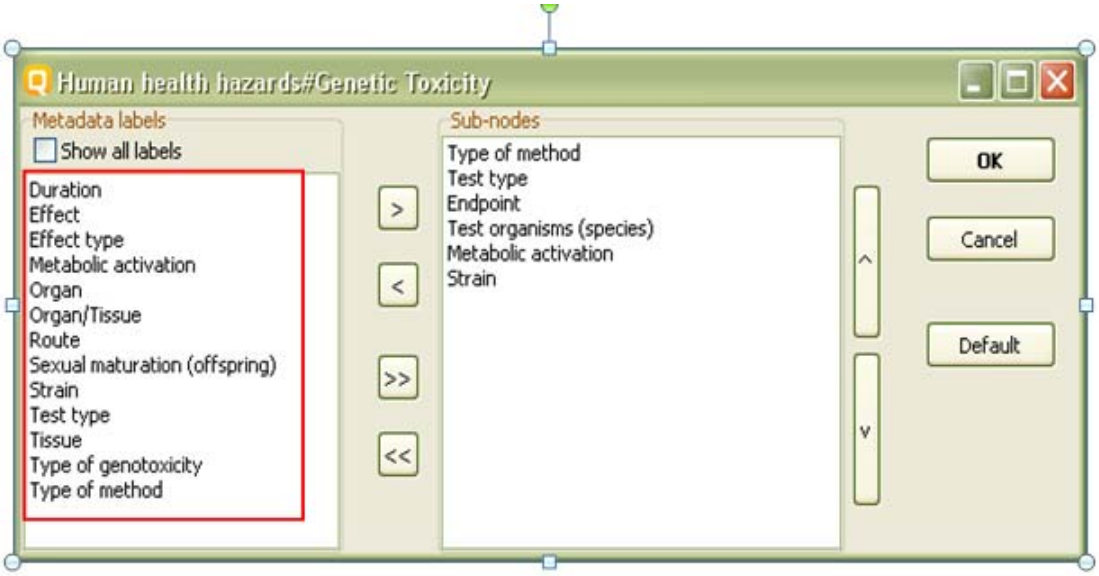
Metadata information

These are fields for metadata such as Duration, Organ, Tissue, Route of administration etc., which are not mandatory for the import:

Metadata information

Endpoint	Test organisms (species)	Duration	Duration Unit	Solubility	Unit	Effect	Lifestage	Water type	Salinity	Temperature	pH	Water alkalinity	Water Hardness	DATA QUALITY
EC 50	Ceriodaphnia	48	h			Immobilis	Juvenile	Freshwater		23				2.2
EC 50	Daphnia mag	1	h			Physiolog	Juvenile	Freshwater		20				3
EC 50	Daphnia mag	24	h			Mortality	Juvenile	Freshwater		20				3
EC 50	Daphnia mag	48	h			Mortality	Juvenile	Freshwater		20				3
EC 50	Vibrio fischer	0.25	h			Behavior	Adult	Saltwater						2.2
EC 50	Ampelisca at	24	h			Mortality		Saltwater						2.2
EC 50	Scrobicularia	24	h			Mortality		Freshwater						2.2
EC 50	Brachionus c	24	h			Mortality		Freshwater						2.2
EC 50	Pimephales p	456	h			Reproduc	Adult	Freshwater		26	8.1	317		1
EC 50	Pimephales p	456	h			Reproduc	Adult	Freshwater		26	8.1	317		1
EC 50	Pimephales p	456	h			Mortality	Adult	Freshwater		26	8.1	317		1
EC 50	Hemicentrotu	2.25	h			Reproduc	Egg	Saltwater		15				3
EC 50	Penaeus van	48	h			Mortality	Juvenile	Saltwater	20	28.5				3
EC 50	Hyalella azte	240	h			Mortality		Freshwater		22				1

Metadata fields can be used for building the dynamic part of the endpoint tree. The feature is accessible through the "Set the hierarchy" option. The user sets what categories metadata he/she wants displayed on the endpoint tree and their hierarchy. Then, when the data are loaded the tree is build with the contents of the corresponding fields.



Metadata field	Examples of metadata field values
Endpoint	LC 50,EC10, EC 50, LOEL, NOEL, Skin sensitisation, Carcinogenicity, Ames, Chromosomal aberration, Estrogen receptor binding….
Duration	years, months, days, hours, minutes, seconds…
Test organisms (species)	Daphnia magna, Lepomis symnetricus, Oncorhynchus mykiss, Poecilia reticulata, Tetrahymena pyriformis….
Effect	Immobilization, Mortality, Reproduction….
Effect type	Maternal toxicity, Developmental toxicity, Fetotoxicity, Embryotoxicity
Metabolic activation	with S9, without S9, no S9 info, with and without
Sexual maturation (offspring)	Male, Female, Male/Female…
Strain	TA 98, TA 100, TA 104, New Zealand White, Swiss, Fischer 344/DuCrj
Test type	bacterial reverse mutation assay (e.g. Ames test), in vitro mammalian cell micronucleus test, bacterial gene mutation assay, acute, subacute, chronic, developmental, static, semi-static, flow-through
Type of genotoxicity	Gene mutaion, Chromosomal aberration, DNA damage and/or repair, genome mutation
Type of method	in vivo, in vitro, other
Organ	Lung, Liver
Route	oral, inhalation, dermal, implantation, intramuscular,

Metadata field	Examples of metadata field values
	intraperitoneal

⚠ When defining the metadata record the user should organize his/her own metadata by using existing field labels. This ensures that the same fields do not multiply under different names. For example effects from the experiment should be placed in a column named "Effect", the type of the test method such as "Ames test" should be placed in a column named "Test type" etc.

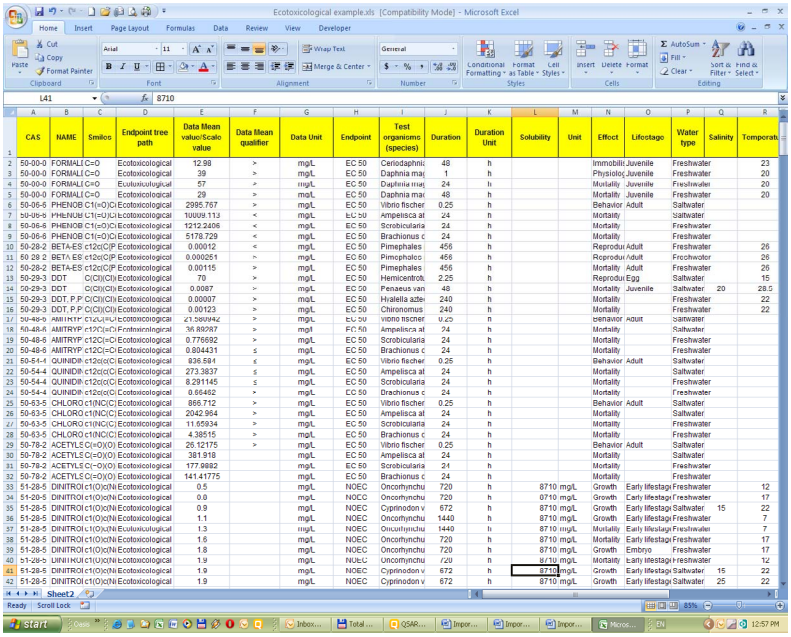
The metadata fields can be organized in "Set tree hierarchy" panel. Right click on endpoint tree to set the hierarchy.

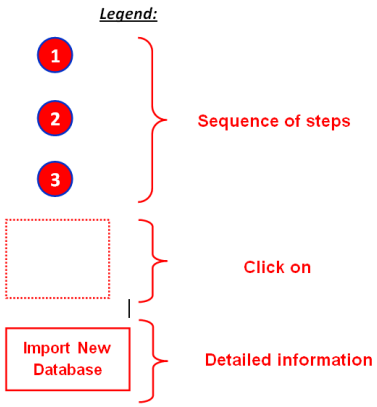
Appendix II: Import example for a database with ecotoxicological information

⚠ The example below uses a file that is already prepared. Guidance on how to prepare file for horizontal import can be found in Appendix I.

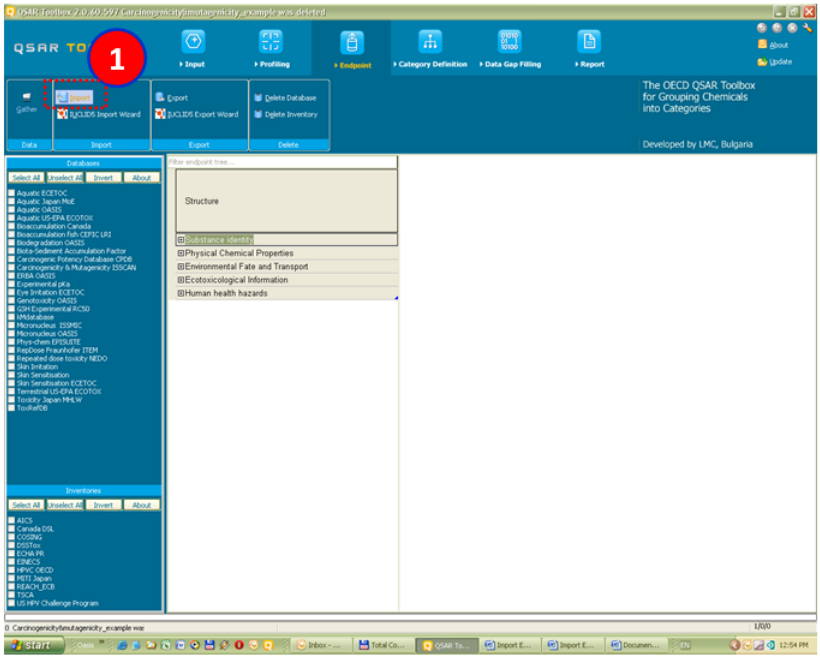
The destination for example files is [Install folder]\Examples

The default path is: C:\Program Files\QSAR Toolbox\QSAR Toolbox 2.1\Examples\Ecotoxicological example.xls

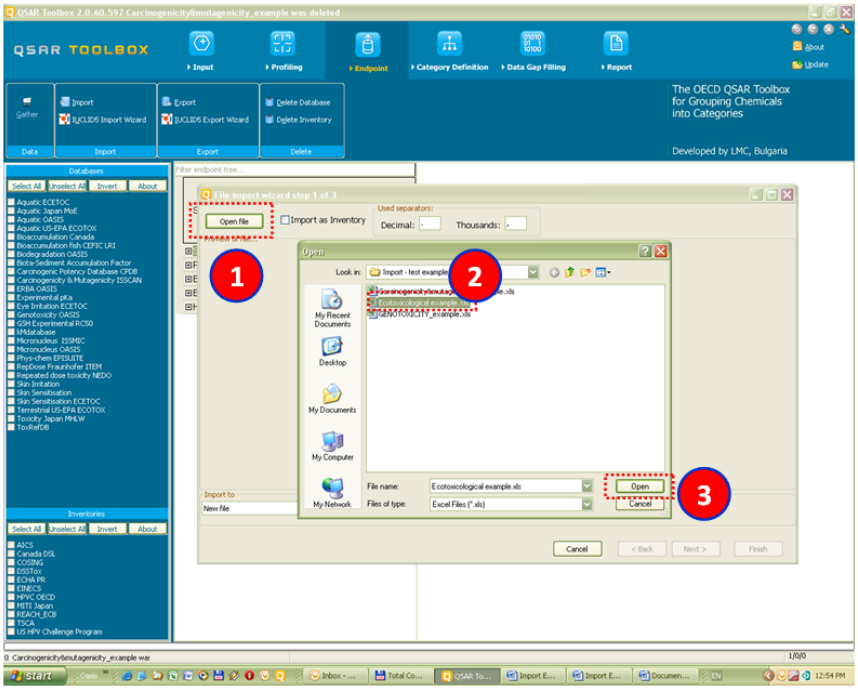


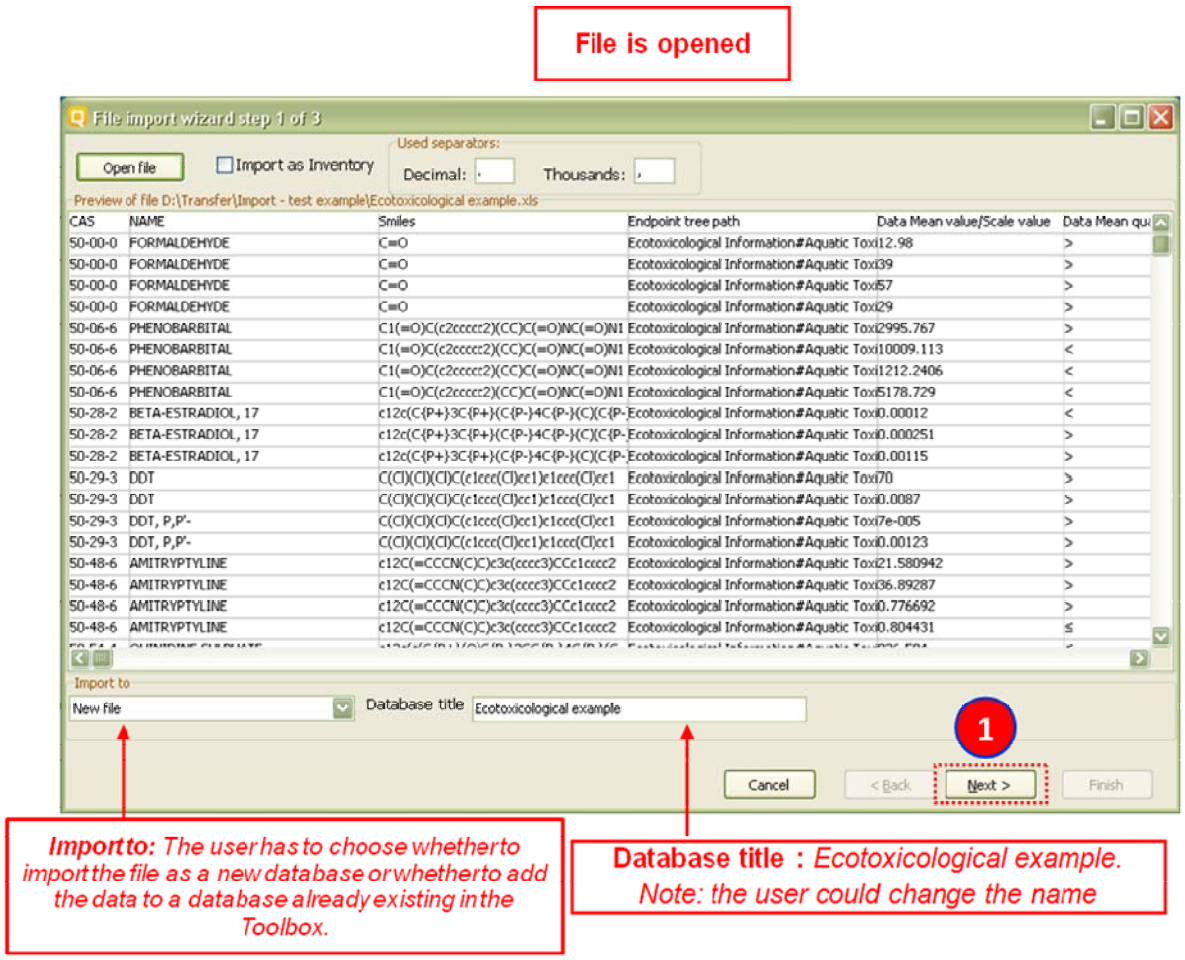


Import New Database



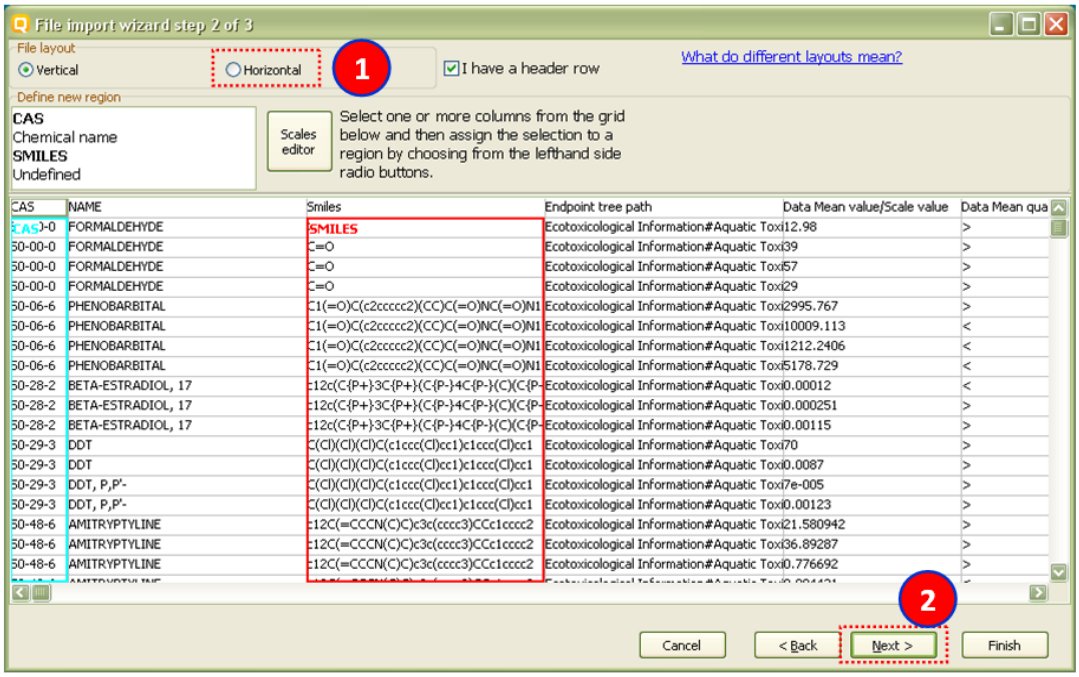
Open example file



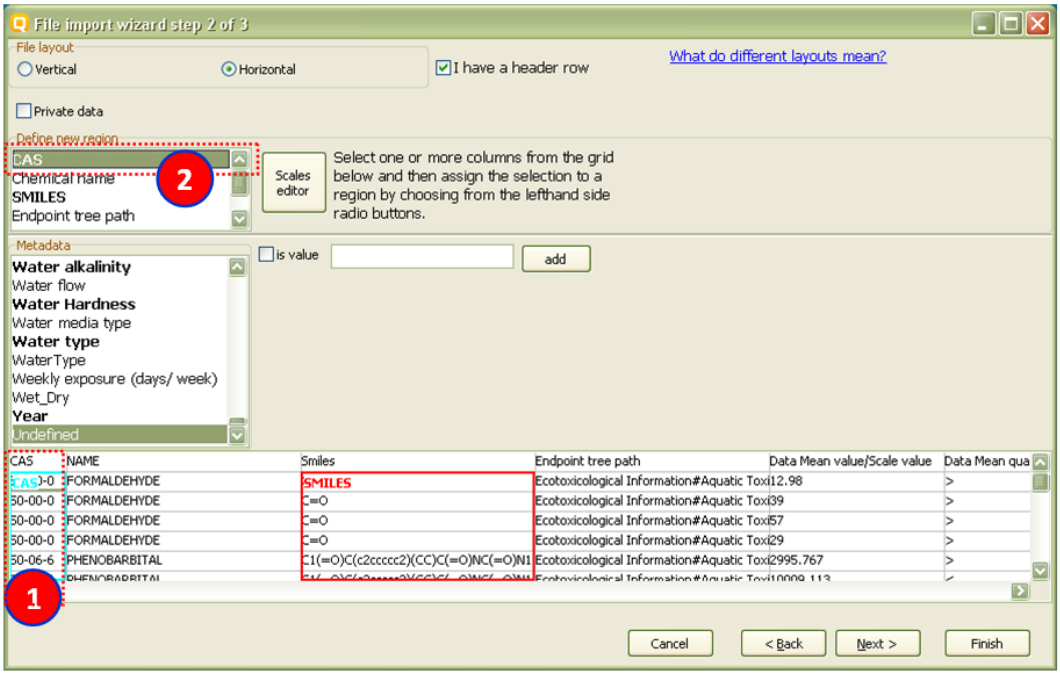


⚠ It is very important that the thousands and decimal separators are properly set while importing. Especially with TXT file this could lead to erroneous parsing of data values.

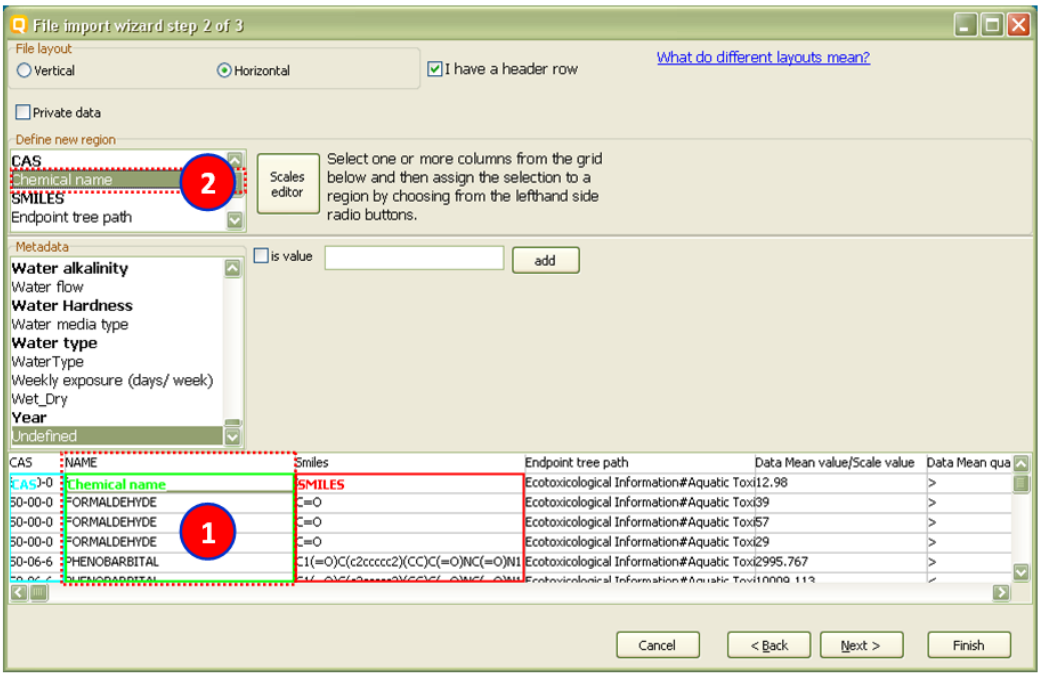
Step 2: Horizontal import



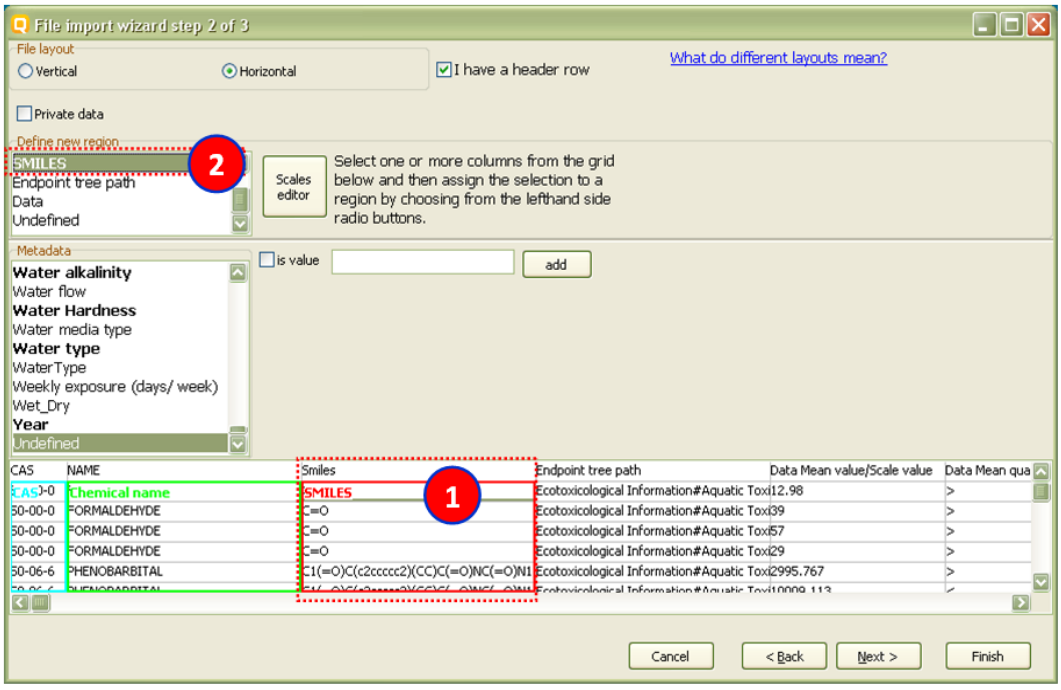
Select: *CAS*



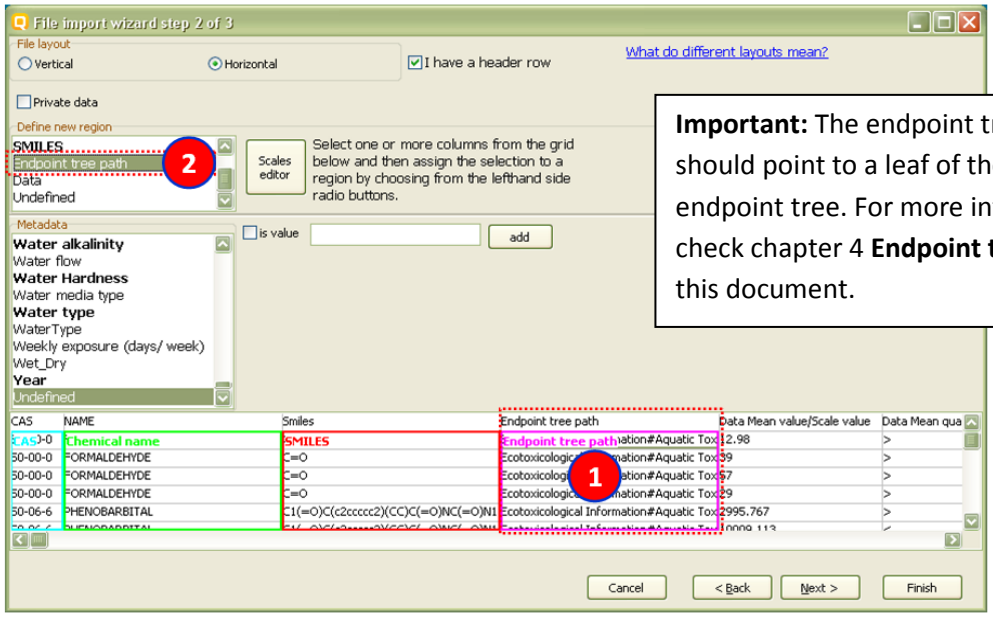
Select: *Chemical name*



Select: *SMILES*

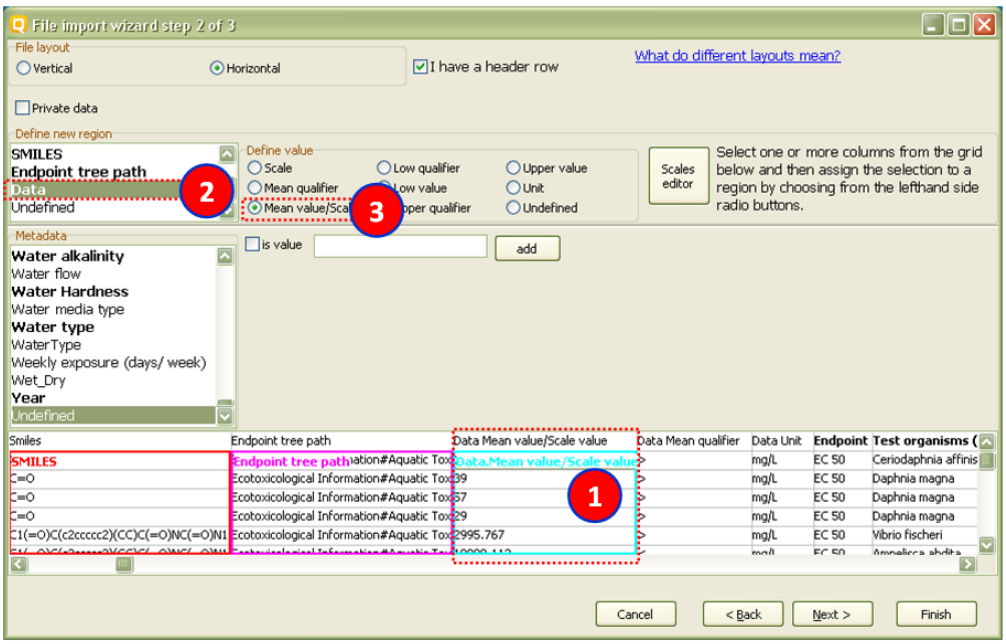


Select : *Endpoint tree path*

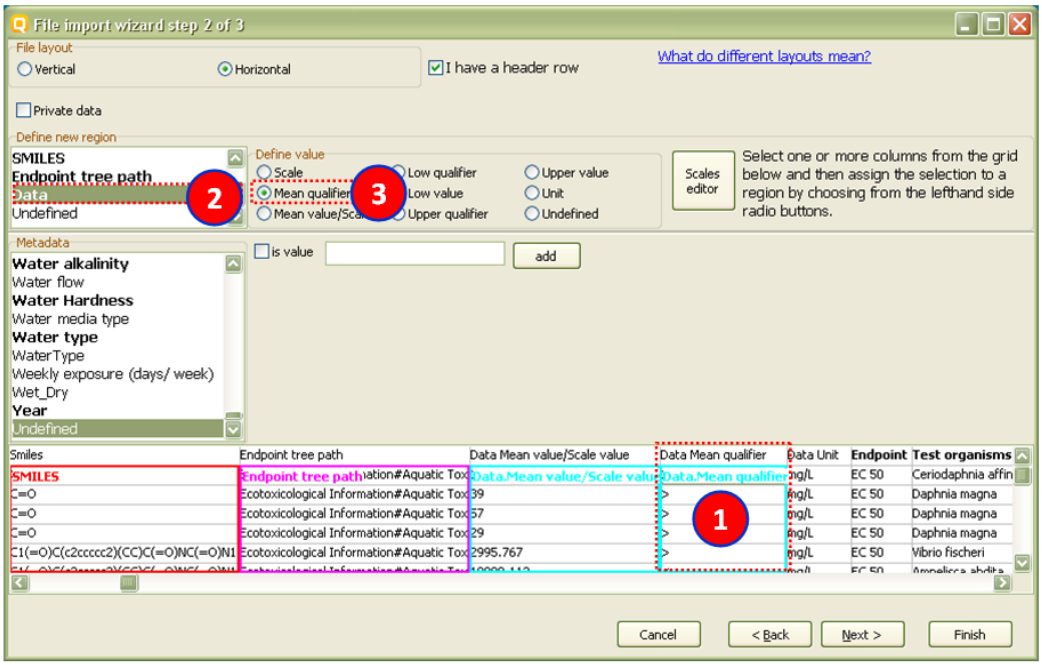


Important: The endpoint tree path should point to a leaf of the **predefined** endpoint tree. For more information check chapter 4 **Endpoint tree path** in this document.

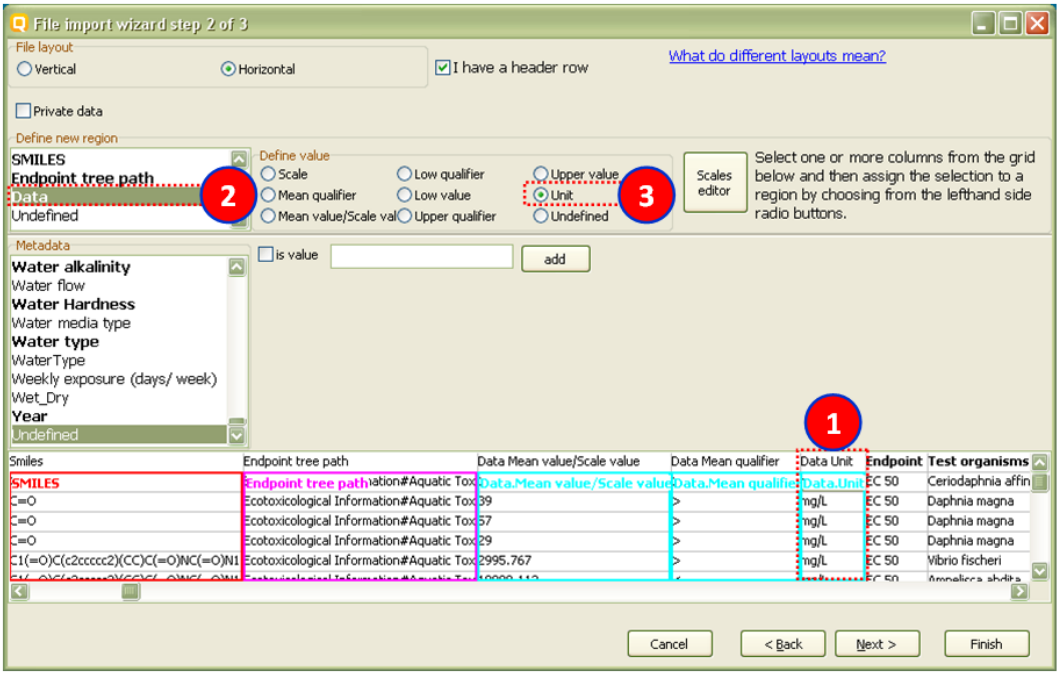
Select: *DATA Mean Value/Scale value*



Select: *DATA Mean qualifier*

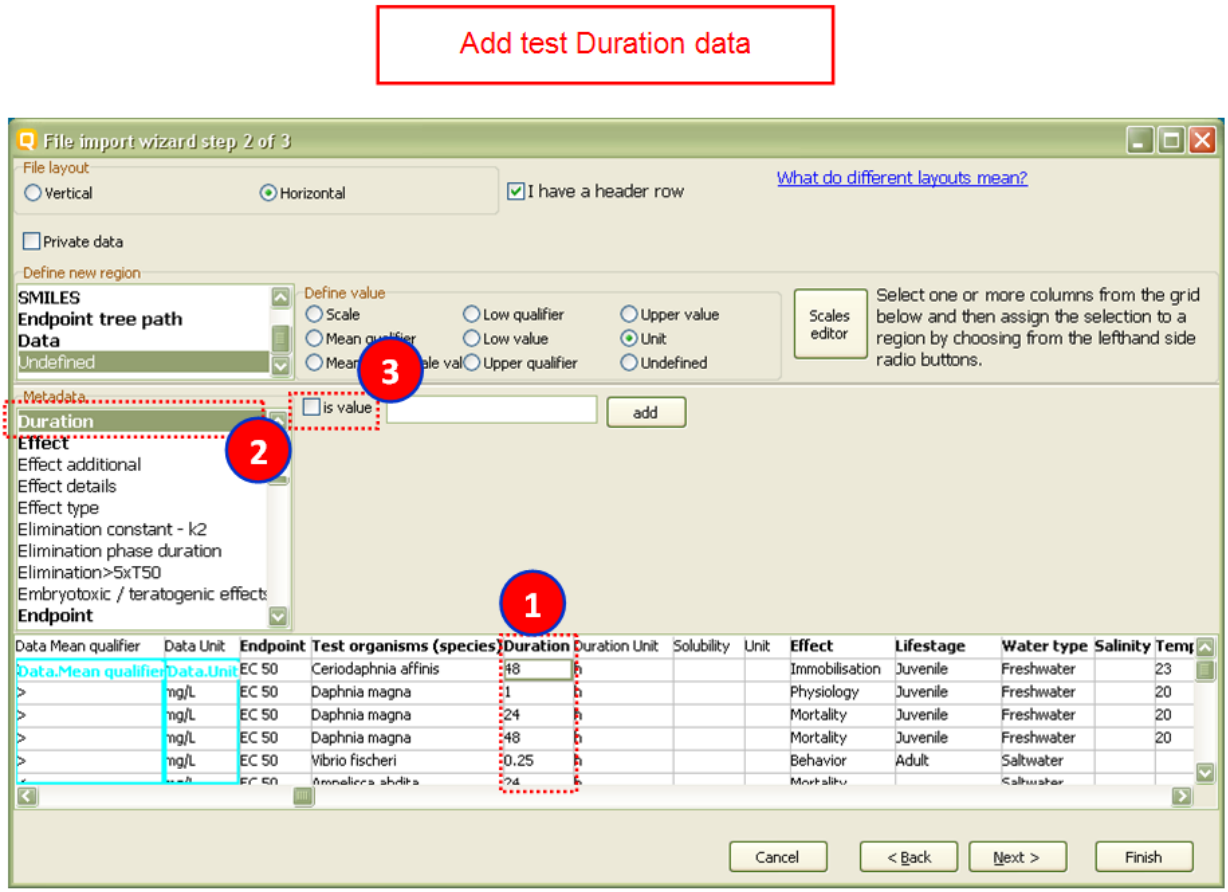


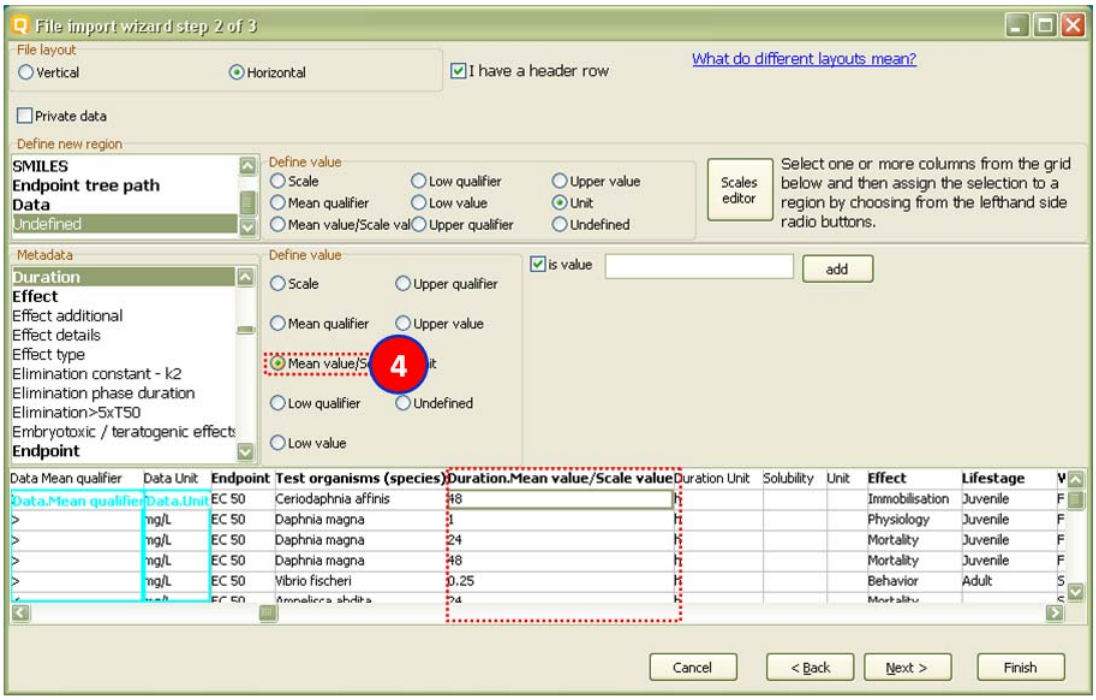
Select: *DATA Unit*



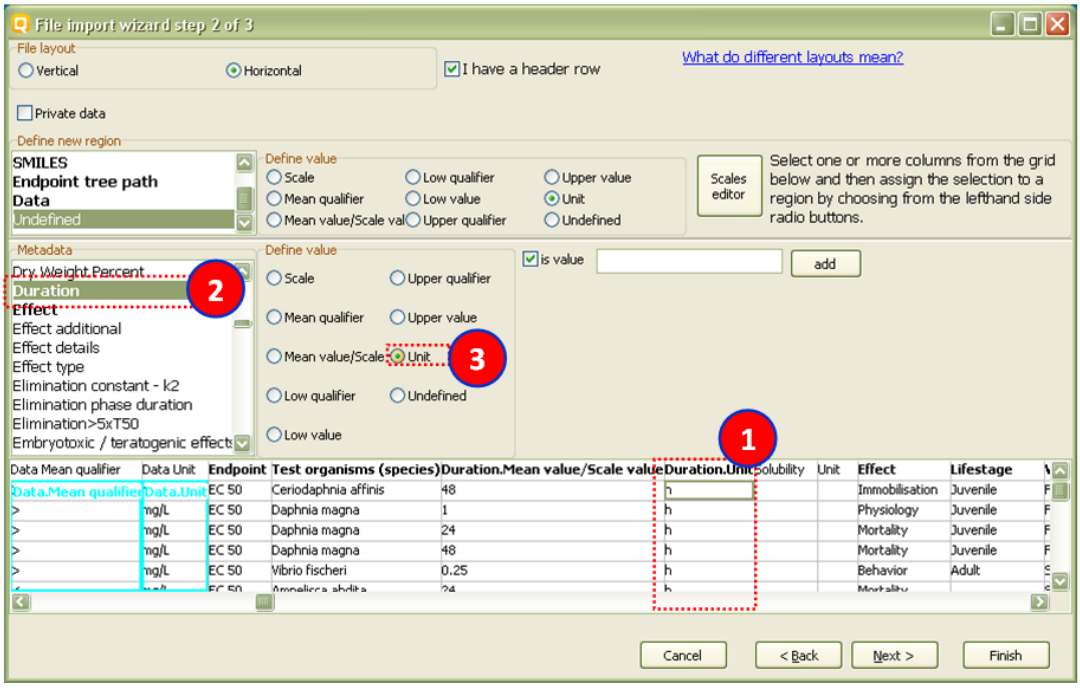
I. The type of the column is specified by clicking on the column and then clicking its type (CAS/Chemical name/SMILES) from the list box in the **Define new region** panel or selecting a metadata field label from the list box in the **Metadata** panel. To remove designations click a column and then click on **Undefined** from the list box.

II. All fields fields defined with the **Define new region** panel are color-distinguished from the fields of the **Metadata** panel.

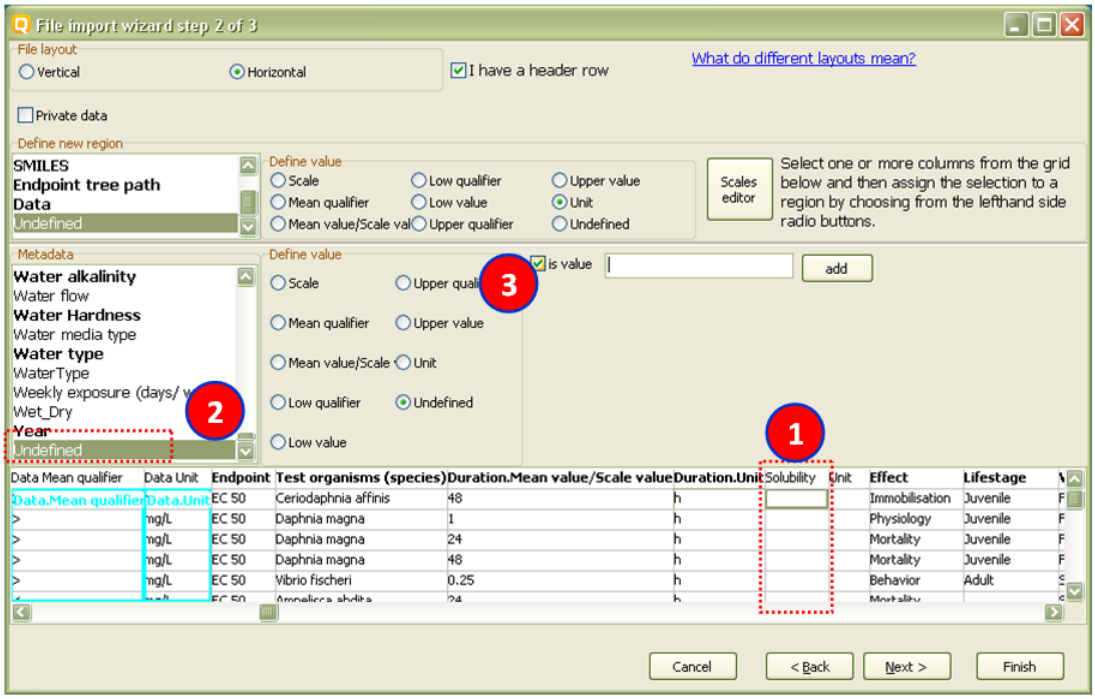


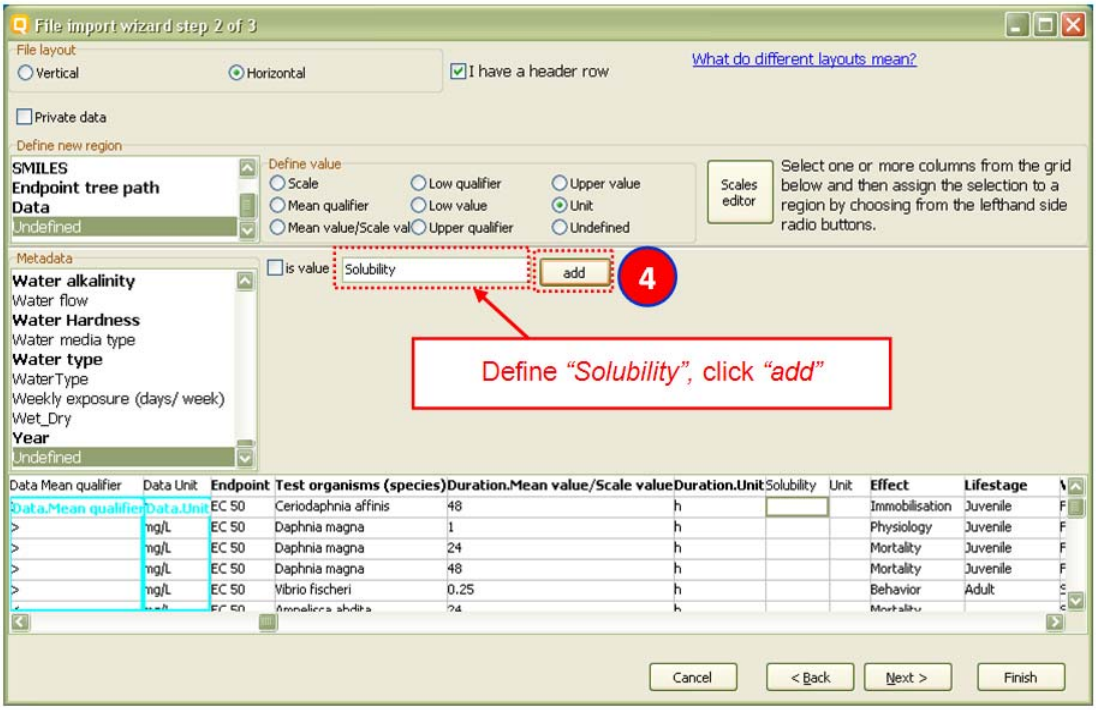


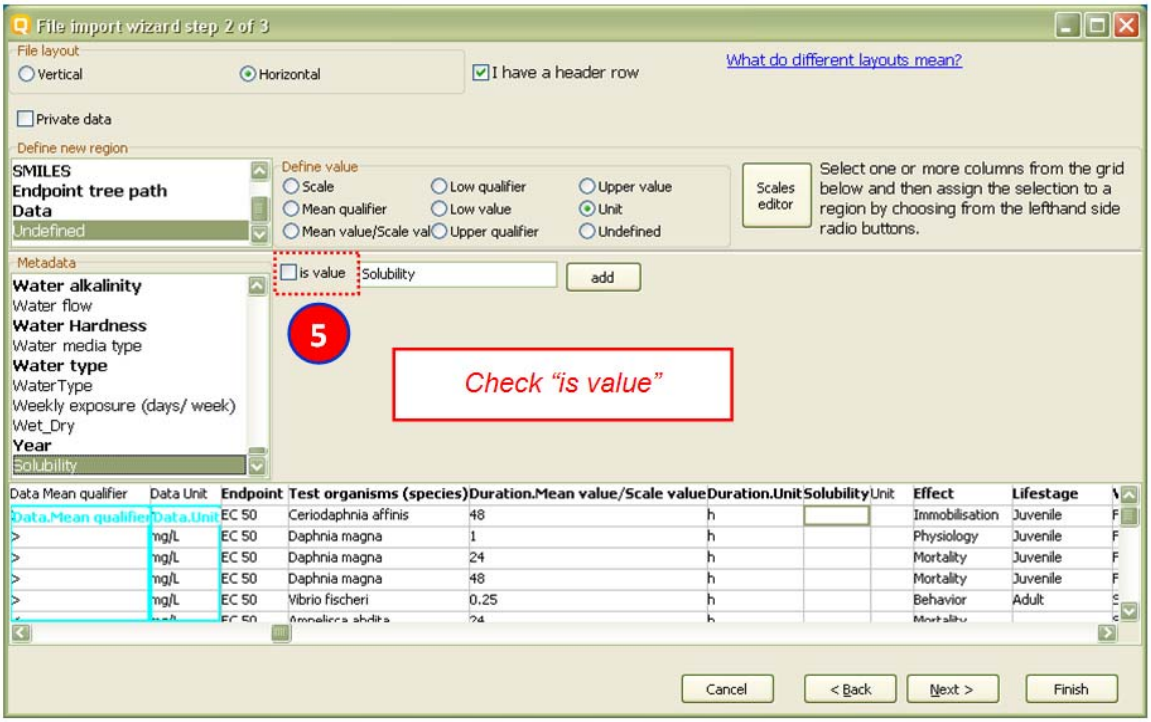
Add test "*Duration unit*"

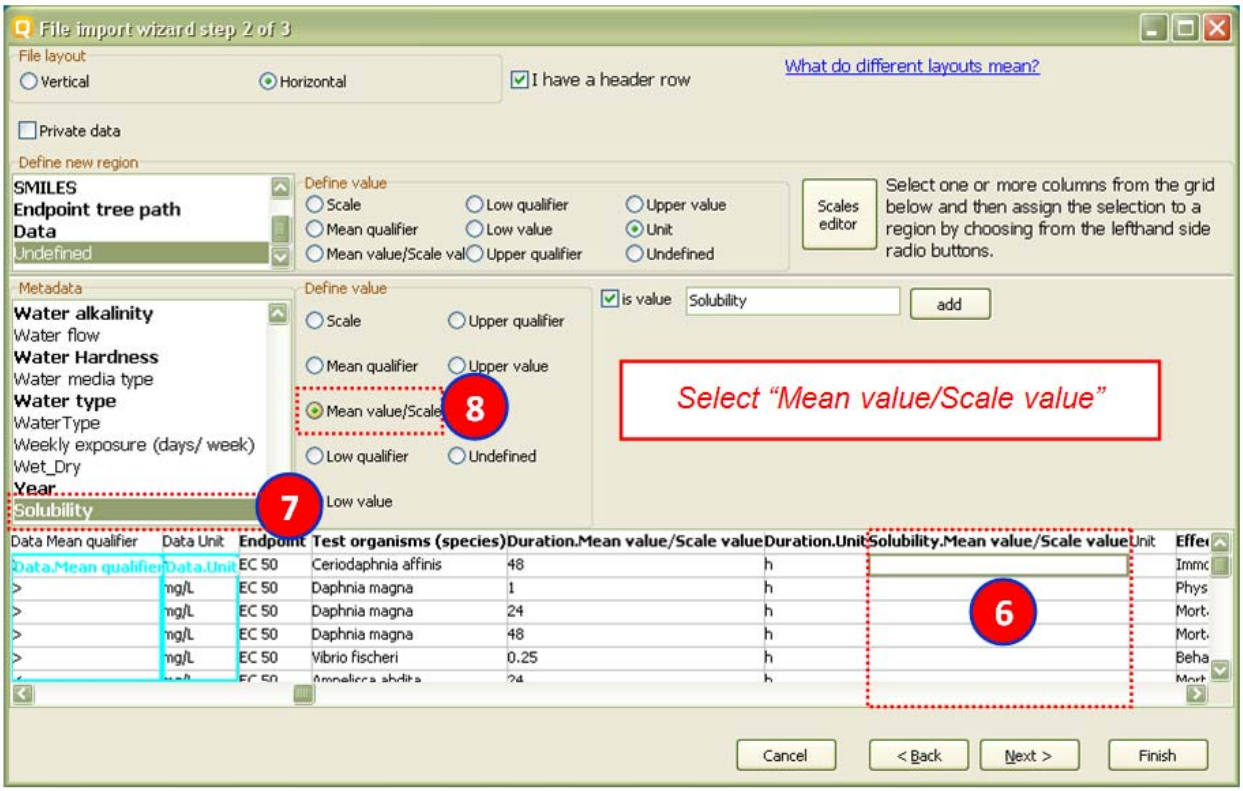


Add undefined parameter - *"Solubility"*






File import wizard step 2 of 3
File layout
Vertical
Horizontal
I have a header row
What do different layouts mean?
Private data
Define new region
SMILES
Endpoint tree path
Data
Undefined
Define value
Scale
Low qualifier
Upper value
Mean qualifier
Low value
Unit
Mean value/Scale val
Upper qualifier
Undefined
Scales editor
Select one or more columns from the grid below and then assign the selection to a region by choosing from the lefthand side radio buttons.
Metadata
Water alkalinity
Water flow
Water Hardness
Water media type
Water type
WaterType
Weekly exposure (days/ week)
Wet_Dry
Year
Solubility
is value
Solubility
add
5
Check "is value"
Data Mean qualifier
Data Unit
Endpoint
Test organisms (species)
Duration.Mean value/Scale value
Duration.Unit
Solubility
Unit
Effect
Lifestage
Data.Mean qualifier
Data.Unit
EC 50
Ceriodaphnia affinis
48
h
Immobilisation
Juvenile
mg/L
EC 50
Daphnia magna
1
h
Physiology
Juvenile
mg/L
EC 50
Daphnia magna
24
h
Mortality
Juvenile
mg/L
EC 50
Daphnia magna
48
h
Mortality
Juvenile
mg/L
EC 50
Vibrio fischeri
0.25
h
Behavior
Adult
Cancel
< Back
Next >
Finish


File import wizard step 2 of 3
File layout
Vertical
Horizontal
I have a header row
What do different layouts mean?
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Define new region
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Define value
Scale
Low qualifier
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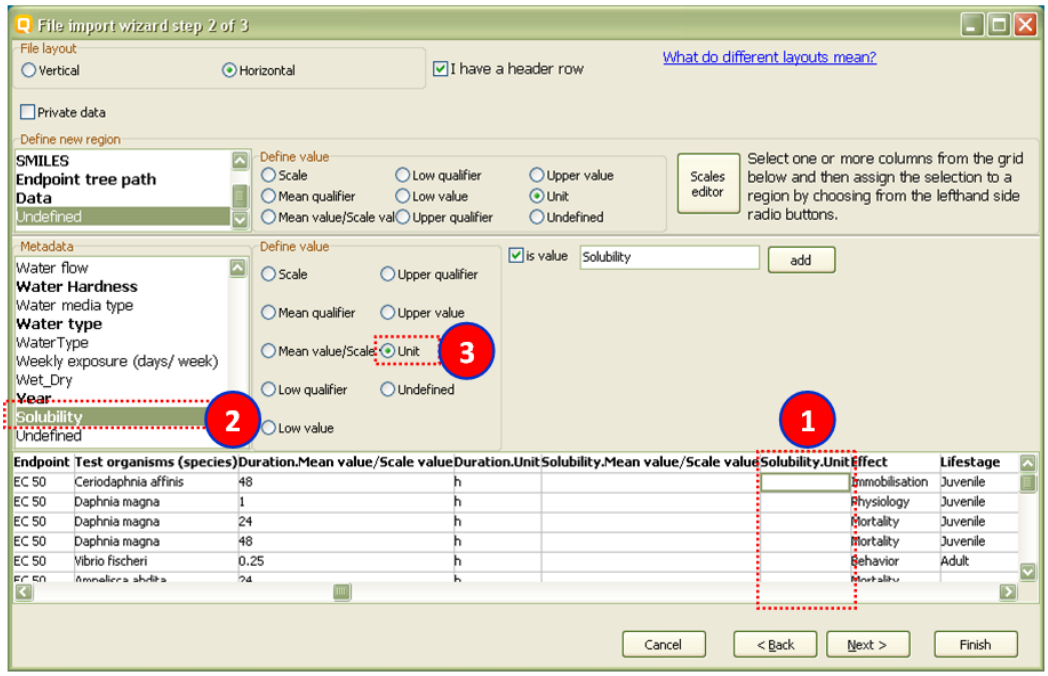
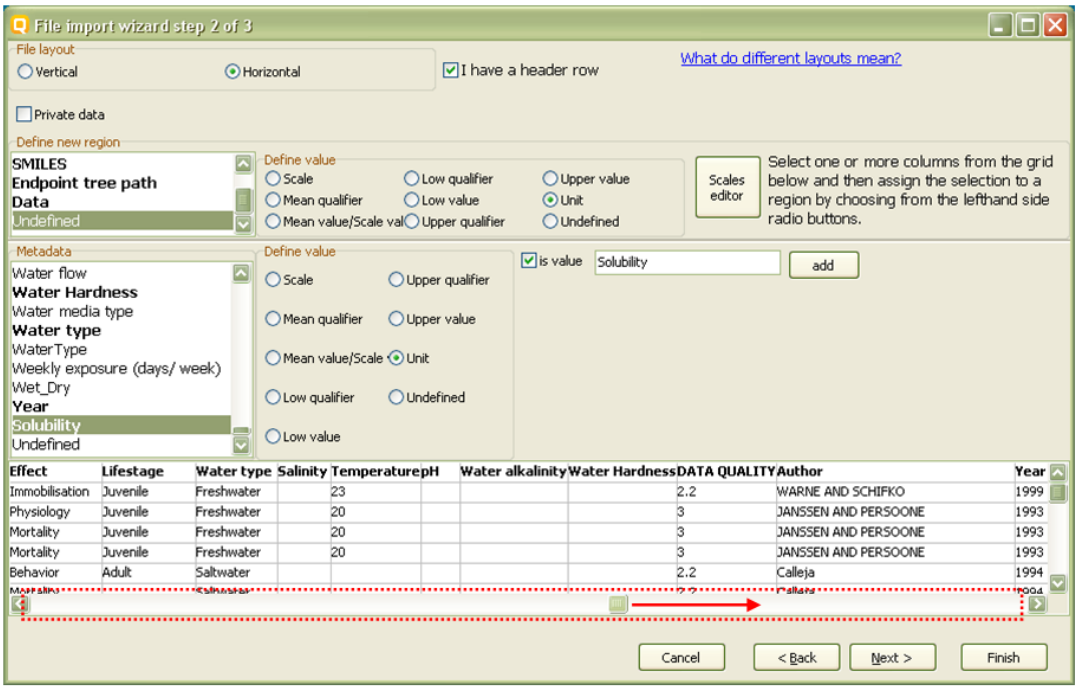
Low value
Unit
Mean value/Scale val
Upper qualifier
Undefined
Scales editor
Select one or more columns from the grid below and then assign the selection to a region by choosing from the lefthand side radio buttons.
Metadata
Water alkalinity
Water flow
Water Hardness
Water media type
Water type
WaterType
Weekly exposure (days/ week)
Wet_Dry
Year
Solubility
Define value
Scale
Upper qualifier
Mean qualifier
Upper value
Mean value/Scale
Low qualifier
Undefined
Low value
8
7
is value
Solubility
add
Select "Mean value/Scale value"
Data Mean qualifier
Data Unit
Endpoint
Test organisms (species)
Duration.Mean value/Scale value
Duration.Unit
Solubility.Mean value/Scale value
Unit
Data.Mean qualifier
Data.Unit
EC 50
Ceriodaphnia affinis
48
h
mg/L
EC 50
Daphnia magna
1
h
mg/L
EC 50
Daphnia magna
24
h
mg/L
EC 50
Daphnia magna
48
h
mg/L
EC 50
Vibrio fischeri
0.25
h
6
Cancel
< Back
Next >
Finish

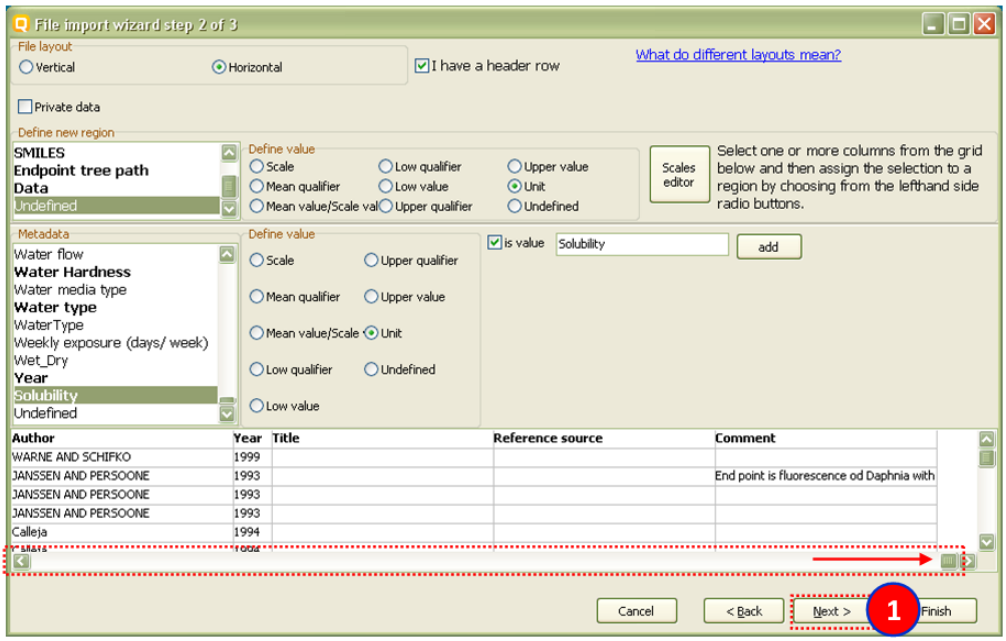
Select *"Unit"* of defined *"Solubility"* parameter



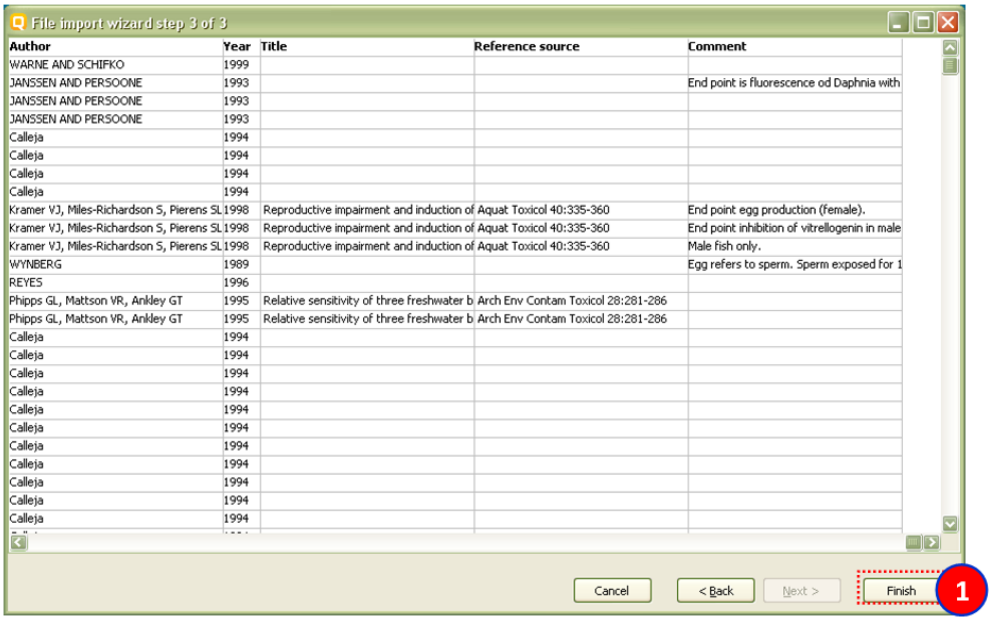
Scroll bar

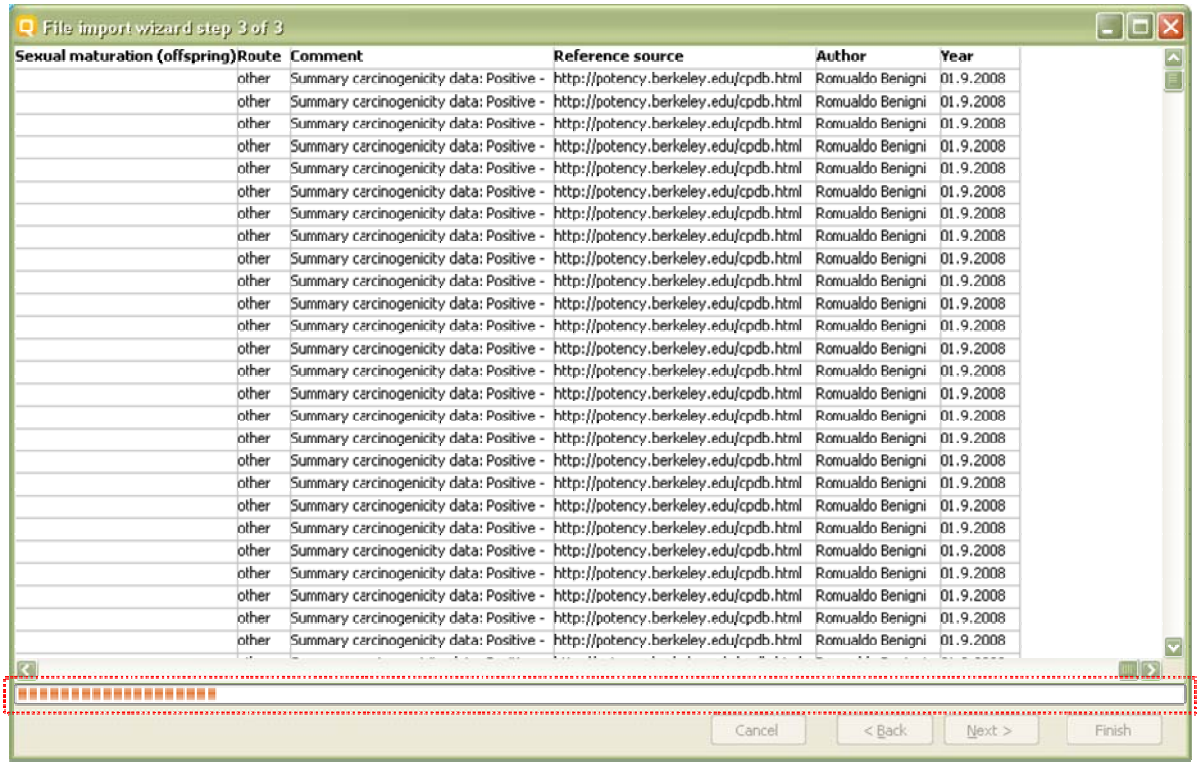


Scroll the bar to review data column designations. Click on *"Next"* button

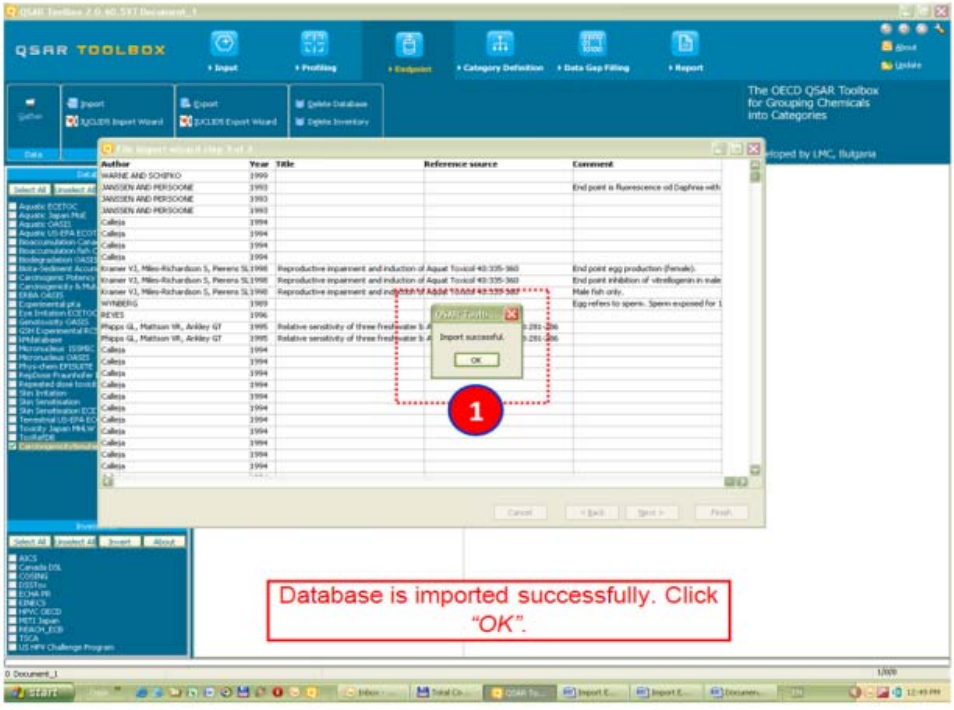


Click on *"Finish"* button

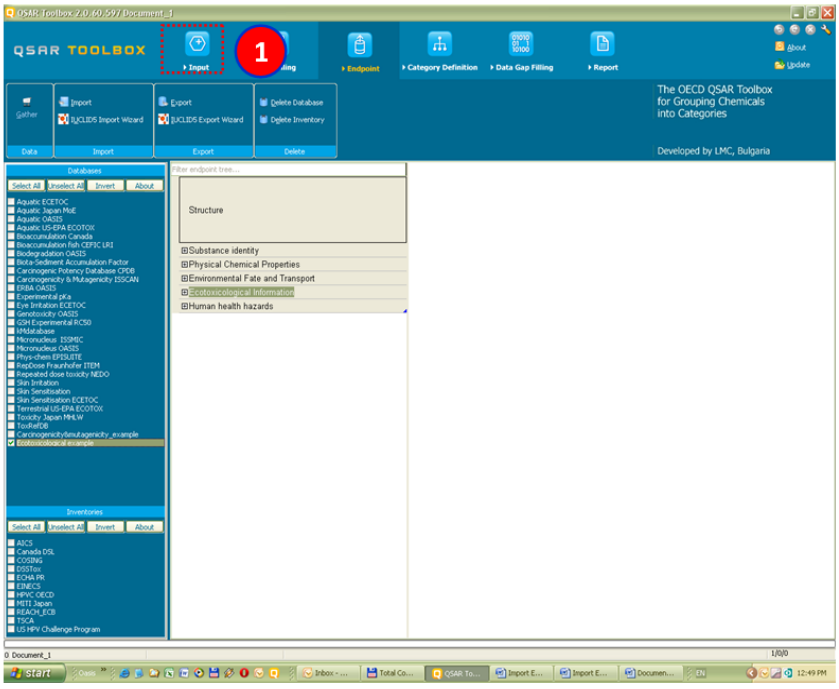


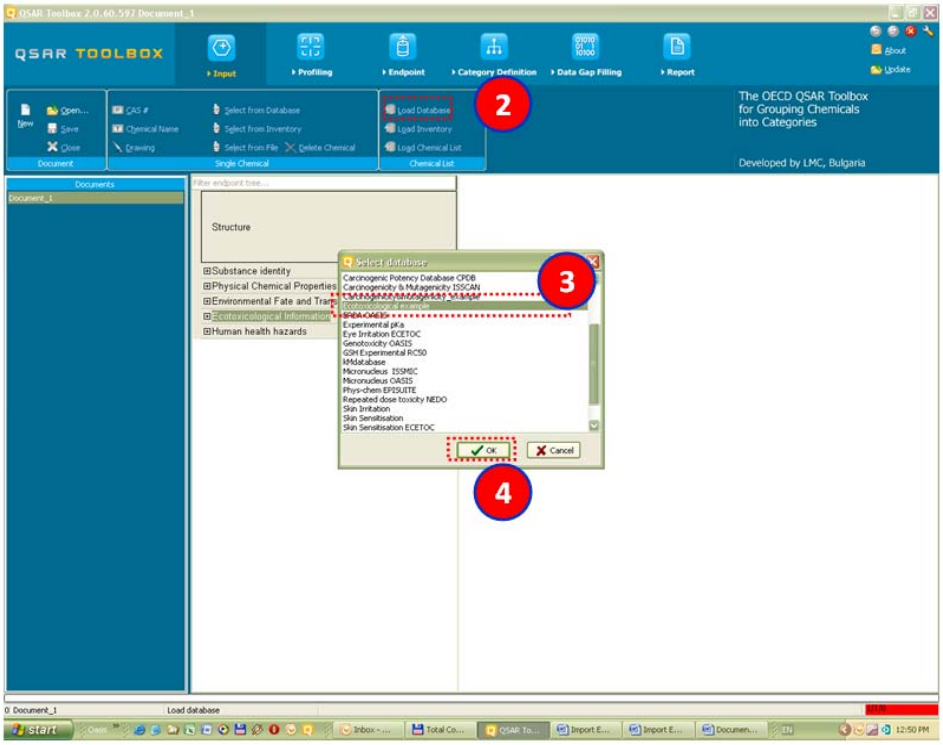


The database is in the process of being imported. For large databases this might take considerable time.

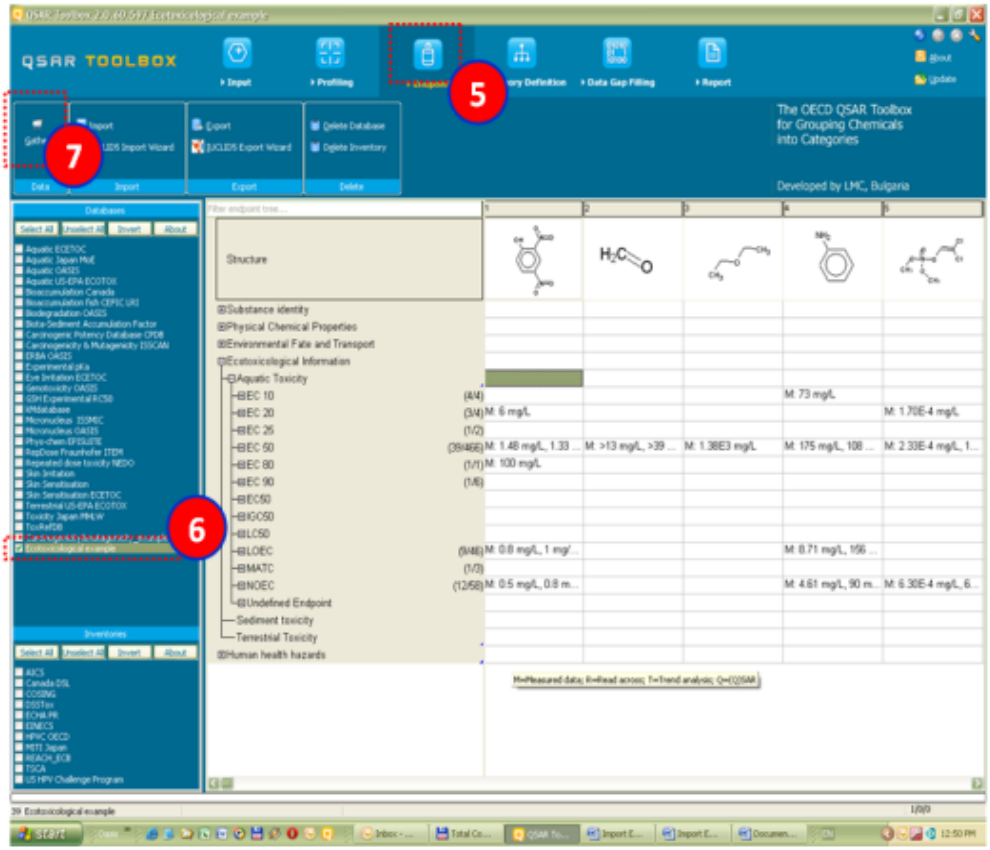


Load imported database





Gather experimental data from imported database

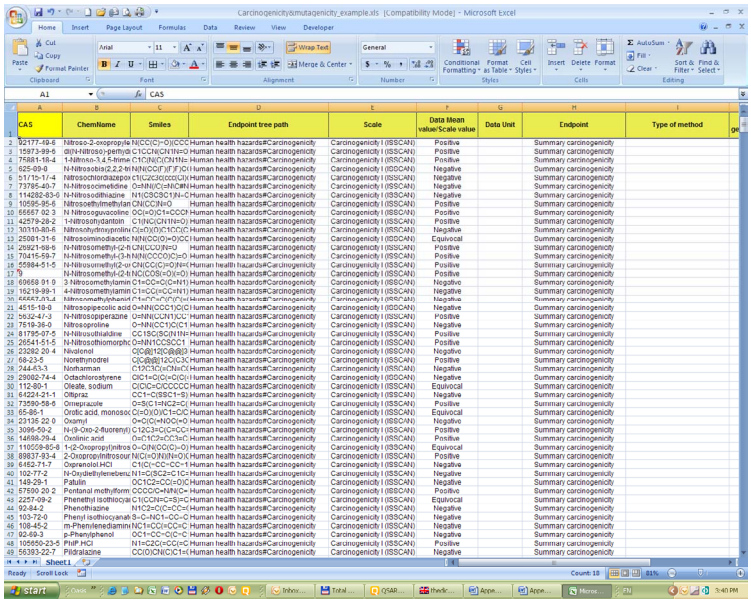


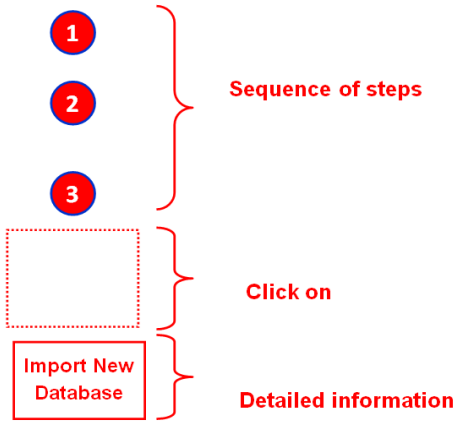
Appendix III: Import example for database with Human health hazards Information

⚠ The example below uses a file that is already prepared. Guidance on how to prepare file for horizontal import can be found in Appendix I.

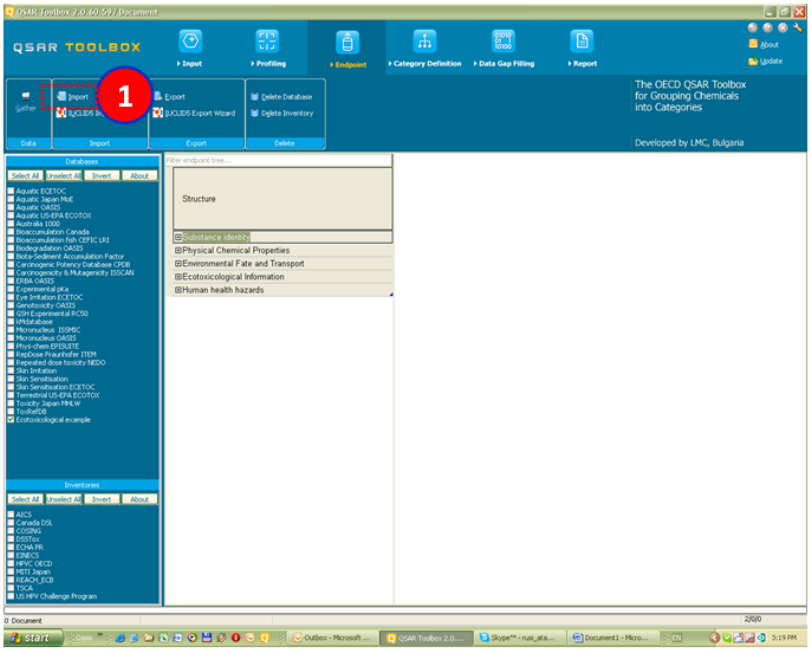
The destination for example files is [Install folder]\Examples

The default path is: C:\Program Files\QSAR Toolbox\QSAR Toolbox 2.1\Examples\ Carcinogenicity&mutagenicity_example.xls

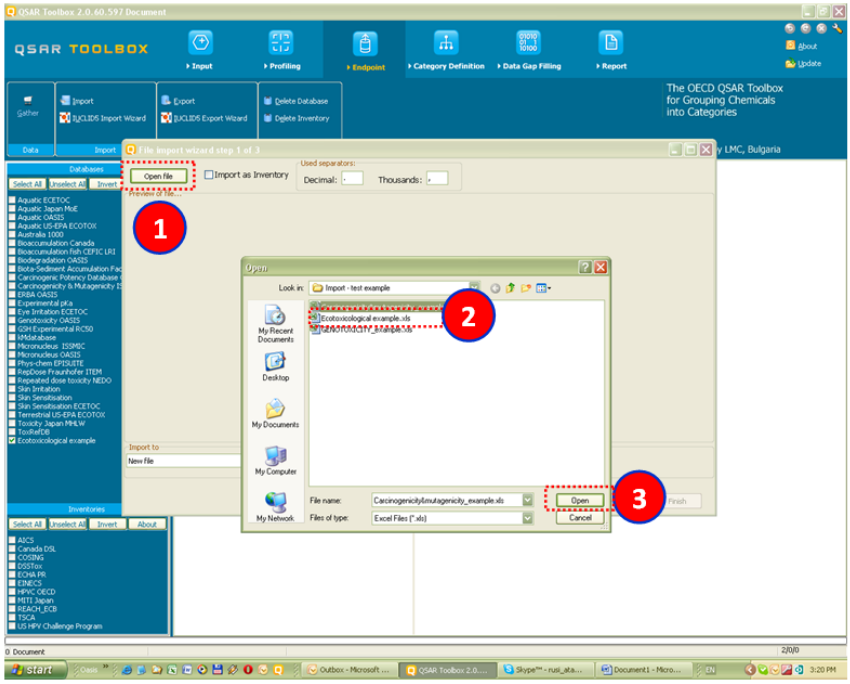


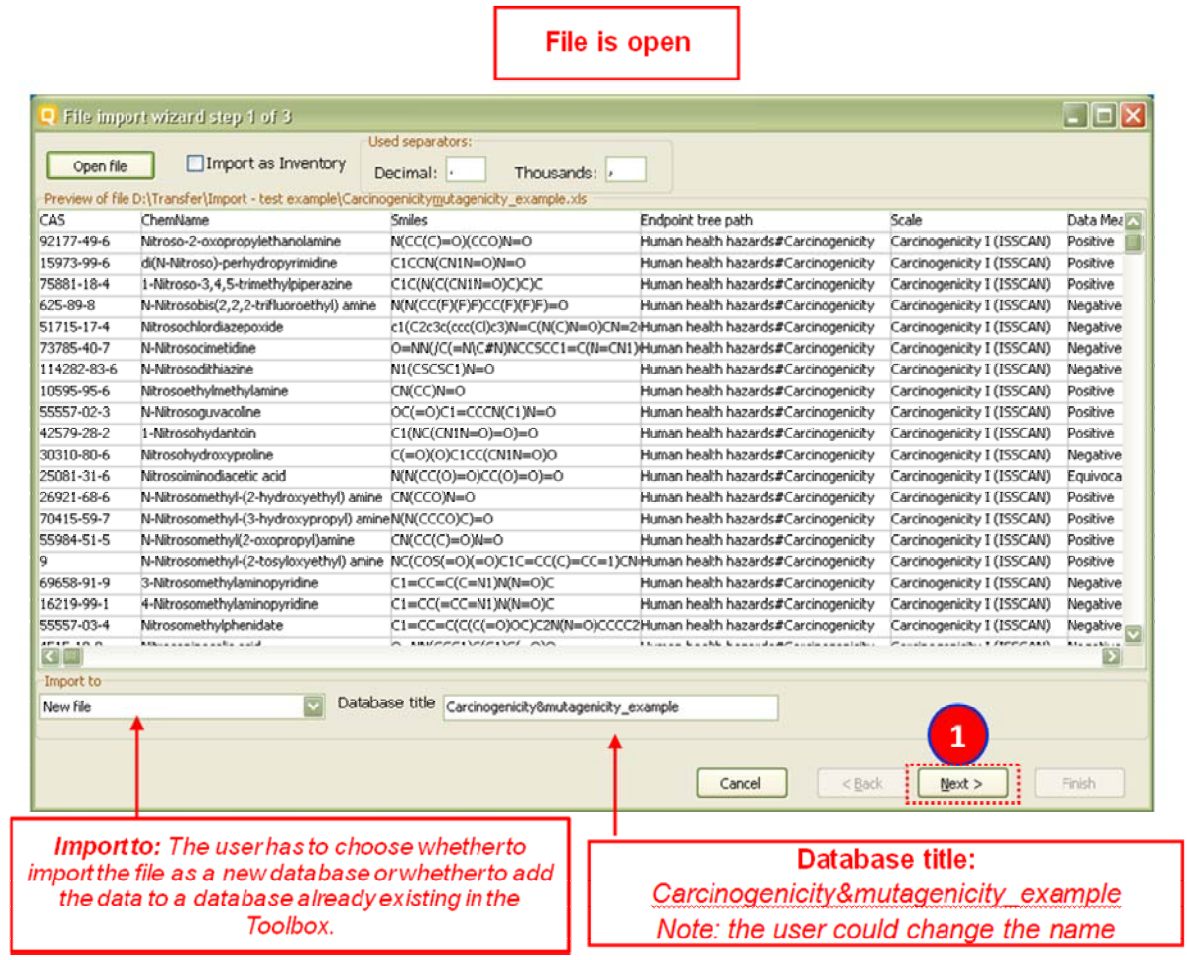


Import New Database



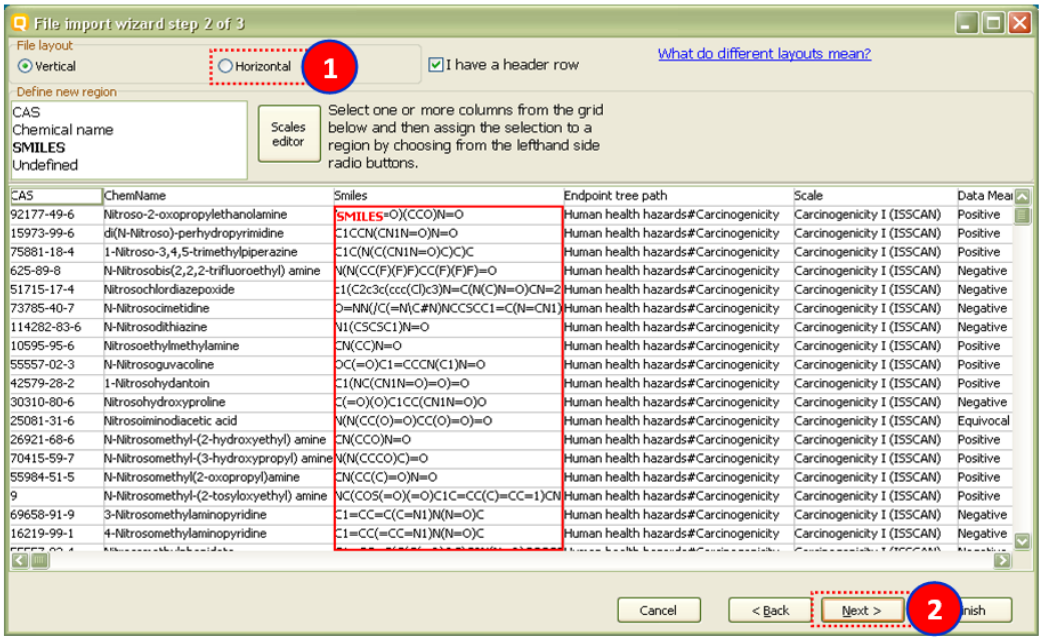
Open example file



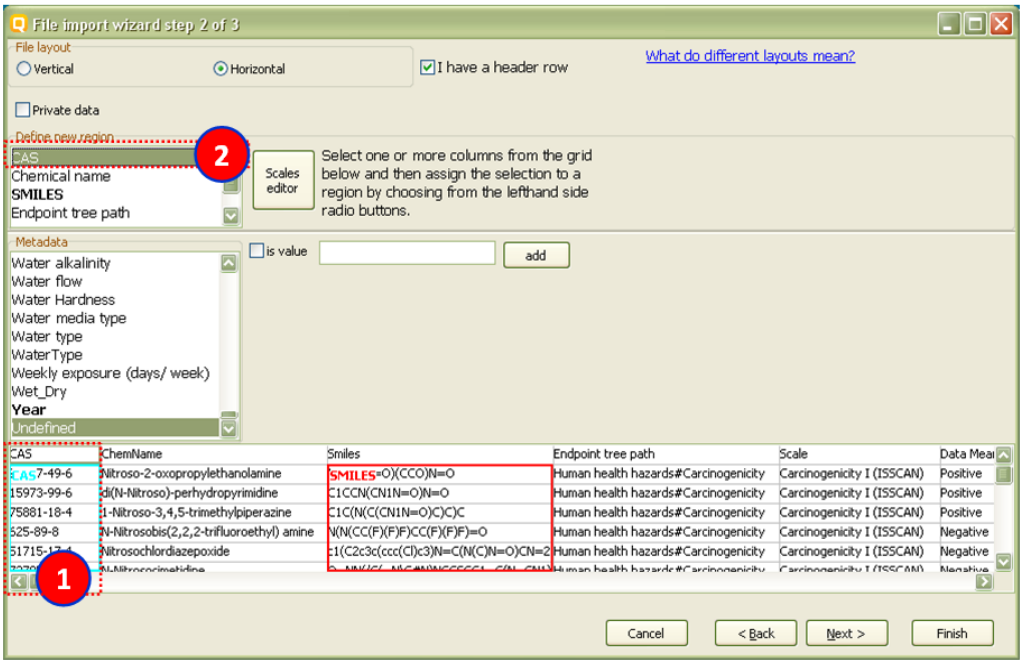


⚠ It is very important that the thousands and decimal separators are properly set while importing. Especially with TXT file this could lead to erroneous parsing of data values.

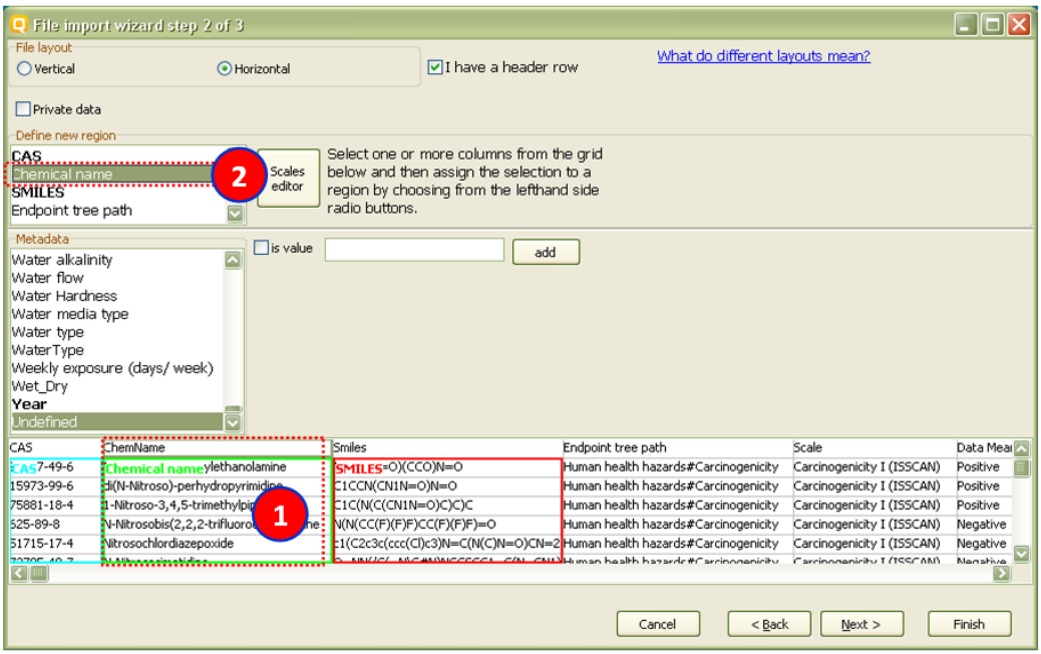
Step 2: Horizontal import



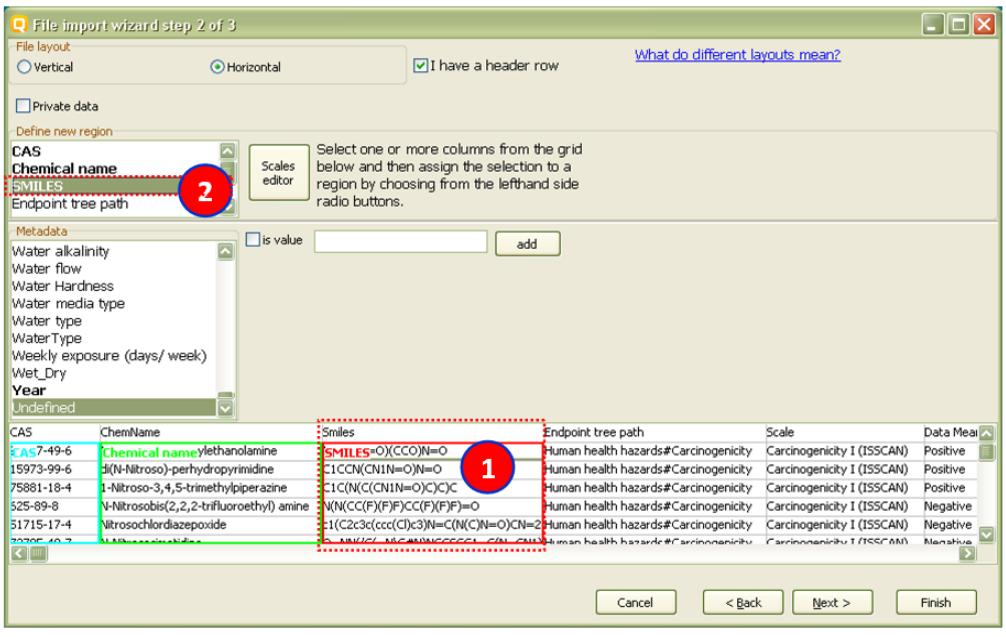
Select : *CAS*



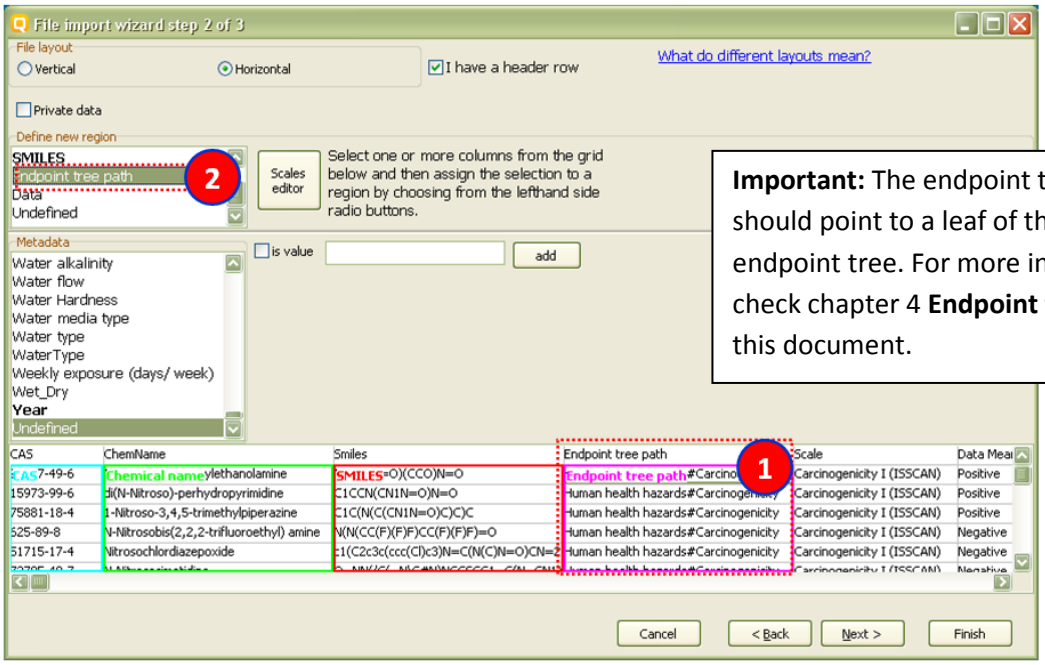
Select : *Chemical name*



Select : *SMILES*

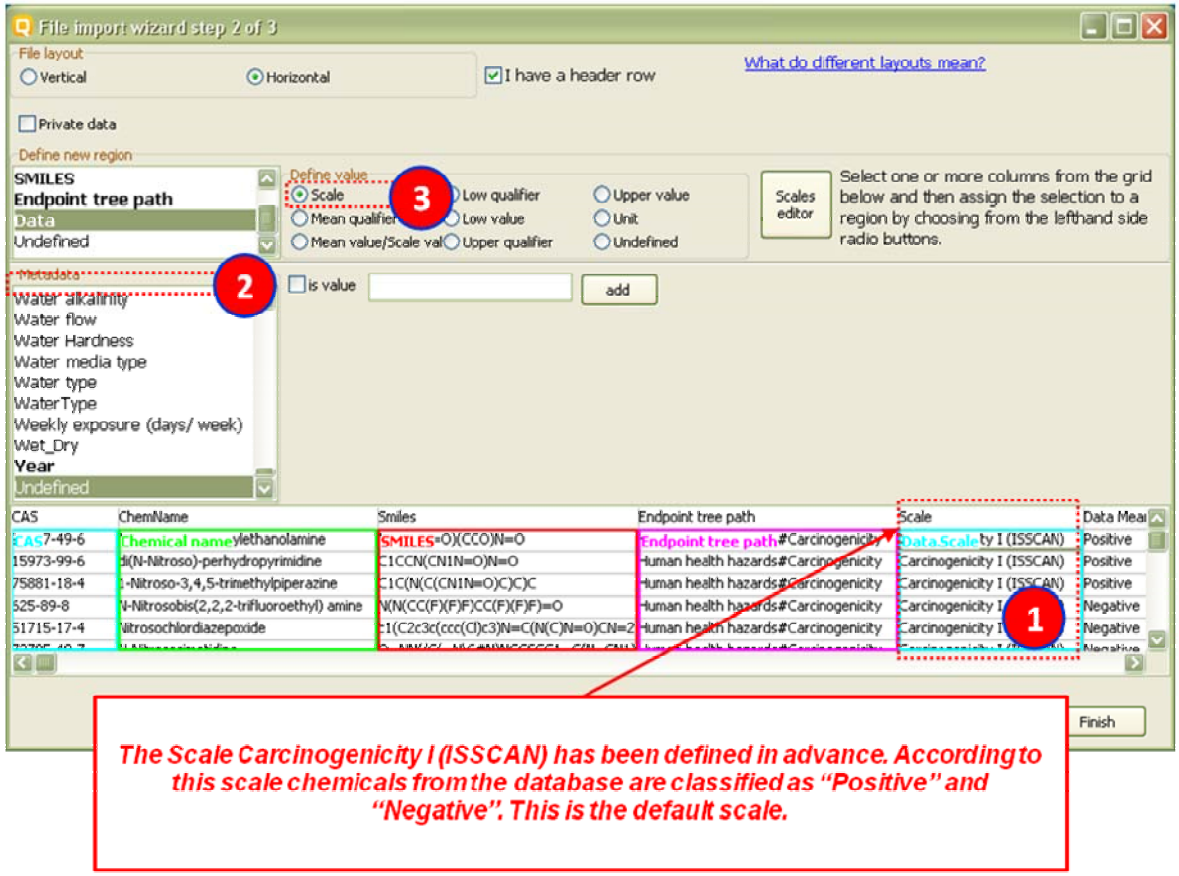


Select : *Endpoint tree path*

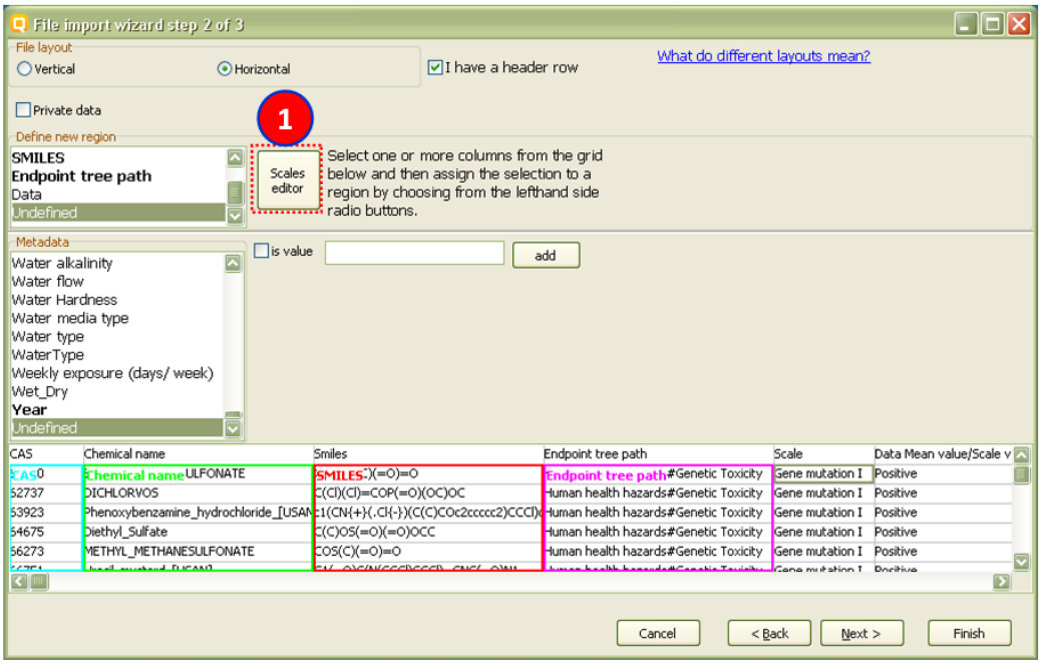


Important: The endpoint tree path should point to a leaf of the **predefined** endpoint tree. For more information check chapter 4 **Endpoint tree path** in this document.

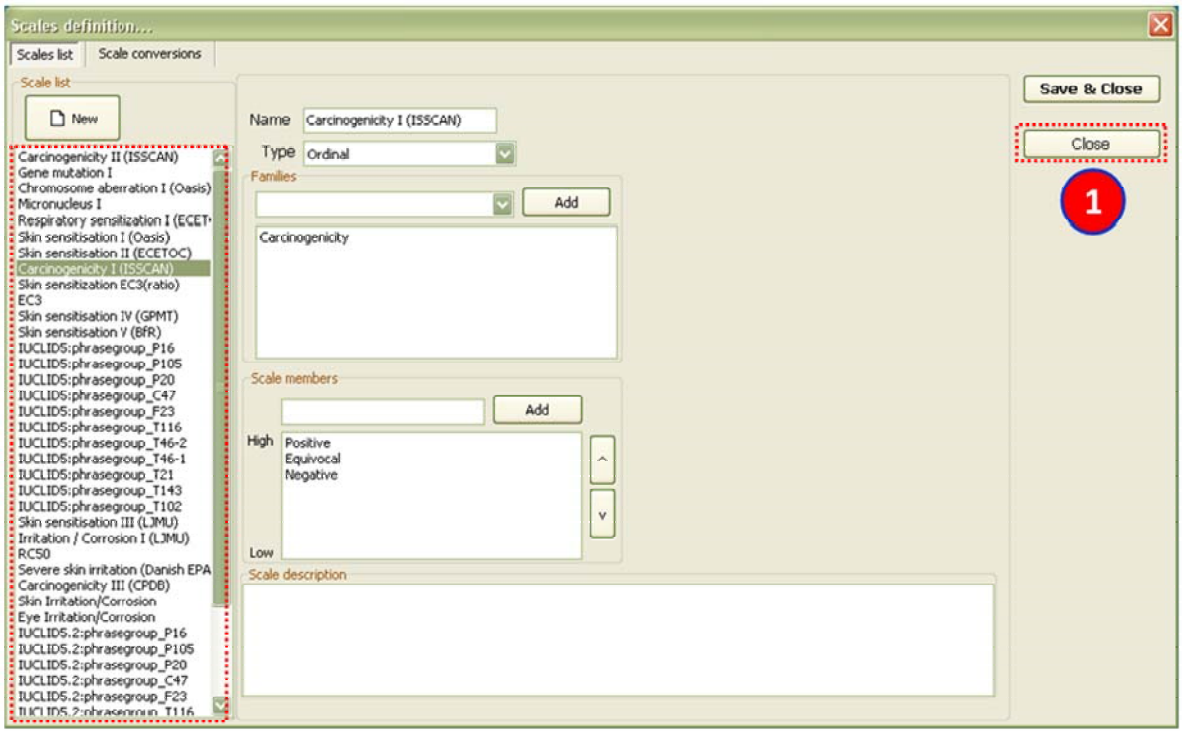
Select : *DATA Scale*



Note : *Scale editor*

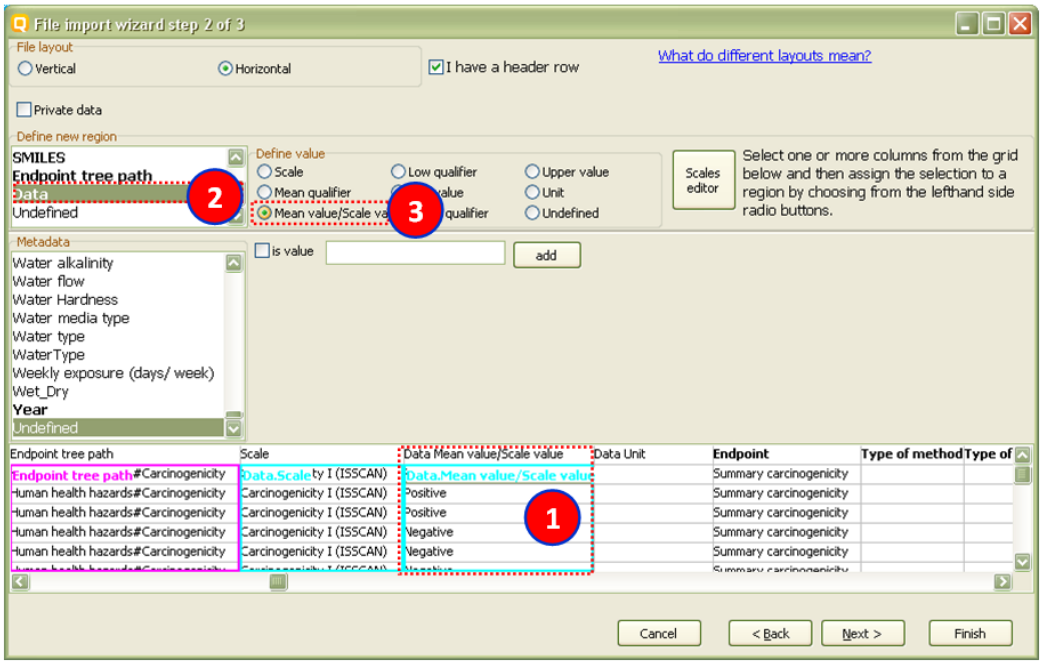


Note : *Scale definition*

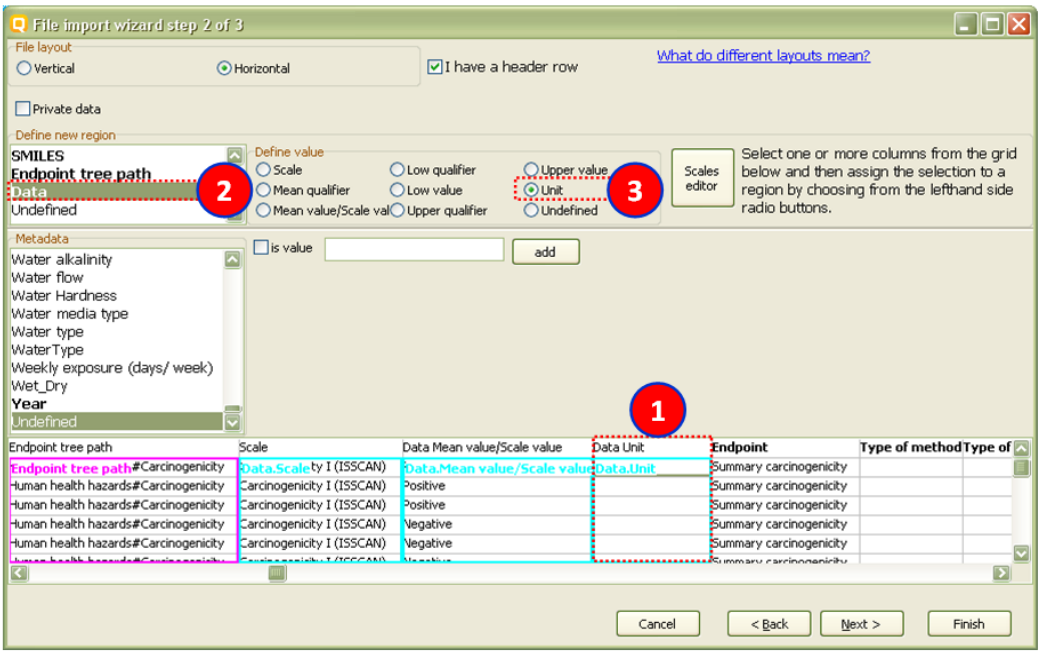


The user should select one of the scales from the Scale list panel or define a new scale.

Select : *DATA Main Value/Scale value*



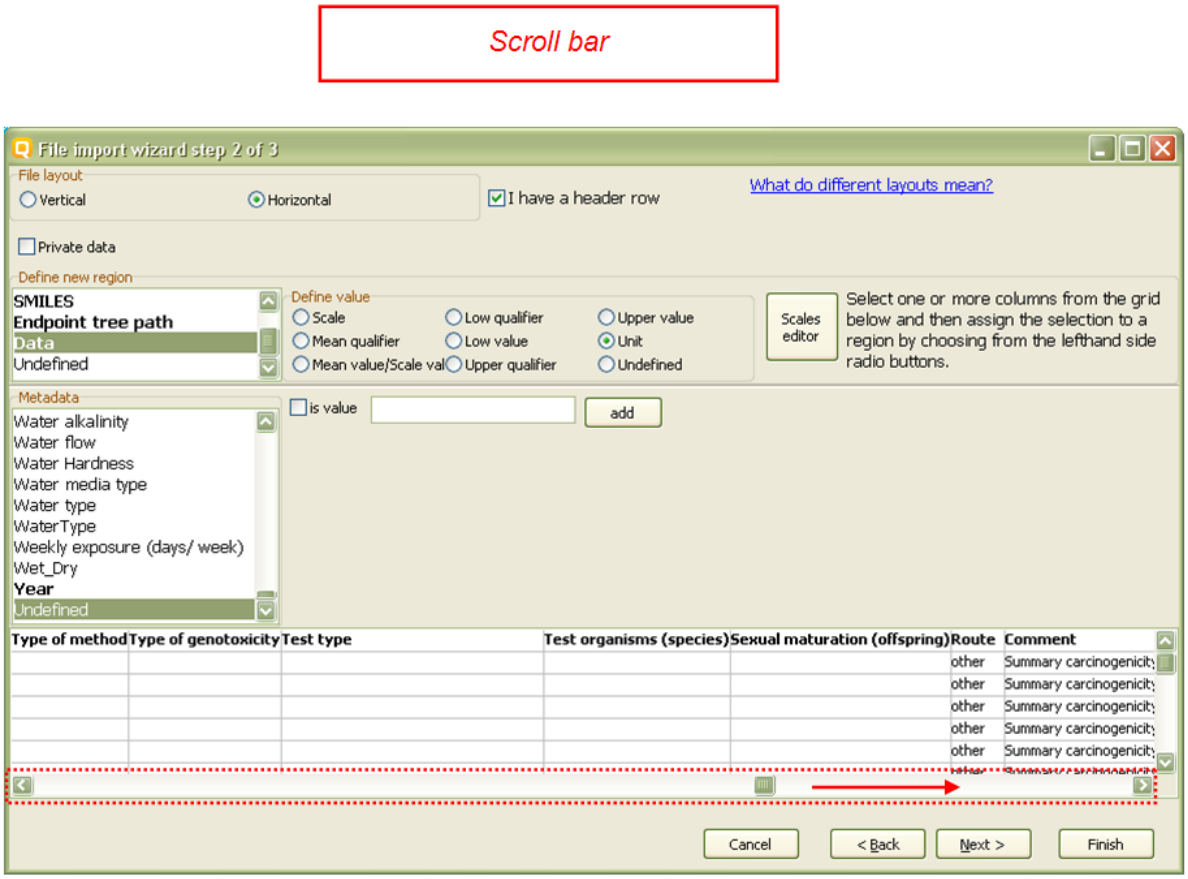
Select : *DATA Unit*



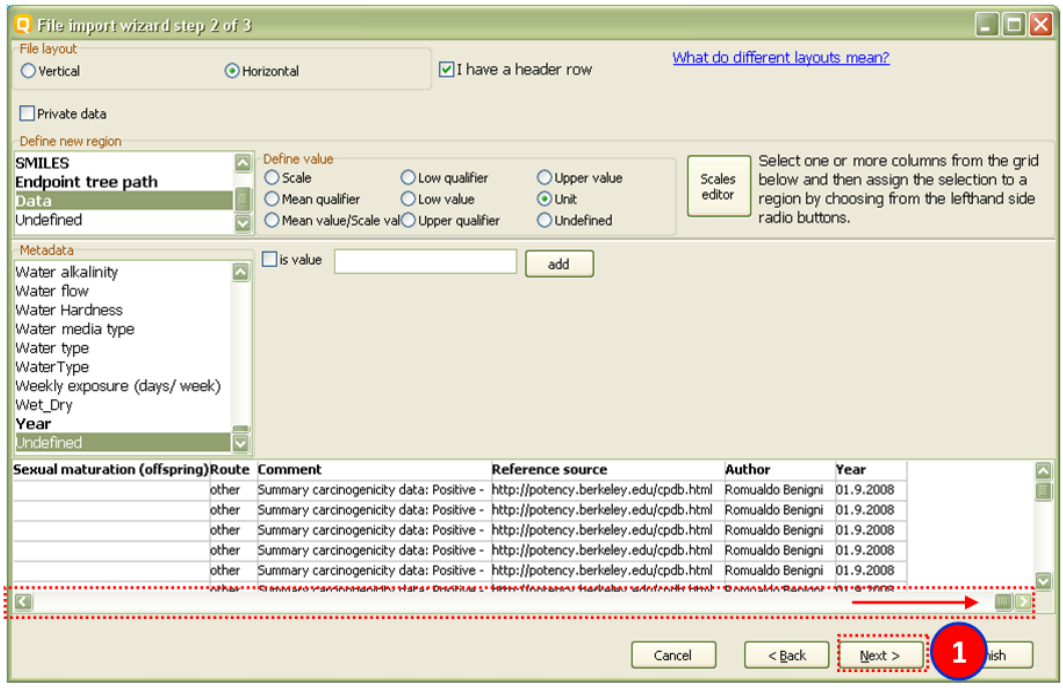
I. The type of the column is specified by clicking on the column and

then clicking its type (CAS/Chemical name/SMILES) from the list box in the **Define new region** panel or selecting a metadata field label from the list box in the **Metadata** panel. To remove designations click a column and then click on **Undefined** from the list box.

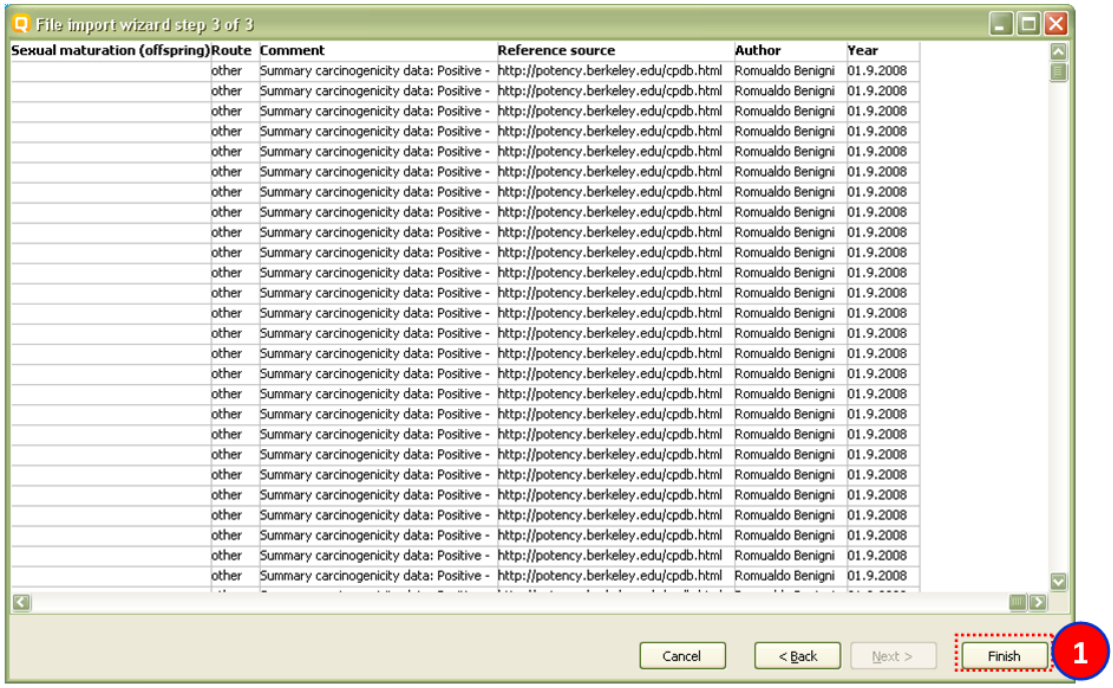
II. All fields fields defined with the **Define new region** panel are color-distinguished from the fields of the **Metadata** panel.



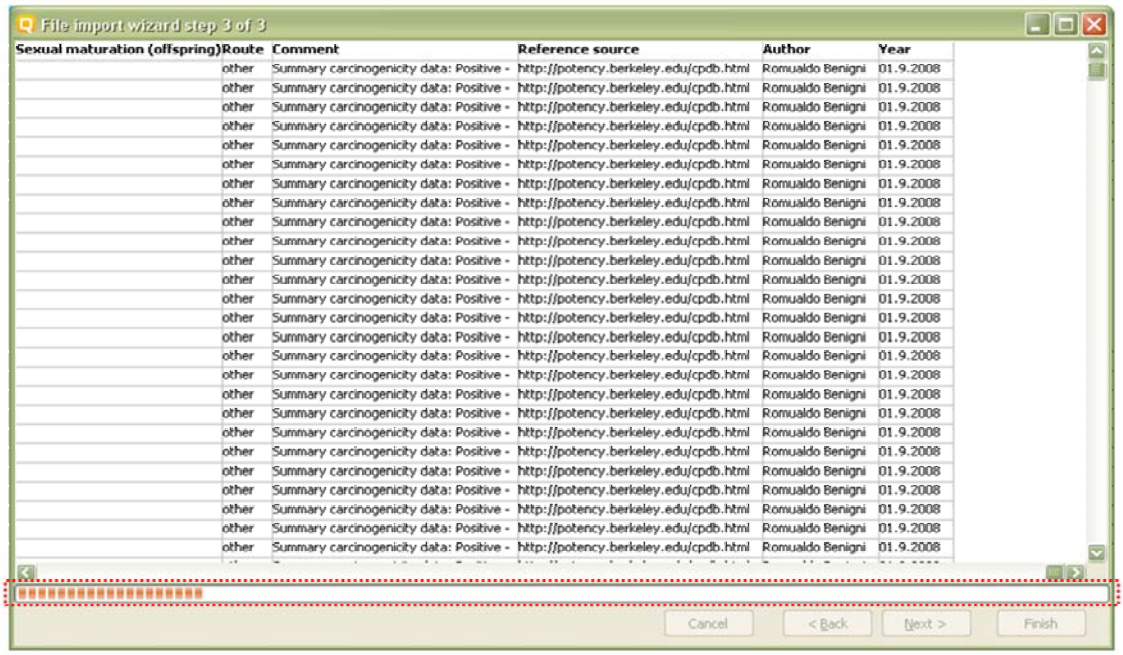
Scroll the bar to review data column designations. Click on *"Next"* button



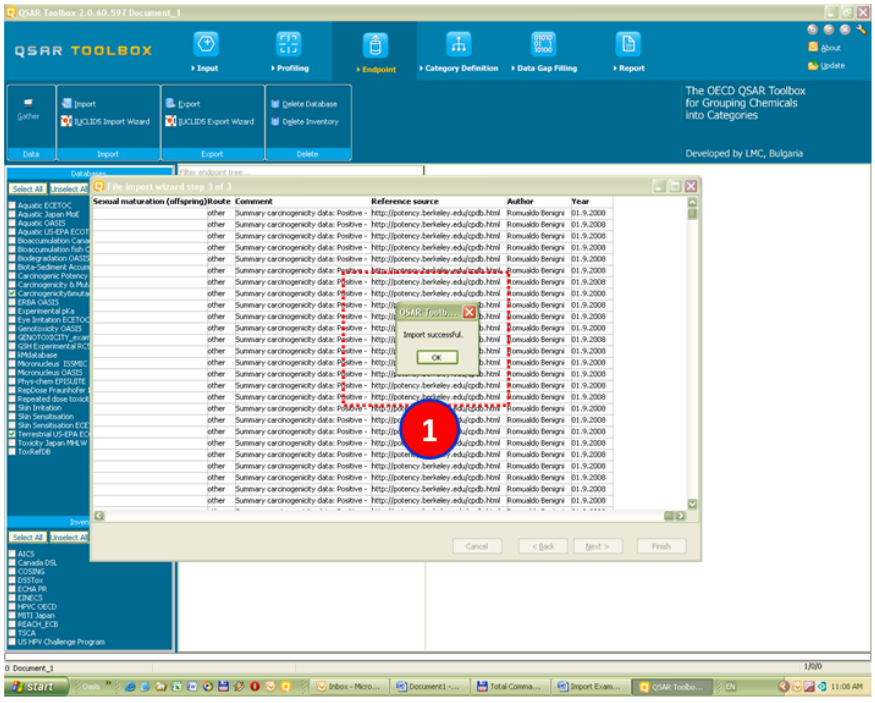
Click on *"Finish"* button



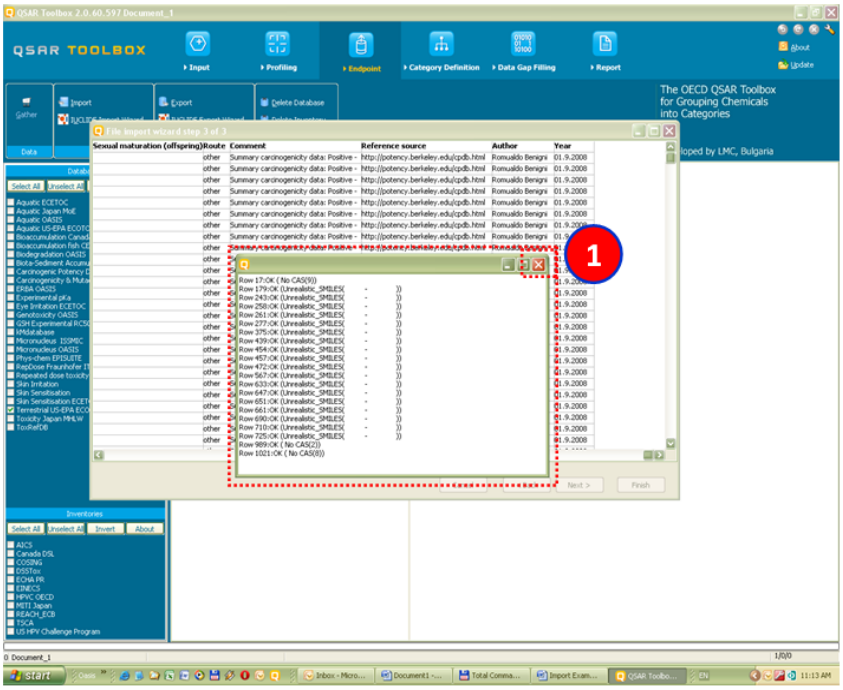
Database is being imported: Progress bar.



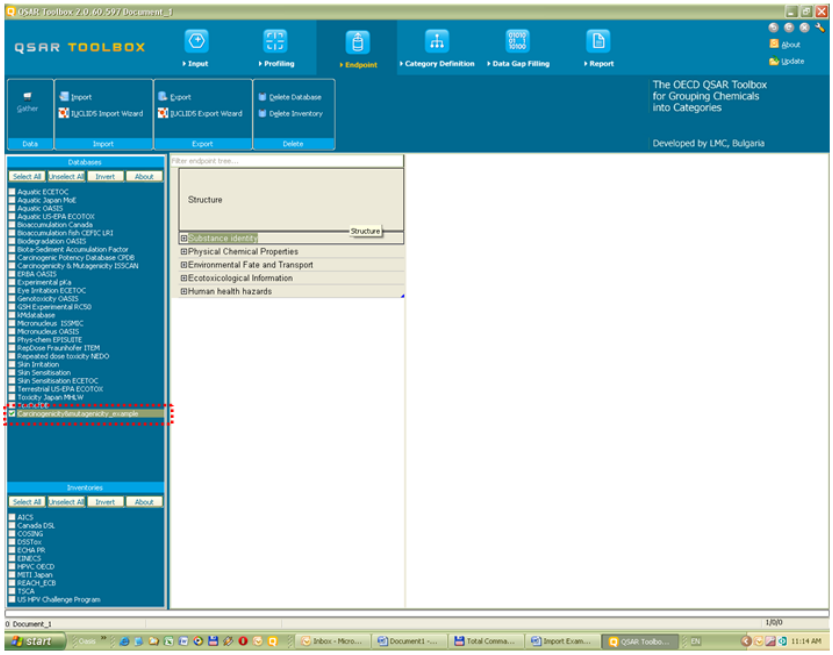
Database is imported successfully. Click *"OK"*.



Error message log file



Imported database

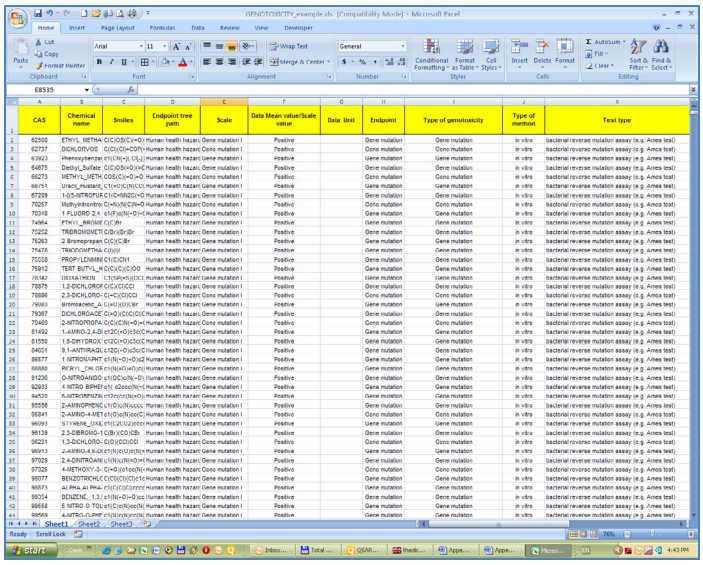


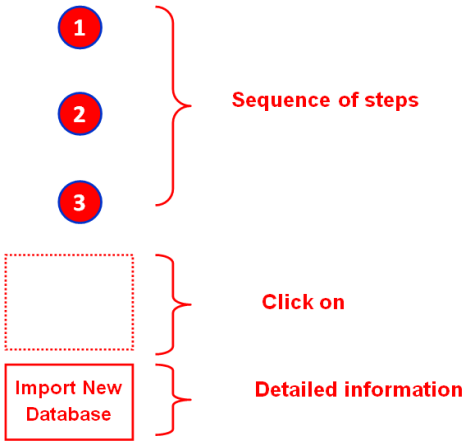
Appendix IV: Import example for database with Human health hazards Information

⚠ The example below uses a file that is already prepared. Guidance on how to prepare file for horizontal import can be found in Appendix I.

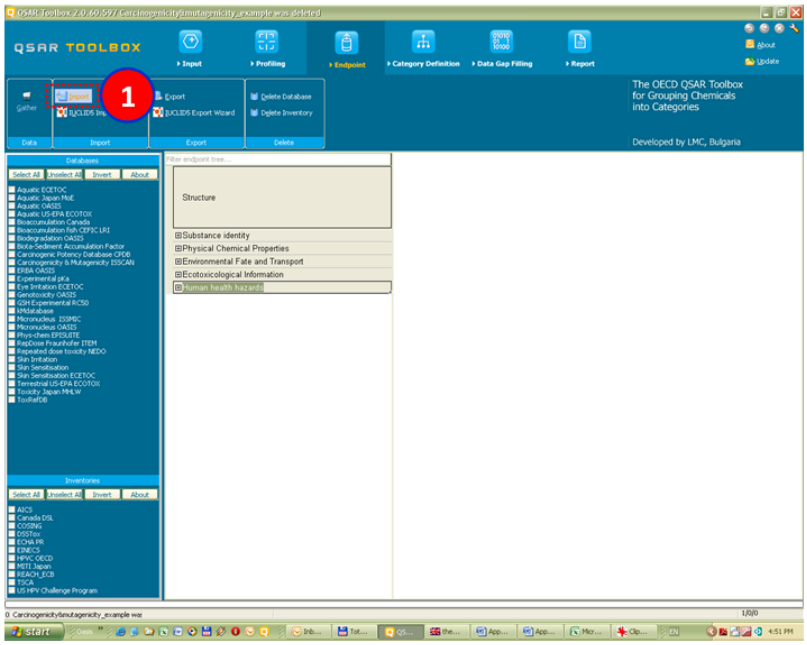
The destination for example files is [Install folder]\Examples.

The default path is C:\Program Files\QSAR Toolbox\QSAR Toolbox 2.1\Examples\GENOTOXICITY_example.xls

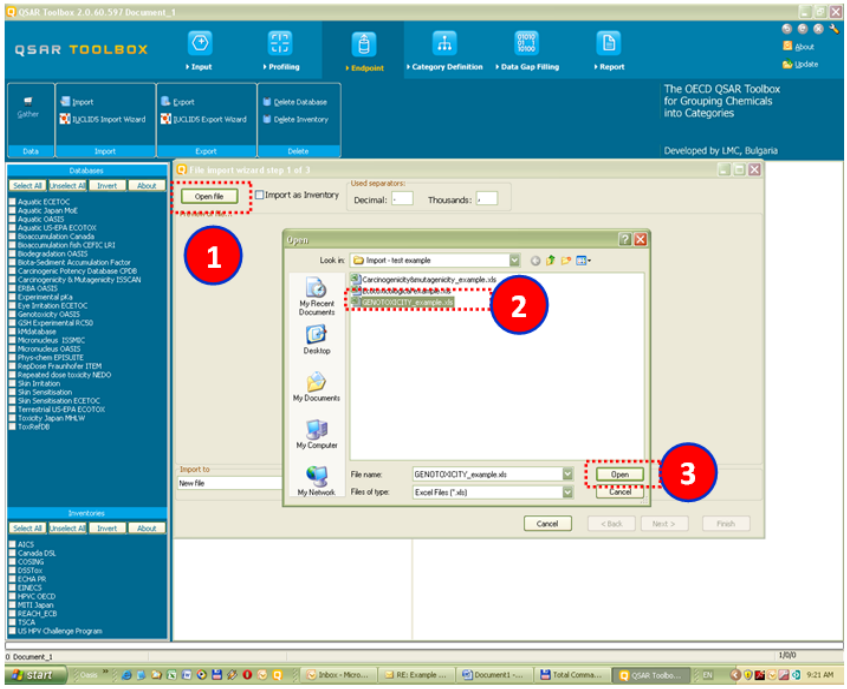


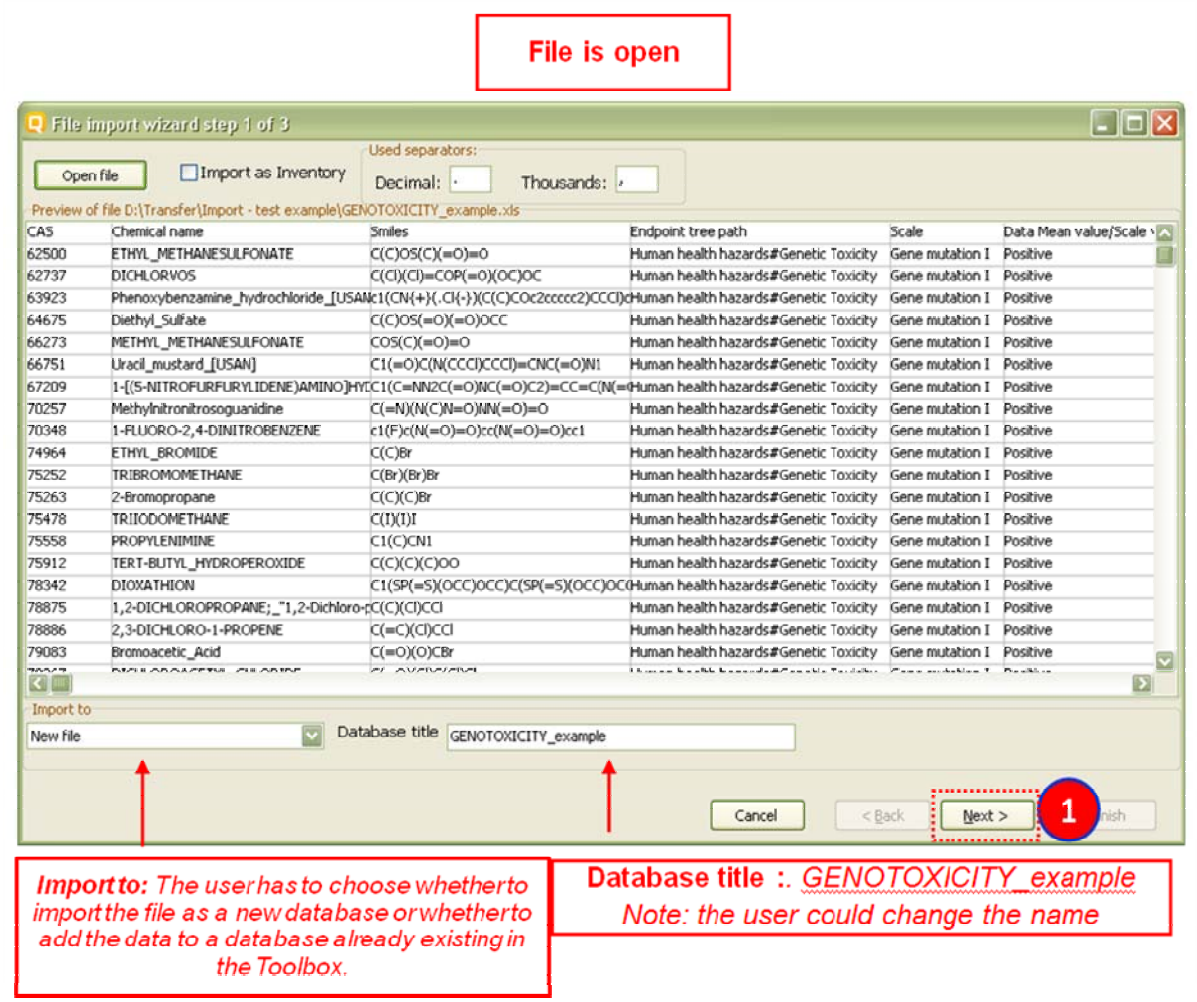


Import New Database



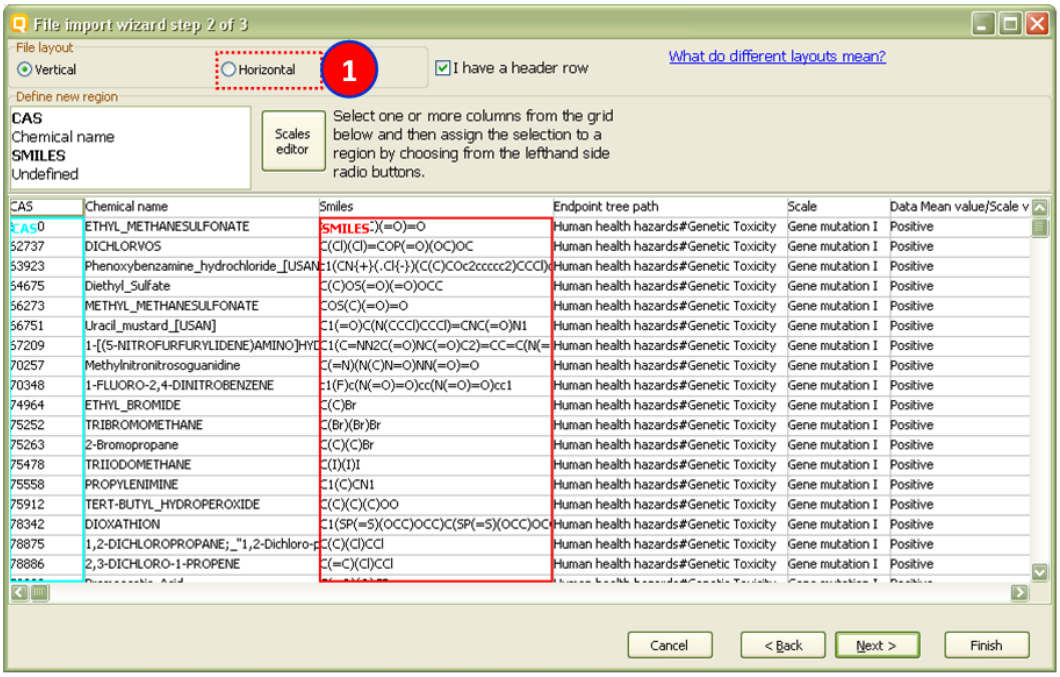
Open example file



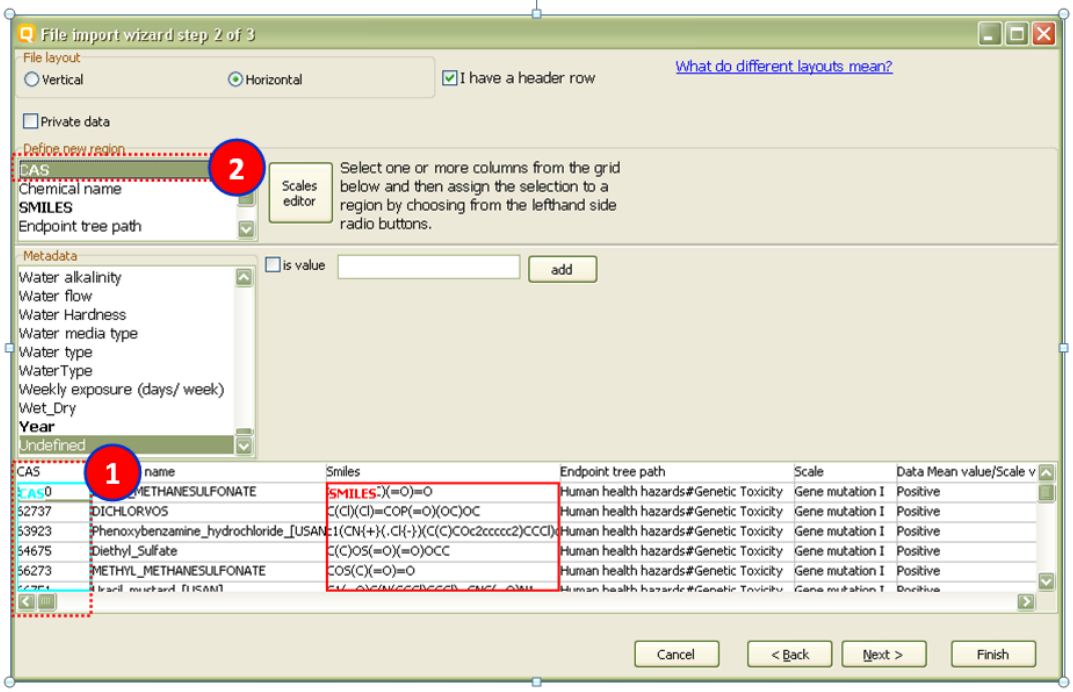


⚠ It is very important that the thousands and decimal separators are properly set while importing. Especially with TXT file this could lead to erroneous parsing of data values.

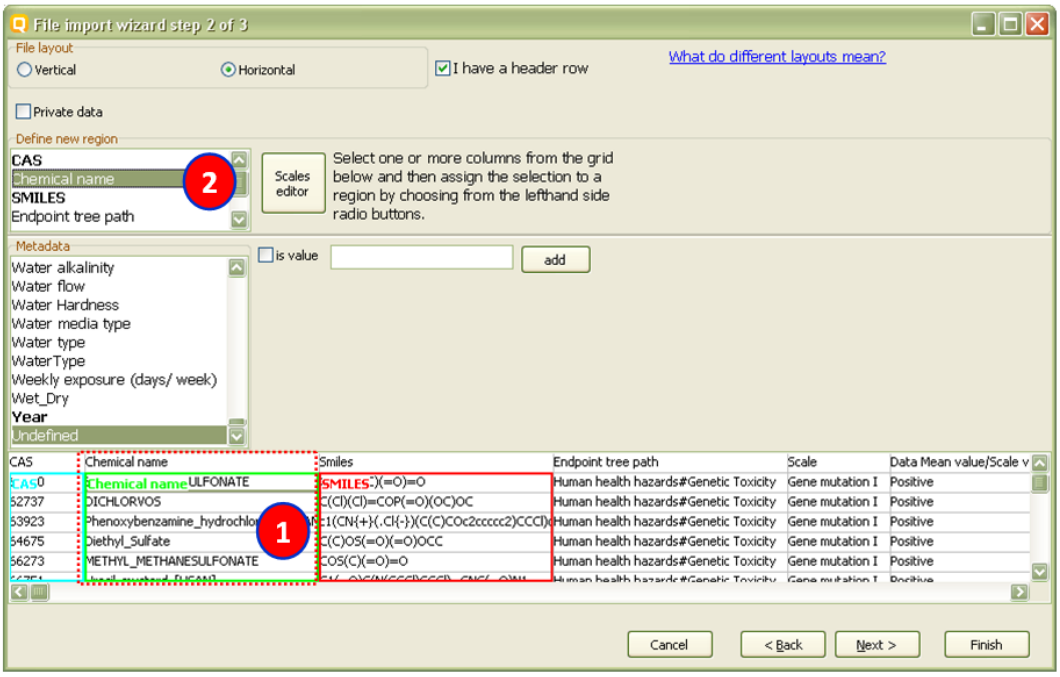
Step 2: Horizontal import



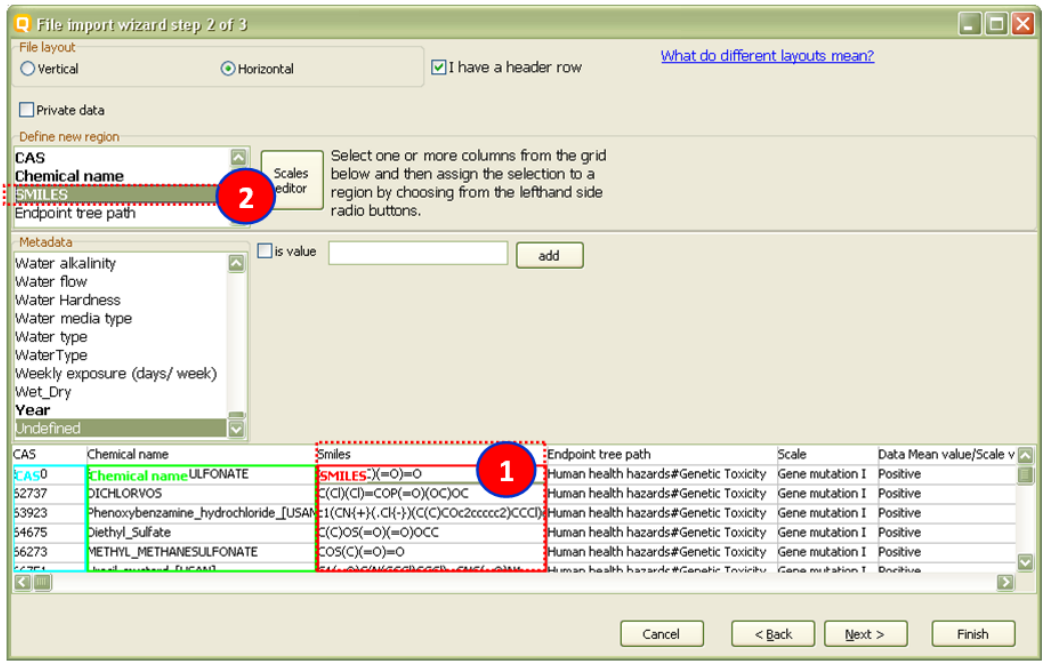
Select : CAS



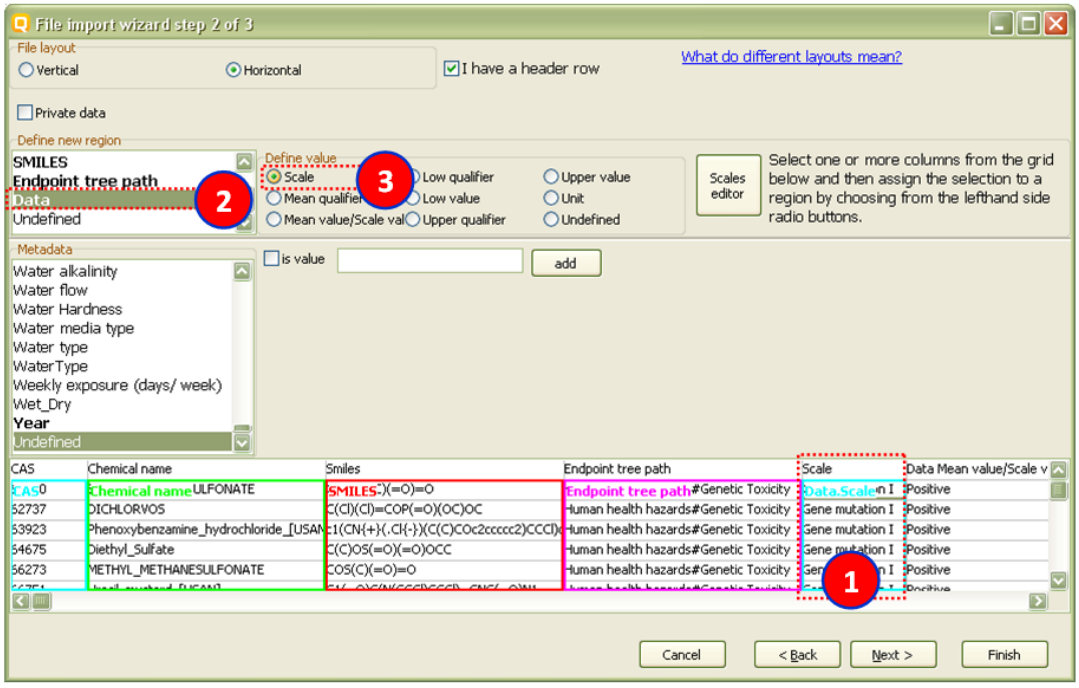
Select : *Chemical name*



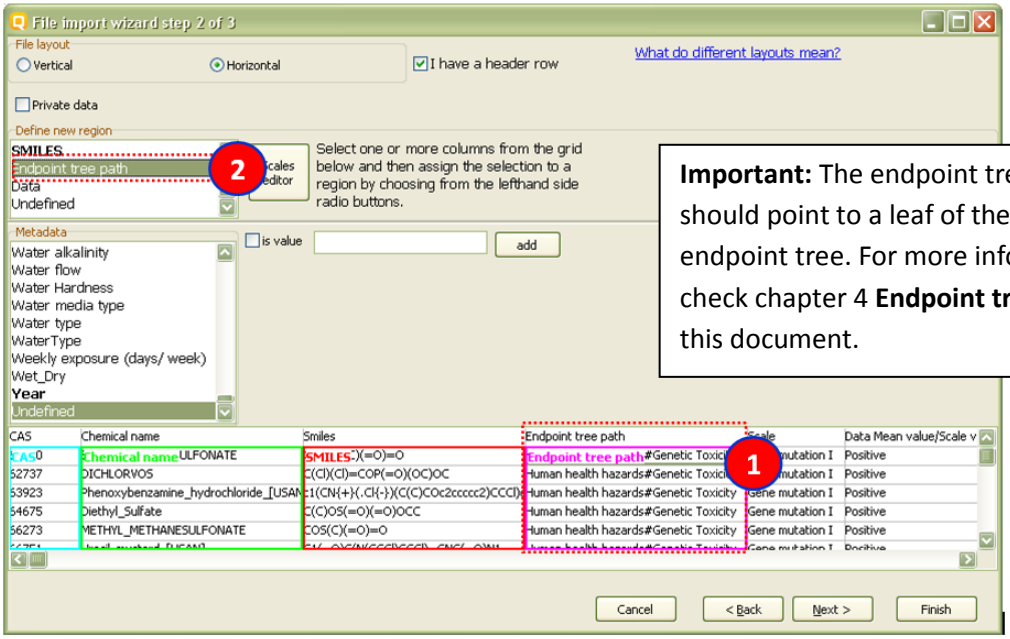
Select : *SMILES*



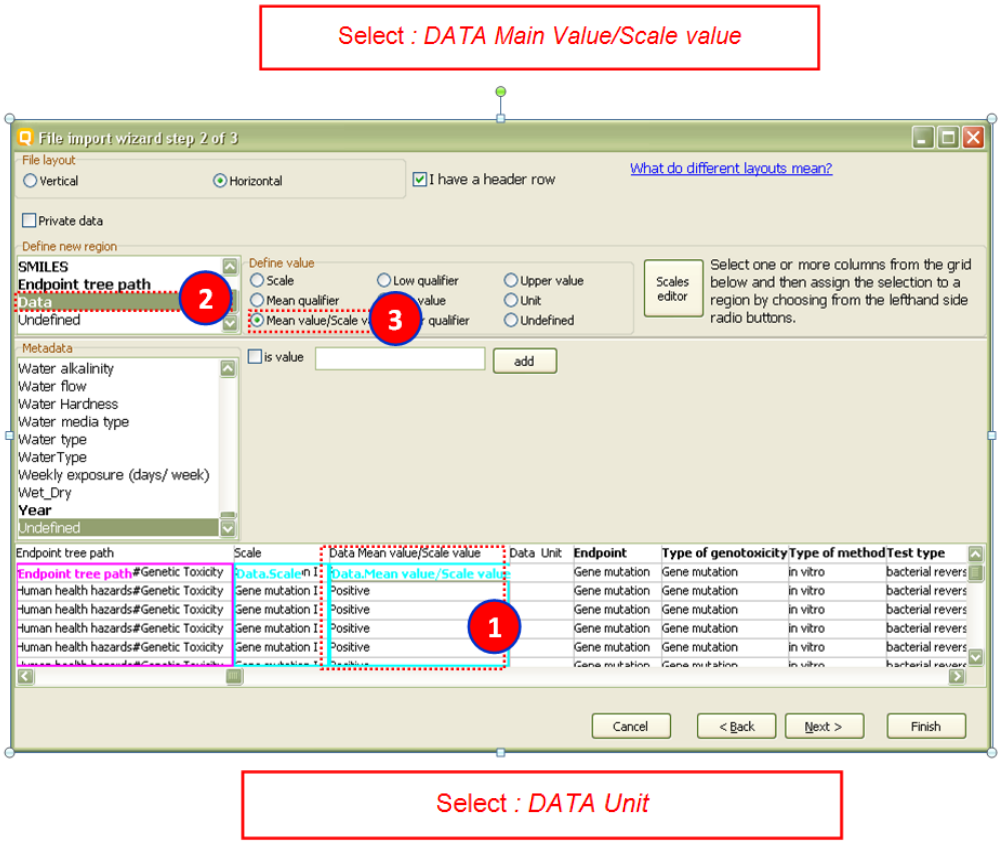
Select : *DATA Scale*

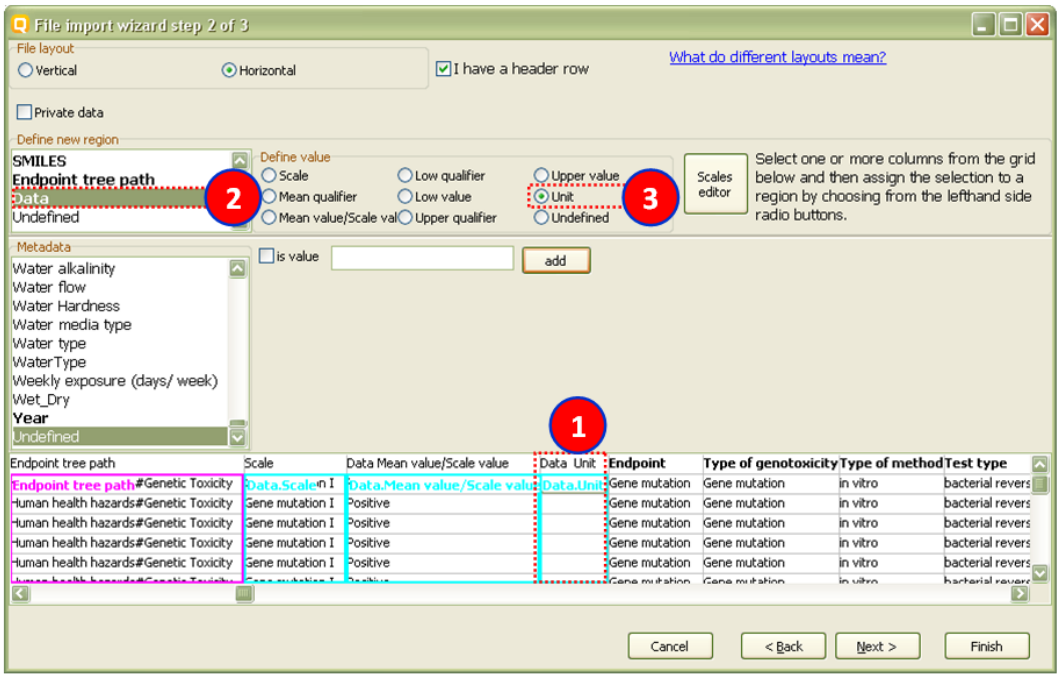


Select : *Endpoint tree path*



Important: The endpoint tree path should point to a leaf of the **predefined** endpoint tree. For more information check chapter 4 **Endpoint tree path** in this document.



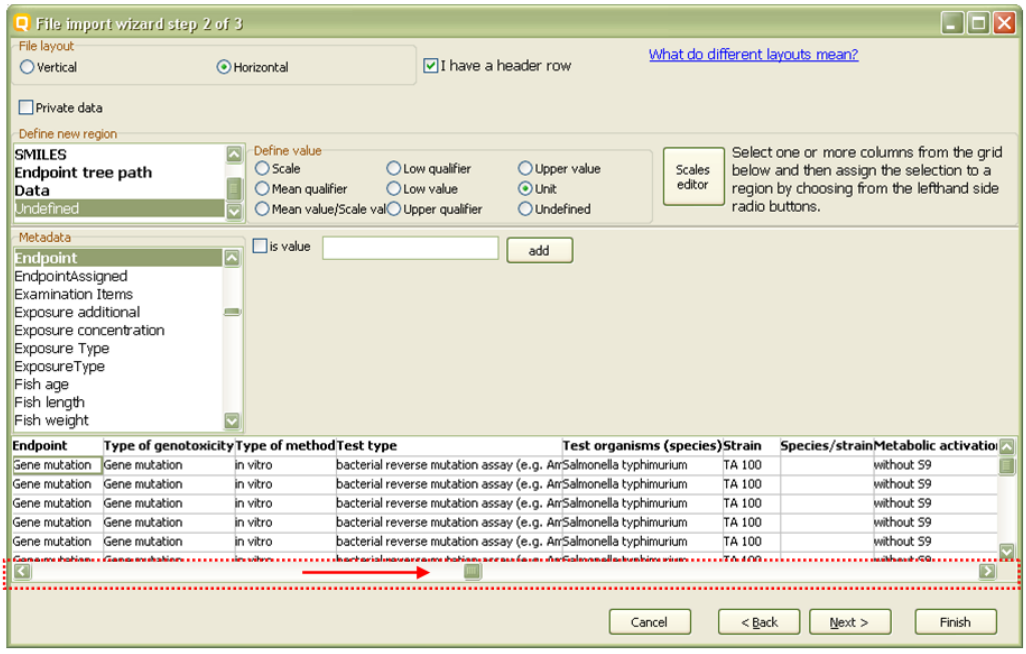


I. The type of the column is specified by clicking on the column and

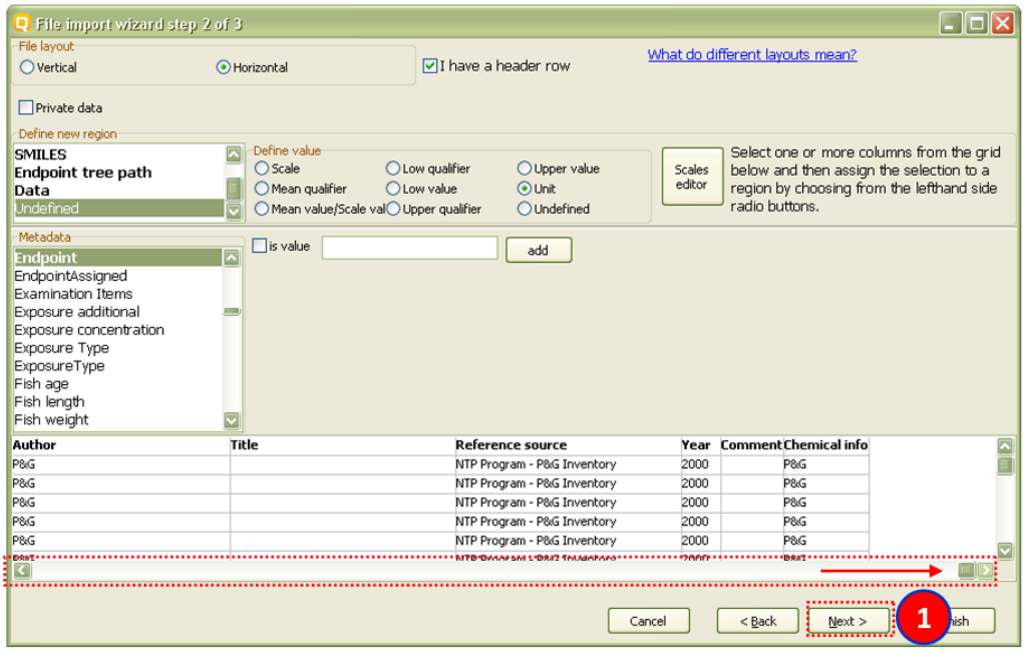
then clicking its type (CAS/Chemical name/SMILES) from the list box in the **Define new region** panel or selecting a metadata field label from the list box in the **Metadata** panel. To remove designations click a column and then click on **Undefined** from the list box.

II. All fields fields defined with the **Define new region** panel are color-distinguished from the fields of the **Metadata** panel.

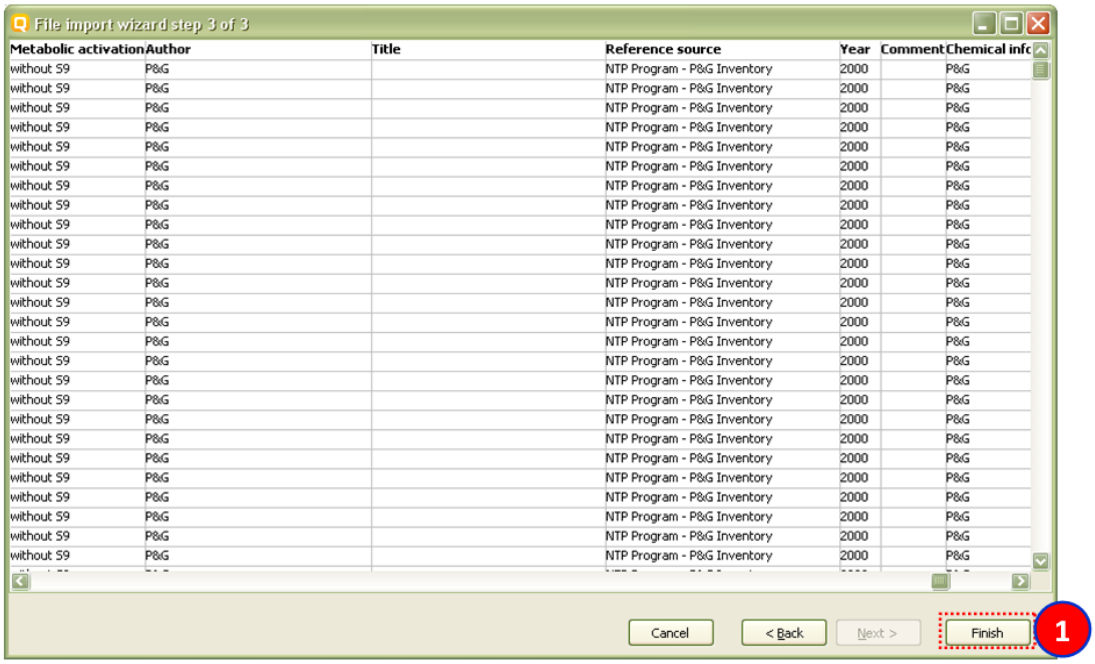
Scroll bar



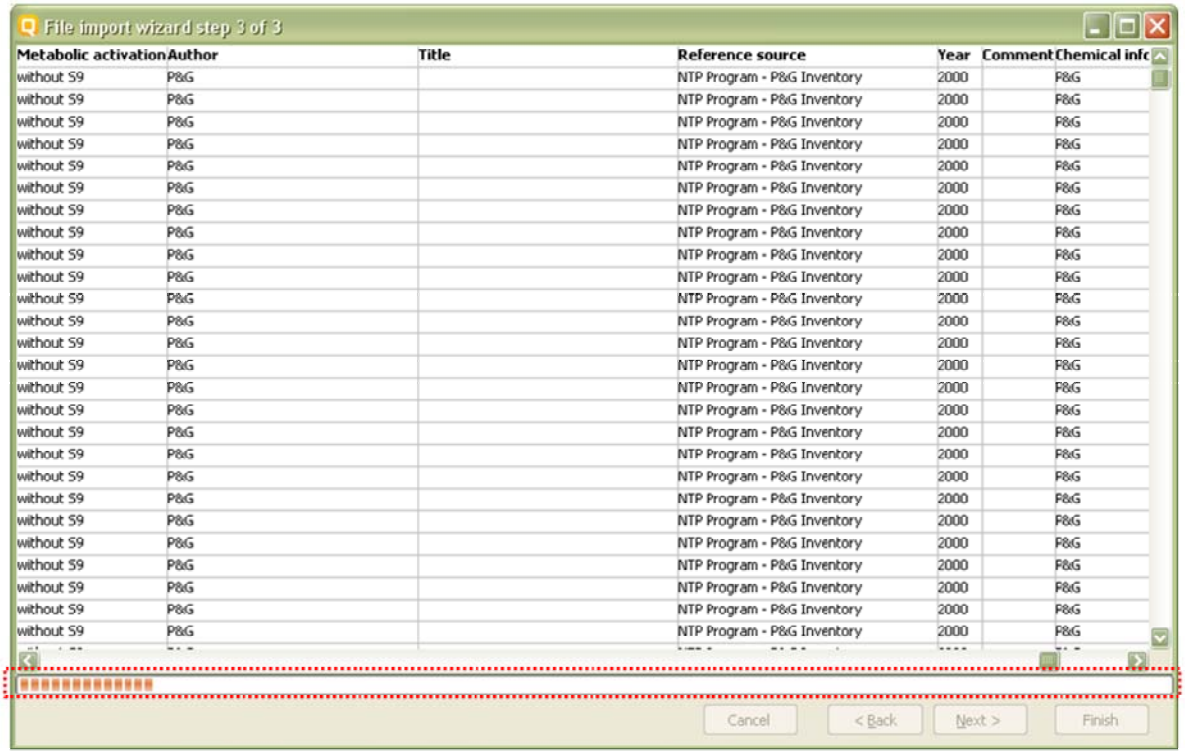
Scroll the bar to review data column designations. Click on *"Next"* button



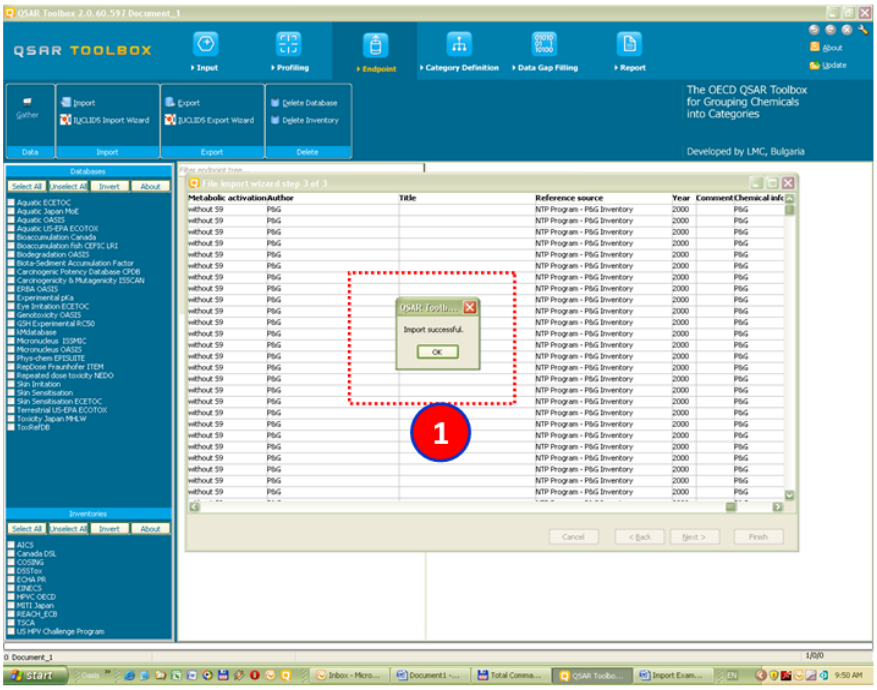
Click on *"Finish"* button



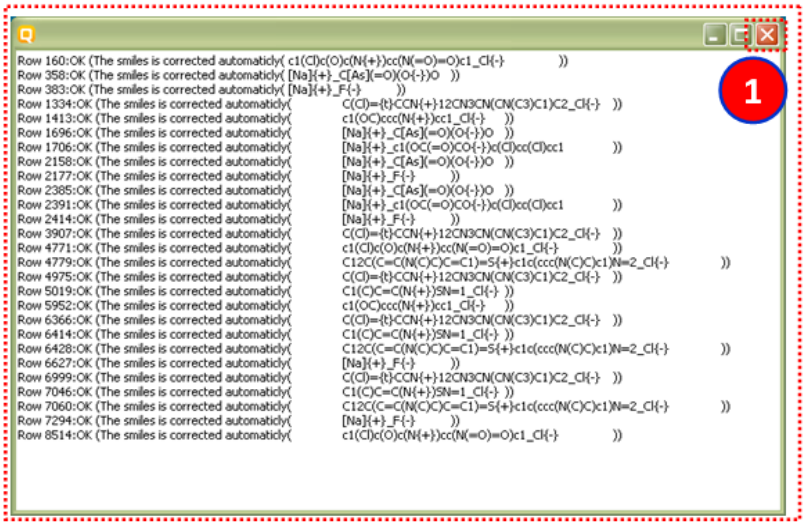
Database is being imported: Progress bar.



Database is imported successfully. Click *"OK"*.



Error message log file



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