

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 |

Issue date: April 2011

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

Table of Contents

| | |
|---|-----------|
| Document history | 1 |
| Document history | 2 |
| 1 Executive summary | 4 |
| 2 QSAR Toolbox data model..... | 4 |
| 3 Import layouts..... | 5 |
| 3.1 Vertical layout..... | 5 |
| 3.2 Horizontal layout | 6 |
| 4 Endpoint tree path | 7 |
| 5 Building the dynamic tree..... | 8 |
| 6 Running the import wizard | 12 |
| 6.1 Vertical | 13 |
| 6.2 Horizontal | 16 |
| Appendix I: Preparing a file for horizontal import | 19 |
| Appendix II: Import example for a database with ecotoxicological information | 31 |
| Appendix III: Import example for database with Human health hazards | |
| Information | 47 |
| Appendix IV: Import example for database with Human health hazards | |
| Information | 59 |

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:

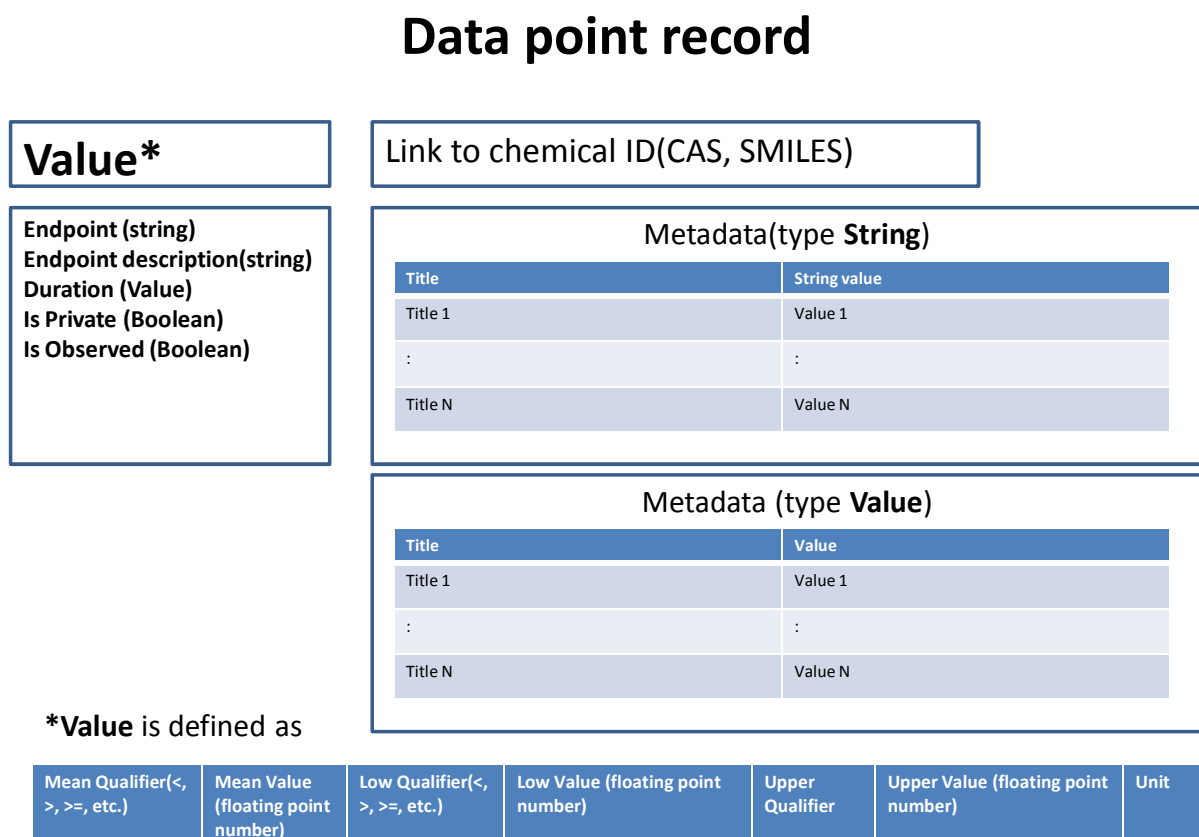


Figure 1: Database structure of the QSAR Toolbox

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.

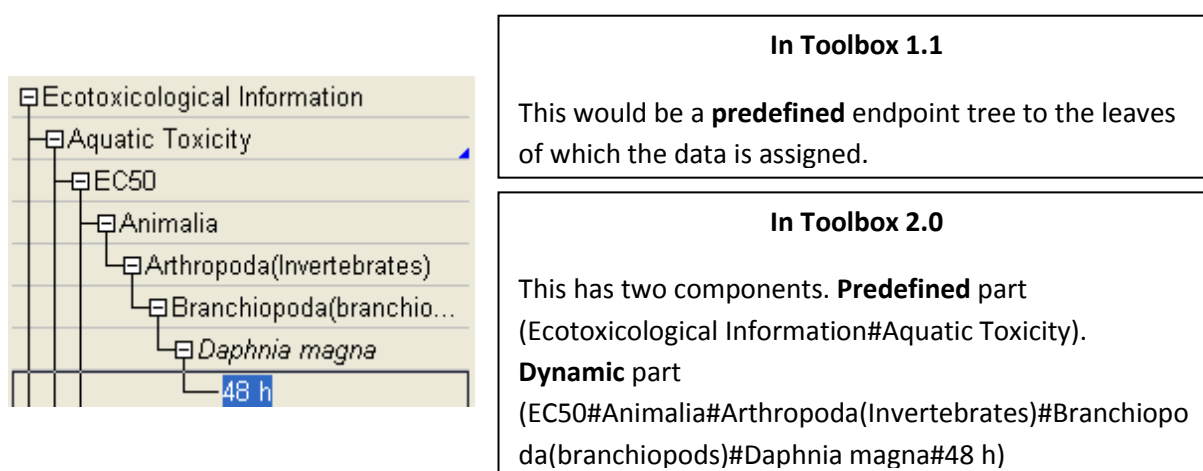


Figure 4: Endpoint tree in Toolbox version 1.1 vs. Endpoint tree in QSAR Toolbox version 2.0

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.

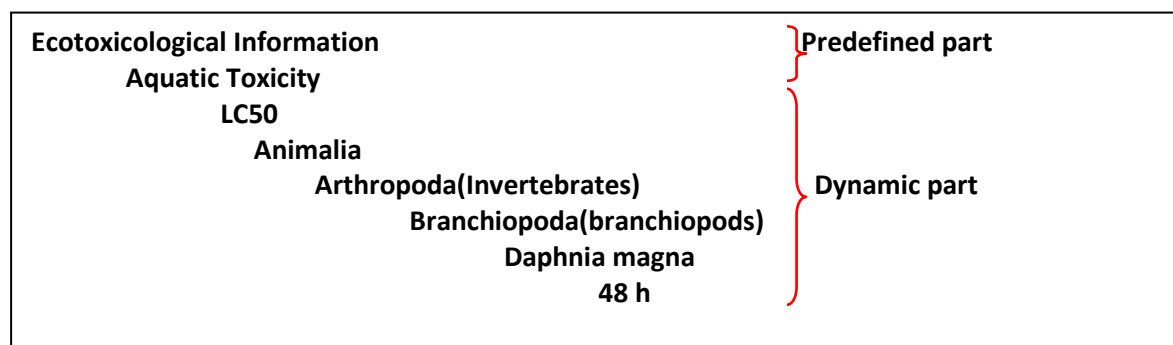
How does the above pertain to the import?

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**

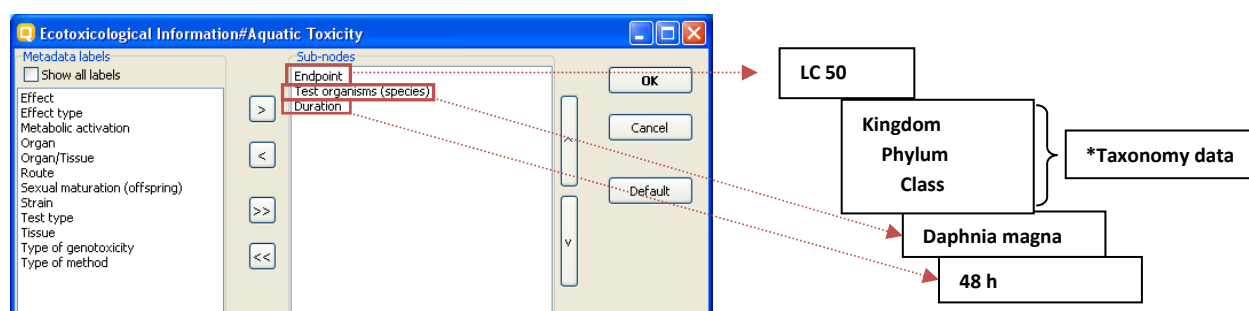
Where do the other fields come from?

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**.



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 mutation, 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.


Endpoint path

| | |
|--|-------------------|
| Endpoint tree path | ation#Aquatic Tox |
| Ecotoxicological Information#Aquatic Tox | |
| Ecotoxicological Information#Aquatic Tox | |
| Ecotoxicological Information#Aquatic Tox | |
| Ecotoxicological Information#Aquatic Tox | |
| Ecotoxicological Information#Aquatic Tox | |
| Ecotoxicological Information#Aquatic Tox | |

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.

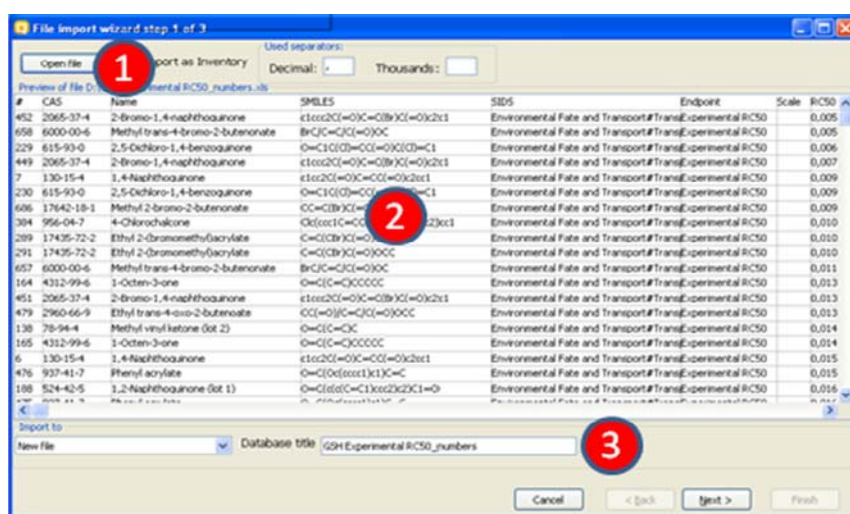


Figure 7: Import wizard step one

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

File import wizard step 2 of 3

File layout:
☒ Vertical ☐ Horizontal ☒ I have a header row [What do different layouts mean?](#)

Define new region

CAS
 Chemical name
 SMILES
 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.

| CAS | Name | SMILES | RC50 value |
|------------|-----------------------------------|--------------------------------|---------------------------|
| CAS-37-4 | Chemical name | thoquinone | SMILES=O)C=C(Br)C(=O)c2c1 |
| 5000-00-6 | Methyl trans-4-bromo-2-butenonate | BrC/C=C/C(=O)OC | 0,0050 |
| 515-93-0 | 2,5-Dichloro-1,4-benzoquinone | O=C1C(Cl)=CC(=O)C(Cl)=C1 | 0,0053 |
| 2065-37-4 | 2-Bromo-1,4-naphthoquinone | O=C1C(Cl)=CC(=O)C(Cl)=C1 | 0,0063 |
| 130-15-4 | 1,4-Naphthoquinone | c1ccc2C(=O)C=C(Br)C(=O)c2c1 | 0,0070 |
| 515-93-0 | 2,5-Dichloro-1,4-benzoquinone | c1cc2C(=O)C=C(C(=O)c2cc1 | 0,0090 |
| 17642-18-1 | Methyl 2-bromo-2-butenonate | CC=C(Br)C(=O)OC | 0,0091 |
| 956-04-7 | 4-Chlorochalcone | Clc(ccc1C=CC(=O)c(ccc2)cc2)cc1 | 0,0097 |
| 17435-72-2 | Ethyl 2-(bromomethyl)acrylate | C=C(CBr)C(=O)OCC | 0,010 |
| 17435-72-2 | Ethyl 2-(bromomethyl)acrylate | C=C(CBr)C(=O)OCC | 0,010 |
| 5000-00-6 | Methyl trans-4-bromo-2-butenonate | BrC/C=C/C(=O)OC | 0,011 |

Cancel < Back Next > Finish

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.

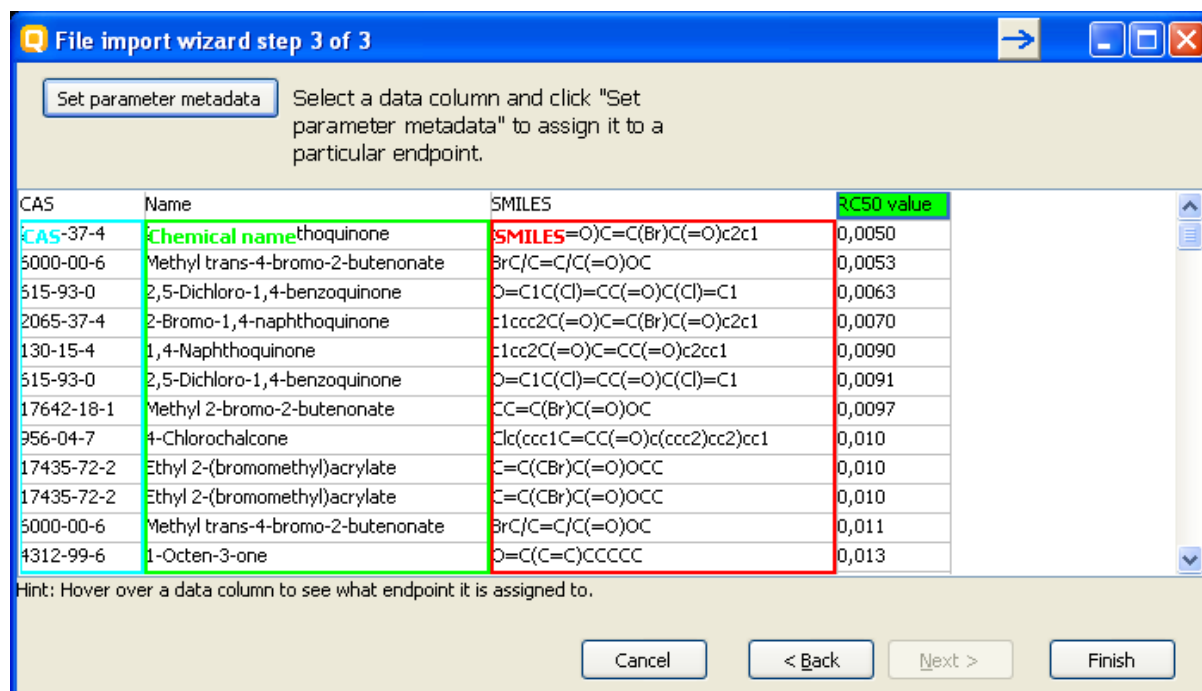


Figure 9: Import wizard step 3 (vertical import)

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).

☐ Scale data
Unit:

☐ Private data

Data tree position

- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
 - Aquatic Toxicity
 - Sediment toxicity
 - Terrestrial Toxicity
- Human health hazards

Metadata fields:

#1: Effect
Value type:
☒ Text
☐ Value

#2: Duration
Value type:
☐ Text
☒ Value
Mean value:
Lower value:
Upper value:
Unit:

#3: Test organisms (species)
Value type:
☒ Text
☐ Value
Abarenicola pacifica

Add field...

OK Cancel

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.



 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 |
|----|----------|--------------------------|----------|---------------|------------|------|-----------|-----------|------------|----------|-------------|-----|------------------|----------------|--------------|----------|------|----------|------------------|-------------|
| 1 | EC 50 | Ceriodaphnia | 48 | h | | | Immobilis | Juvenile | Freshwater | | 23 | | | | 2.2 | WARNE | 1999 | | | |
| 2 | EC 50 | Daphnia magna | 1 | h | | | Physiol | Juvenile | Freshwater | | 20 | | | | 3 | JANSSEN | 1993 | | | End point |
| 3 | EC 50 | Daphnia magna | 24 | h | | | Mortality | Juvenile | Freshwater | | 20 | | | | 3 | JANSSEN | 1993 | | | |
| 4 | EC 50 | Daphnia magna | 48 | h | | | Mortality | Juvenile | Freshwater | | 20 | | | | 3 | JANSSEN | 1993 | | | |
| 5 | EC 50 | Vibrio fischeri | 0.25 | h | | | Behavior | Adult | Saltwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 6 | EC 50 | Ampelisca alba | 24 | h | | | Mortality | | Saltwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 7 | EC 50 | Scrobicularia | 24 | h | | | Mortality | | Freshwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 8 | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 9 | EC 50 | Pimephales | 456 | h | | | Reproduct | Adult | Freshwater | | 26 | 8.1 | 317 | | 1 | Kramer V | 1998 | Reprodu | Aquat Toxicol | 4 End point |
| 10 | EC 50 | Pimephales | 456 | h | | | Reproduct | Adult | Freshwater | | 26 | 8.1 | 317 | | 1 | Kramer V | 1998 | Reprodu | Aquat Toxicol | 4 End point |
| 11 | EC 50 | Pimephales | 456 | h | | | Mortality | Adult | Freshwater | | 26 | 8.1 | 317 | | 1 | Kramer V | 1998 | Reprodu | Aquat Toxicol | 4 Male fish |
| 12 | EC 50 | Hemicentrotus | 2.25 | h | | | Reproduct | Egg | Saltwater | | 15 | | | | 3 | WYNBEF | 1989 | | | Egg refer |
| 13 | EC 50 | Penaeus van | 48 | h | | | Mortality | Juvenile | Saltwater | 20 | 28.5 | | | | 3 | REYES | 1996 | | | |
| 14 | EC 50 | Hyalella azteca | 240 | h | | | Mortality | | Freshwater | | 22 | | | | 1 | Phipps G | 1995 | Relative | Arch Env Cont | |
| 15 | EC 50 | Chironomus | 240 | h | | | Mortality | | Freshwater | | 22 | | | | 1 | Phipps G | 1995 | Relative | Arch Env Cont | |
| 16 | EC 50 | Vibrio fischeri | 0.25 | h | | | Behavior | Adult | Saltwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 17 | EC 50 | Ampelisca alba | 24 | h | | | Mortality | | Saltwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 18 | EC 50 | Scrobicularia | 24 | h | | | Mortality | | Freshwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 19 | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 20 | EC 50 | Vibrio fischeri | 0.25 | h | | | Behavior | Adult | Saltwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 21 | EC 50 | Ampelisca alba | 24 | h | | | Mortality | | Saltwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 22 | EC 50 | Scrobicularia | 24 | h | | | Mortality | | Freshwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 23 | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 24 | EC 50 | Vibrio fischeri | 0.25 | h | | | Behavior | Adult | Saltwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 25 | EC 50 | Ampelisca alba | 24 | h | | | Mortality | | Saltwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 26 | EC 50 | Scrobicularia | 24 | h | | | Mortality | | Freshwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 27 | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | | | | | 2.2 | Calleja | 1994 | | | |
| 28 | EC 50 | Vibrio fischeri | 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.

Endpoint tree path

Structural information

Experimental Data

Metadata information

| CAS | NAME | Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qualifier | Data Unit | Endpoint | Test organisms (species) | Duration | Duration Unit | Solubility | Unit | Effect | Lifestage | Water type | Salinity | Temperat |
|---------|---------------------|--------|--------------------|-----------------------------|---------------------|-----------|----------|--------------------------|----------|---------------|------------|------|-----------|----------------|------------|----------|----------|
| 50-00-0 | FORMALI C=O | | Ecotoxicological | 12.98 | > | mg/L | EC 50 | Ceriodaphnia | 48 | h | | | Immobili | Juvenile | Freshwater | | 23 |
| 50-00-0 | FORMALI C=O | | Ecotoxicological | 39 | > | mg/L | EC 50 | Daphnia maj | 1 | h | | | Physiol | Juvenile | Freshwater | | 20 |
| 50-00-0 | FORMALI C=O | | Ecotoxicological | 57 | > | mg/L | EC 50 | Daphnia maj | 24 | h | | | Mortality | Juvenile | Freshwater | | 20 |
| 50-00-0 | FORMALI C=O | | Ecotoxicological | 29 | > | mg/L | EC 50 | Daphnia maj | 48 | h | | | Mortality | Juvenile | Freshwater | | 20 |
| 50-06-6 | PHEXOB C11=O/C | | Ecotoxicological | 2095.767 | > | mg/L | EC 50 | Vibrio fischer | 0.25 | h | | | Behavior | Adult | Saltwater | | |
| 50-06-6 | PHEXOB C11=O/C | | Ecotoxicological | 10009.113 | < | mg/L | EC 50 | Ampelica al | 24 | h | | | Mortality | | Saltwater | | |
| 50-06-6 | PHEXOB C11=O/C | | Ecotoxicological | 1212.5406 | < | mg/L | EC 50 | Scrobicula | 24 | h | | | Mortality | | Freshwater | | |
| 50-06-6 | PHEXOB C11=O/C | | Ecotoxicological | 5178.729 | < | mg/L | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | |
| 50-28-2 | BETA-ES c12c(C) | | Ecotoxicological | 0.00012 | < | mg/L | EC 50 | Pimephales | 456 | h | | | Reprodu | Adult | Freshwater | | 26 |
| 50-28-2 | BETA-ES c12c(C) | | Ecotoxicological | 0.000251 | < | mg/L | EC 50 | Pimephales | 456 | h | | | Reprodu | Adult | Freshwater | | 26 |
| 50-28-2 | BETA-ES c12c(C) | | Ecotoxicological | 0.00115 | > | mg/L | EC 50 | Pimephales | 456 | h | | | Mortality | Adult | Freshwater | | 26 |
| 50-29-3 | DOT C(C)C(C)C | | Ecotoxicological | 70 | > | mg/L | EC 50 | Hemicent | 2.25 | h | | | Reprodu | Egg | Saltwater | | 15 |
| 50-29-3 | DOT C(C)C(C)C | | Ecotoxicological | 0.0087 | > | mg/L | EC 50 | Penseus van | 48 | h | | | Mortality | Juvenile | Saltwater | 20 | 28.5 |
| 50-29-3 | DOT, P, P C(C)C(C)C | | Ecotoxicological | 0.00007 | > | mg/L | EC 50 | Hyalella azei | 240 | h | | | Mortality | | Freshwater | | 22 |
| 50-29-3 | DOT, P, P C(C)C(C)C | | Ecotoxicological | 0.00123 | > | mg/L | EC 50 | Chironomus | 240 | h | | | Mortality | | Freshwater | | 22 |
| 50-48-6 | AMITRYP c12c(C) | | Ecotoxicological | 21.580942 | > | mg/L | EC 50 | Vibrio fischer | 0.25 | h | | | Behavior | Adult | Saltwater | | |
| 50-48-6 | AMITRYP c12c(C) | | Ecotoxicological | 36.89287 | > | mg/L | EC 50 | Ampelica al | 24 | h | | | Mortality | | Saltwater | | |
| 50-48-6 | AMITRYP c12c(C) | | Ecotoxicological | 0.776692 | > | mg/L | EC 50 | Scrobicula | 24 | h | | | Mortality | | Freshwater | | |
| 50-48-6 | AMITRYP c12c(C) | | Ecotoxicological | 0.804431 | s | mg/L | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | |
| 50-54-4 | QUINIDI c12c(C) | | Ecotoxicological | 836.684 | s | mg/L | EC 50 | Vibrio fischer | 0.25 | h | | | Behavior | Adult | Saltwater | | |
| 50-54-4 | QUINIDI c12c(C) | | Ecotoxicological | 273.3837 | s | mg/L | EC 50 | Ampelica al | 24 | h | | | Mortality | | Saltwater | | |
| 50-54-4 | QUINIDI c12c(C) | | Ecotoxicological | 8.291145 | s | mg/L | EC 50 | Scrobicula | 24 | h | | | Mortality | | Freshwater | | |
| 50-54-4 | QUINIDI c12c(C) | | Ecotoxicological | 8.65462 | s | mg/L | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | |
| 50-63-5 | CHLORO c11NC(C) | | Ecotoxicological | 866.712 | > | mg/L | EC 50 | Vibrio fischer | 0.25 | h | | | Behavior | Adult | Saltwater | | |
| 50-63-5 | CHLORO c11NC(C) | | Ecotoxicological | 2042.964 | > | mg/L | EC 50 | Ampelica al | 24 | h | | | Mortality | | Saltwater | | |
| 50-63-5 | CHLORO c11NC(C) | | Ecotoxicological | 11.65934 | > | mg/L | EC 50 | Scrobicula | 24 | h | | | Mortality | | Freshwater | | |
| 50-63-5 | CHLORO c11NC(C) | | Ecotoxicological | 4.38515 | > | mg/L | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | |
| 50-78-2 | ACETYLE C(=O)O | | Ecotoxicological | 26.12175 | > | mg/L | EC 50 | Vibrio fischer | 0.25 | h | | | Behavior | Adult | Saltwater | | |
| 50-78-2 | ACETYLE C(=O)O | | Ecotoxicological | 381.918 | > | mg/L | EC 50 | Ampelica al | 24 | h | | | Mortality | | Saltwater | | |
| 50-78-2 | ACETYLE C(=O)O | | Ecotoxicological | 177.9882 | > | mg/L | EC 50 | Scrobicula | 24 | h | | | Mortality | | Freshwater | | |
| 50-78-2 | ACETYLE C(=O)O | | Ecotoxicological | 141.41775 | > | mg/L | EC 50 | Brachionus c | 24 | h | | | Mortality | | Freshwater | | |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 0.5 | > | mg/L | NOEC | Oncorhynch | 720 | h | 8710 mg/L | | Growth | Early lifestag | Freshwater | | 12 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 0.8 | > | mg/L | NOEC | Oncorhynch | 720 | h | 8710 mg/L | | Growth | Early lifestag | Freshwater | | 17 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 0.9 | > | mg/L | NOEC | Cyprinodon v | 672 | h | 8710 mg/L | | Growth | Early lifestag | Saltwater | 15 | 22 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 1.1 | > | mg/L | NOEC | Oncorhynch | 1440 | h | 8710 mg/L | | Growth | Early lifestag | Freshwater | | 7 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 1.3 | > | mg/L | NOEC | Oncorhynch | 1440 | h | 8710 mg/L | | Mortality | Early lifestag | Freshwater | | 7 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 1.6 | > | mg/L | NOEC | Oncorhynch | 720 | h | 8710 mg/L | | Mortality | Early lifestag | Freshwater | | 17 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 1.8 | > | mg/L | NOEC | Oncorhynch | 720 | h | 8710 mg/L | | Growth | Embryo | Freshwater | | 17 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 1.9 | > | mg/L | NOEC | Oncorhynch | 720 | h | 8710 mg/L | | Mortality | Early lifestag | Freshwater | | 12 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 1.9 | > | mg/L | NOEC | Cyprinodon v | 672 | h | 8710 mg/L | | Growth | Early lifestag | Saltwater | 15 | 22 |
| 51-28-5 | DINITROI c1(O)N | | Ecotoxicological | 1.9 | > | mg/L | NOEC | Cyprinodon v | 672 | h | 8710 mg/L | | Growth | Early lifestag | Saltwater | 25 | 22 |

Endpoint data region

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-}4C |
| 50-28-2 | BETA-ESTRADIOL, 1 | c12c(C{P+}3C{P+})(C{P-}4C |
| 50-28-2 | BETA-ESTRADIOL, 1 | c12c(C{P+}3C{P+})(C{P-}4C |
| 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 |
| Ecotoxicological Information#Aquatic Toxicity |

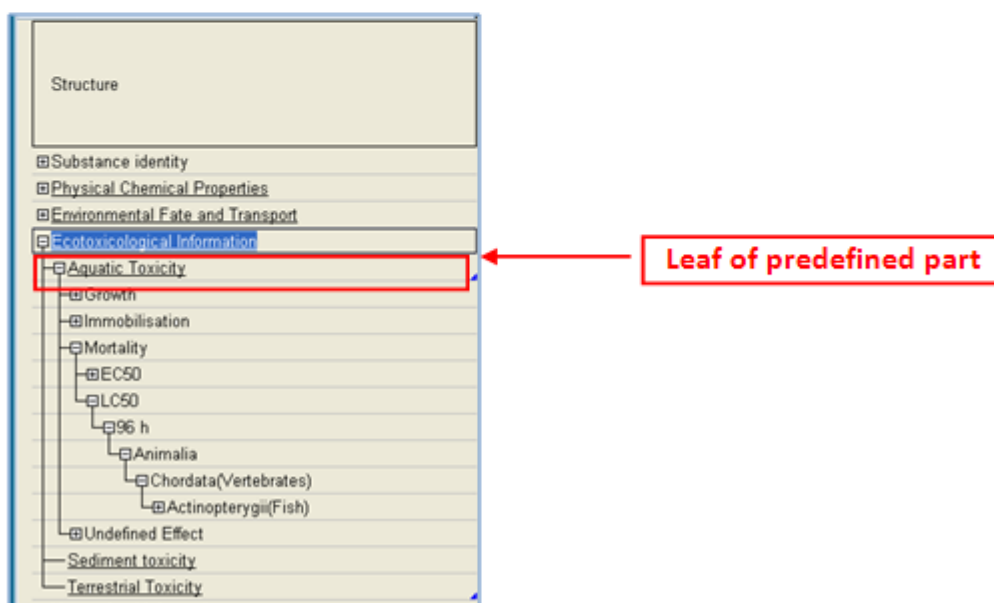
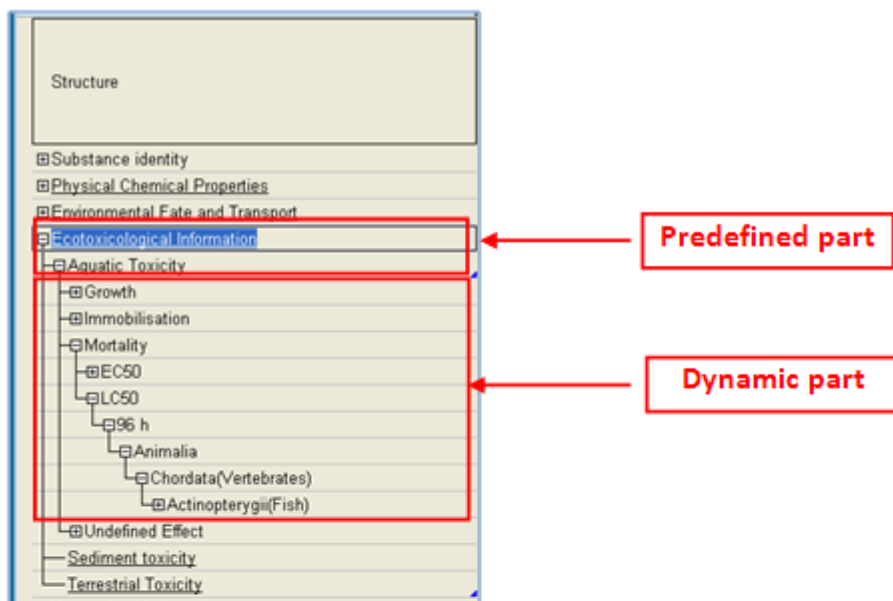
Important: The endpoint tree path should point to a leaf of the **predefined** endpoint tree. For more information check chapter 4 **Endpoint tree path** of this document.

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*)

Endpoint 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 operates with the following data structure:

Data point record

Value*

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

Link to chemical ID(CAS, SMILES)

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:

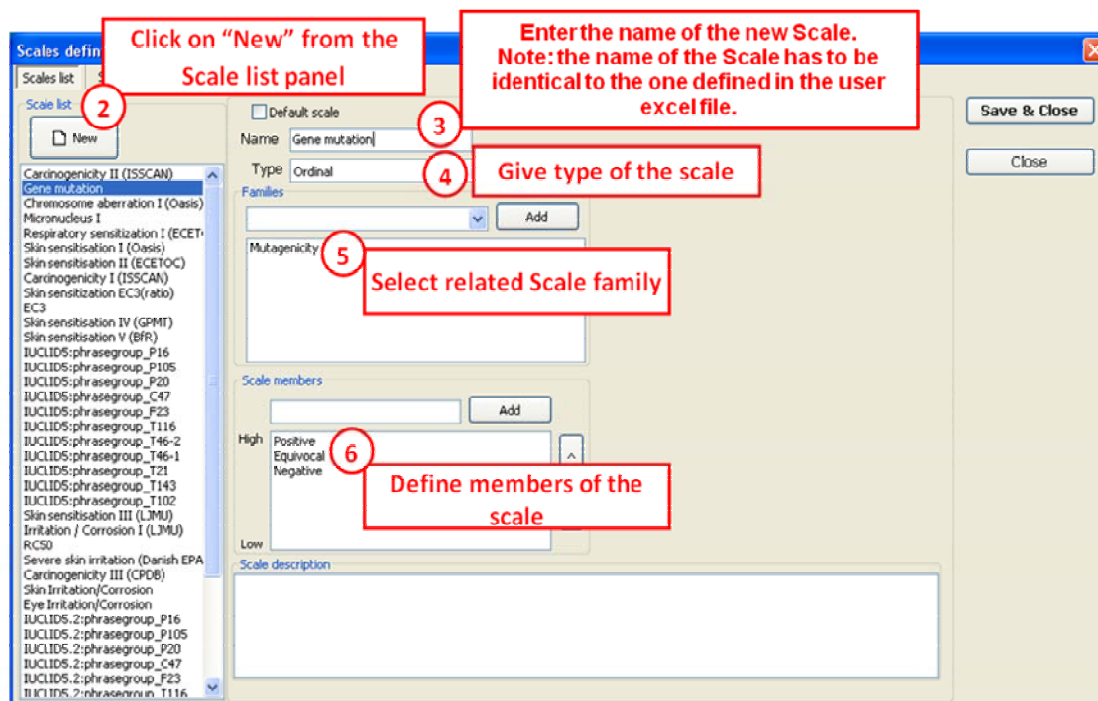
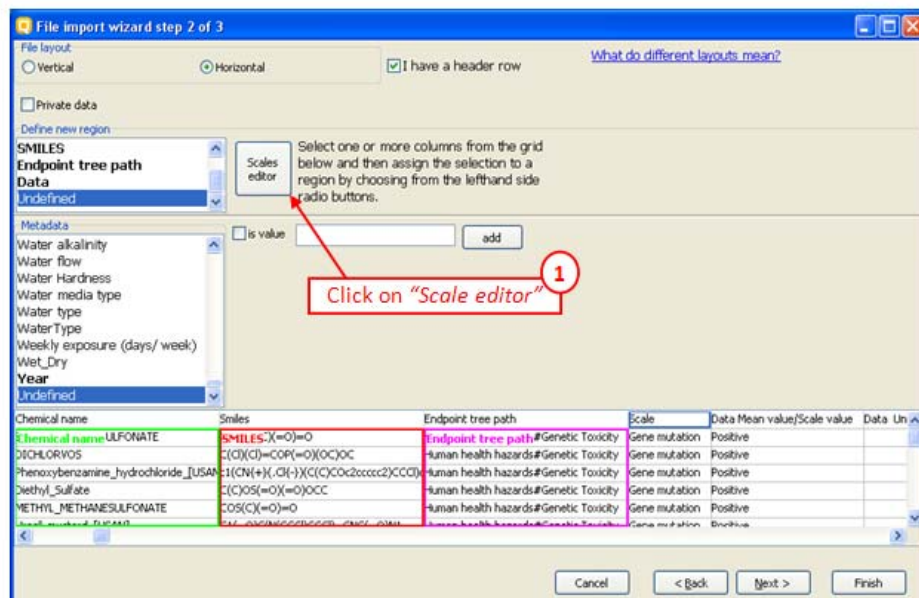
1. The file for import should have a **Scale** column for the scale name. This should contain a name of a scale **exactly** as defined in the scales list in the QSAR Toolbox database for example "Gene mutation I" is a scale from the QSAR Toolbox database scale list (*red colored fields*):

The screenshot shows the 'Scales definition...' dialog box with the 'Scales list' tab selected. In the list, 'Gene mutation I' is highlighted. The 'Name' field is 'Gene mutation I' and the 'Type' is 'Ordinal'. The 'Scale members' are listed as 'Positive', 'Equivocal', and 'Negative'. A red arrow points from the 'Gene mutation I' entry in the list to the 'Scale' column in the data table. A blue arrow points from the 'Scale members' box to the 'Data Mean value/Scale value' column in the data table.

| | A | B | C | D | E | F |
|----|-------|------------------|--------------------------|---------------------|-----------------|-----------------------------|
| | CAS | Chemical name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale value |
| 1 | | | | | | |
| 2 | 62500 | ETHYL_METHA | C(C)OS(C)(=O) | Human health hazard | Gene mutation I | Positive |
| 3 | 62737 | DICHLORVOS | C(Cl)(Cl)=COP(=O) | Human health hazard | Gene mutation I | Positive |
| 4 | 63923 | Phenoxybenzai | c1(CN(-)(Cl)Cl)c2ccccc12 | Human health hazard | Gene mutation I | Positive |
| 5 | 64875 | Diethyl_Sulfate | C(C)OS(=O)(=O)C | Human health hazard | Gene mutation I | Positive |
| 6 | 66273 | METHYL_METH | COS(C)(=O)=O | Human health hazard | Gene mutation I | Positive |
| 7 | 66751 | Uracil_mustard | C1(=O)C(N)CCC(=O)N1 | Human health hazard | Gene mutation I | Positive |
| 8 | 67209 | 1-[(5-NITROFUR | C1(=O)N(C2=O)C=CC2)N1 | Human health hazard | Gene mutation I | Equivocal |
| 9 | 70257 | Methylnitronitro | C(=N)(N)C(N)=O | Human health hazard | Gene mutation I | Positive |
| 10 | 70348 | 1-FLUORO-2,4- | c1(F)c(N(=O)=O)c2ccccc12 | Human health hazard | Gene mutation I | Positive |
| 11 | 74964 | ETHYL_BROMI | C(C)Br | Human health hazard | Gene mutation I | Positive |
| 12 | 75252 | TRIBROMOMETI | C(Br)(Br)Br | Human health hazard | Gene mutation I | Positive |
| 13 | 75263 | 2-Bromopropan | C(C)C(Br) | Human health hazard | Gene mutation I | Positive |
| 14 | 75478 | TRIDODIMETHA | C(Cl)(Cl)Cl | Human health hazard | Gene mutation I | Positive |
| 15 | 75558 | PROPYLENIMINI | C1(C)CN1 | Human health hazard | Gene mutation I | Negative |
| 16 | 75912 | TERT-BUTYL_H | C(C)(C)C(C)OO | Human health hazard | Gene mutation I | Positive |
| 17 | 78342 | DIOXATHION | C1(S(=S)(OCC)CCN1 | Human health hazard | Gene mutation I | Positive |
| 18 | 78875 | 1,2-DICHLOROF | C(Cl)ClCl | Human health hazard | Gene mutation I | Positive |

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

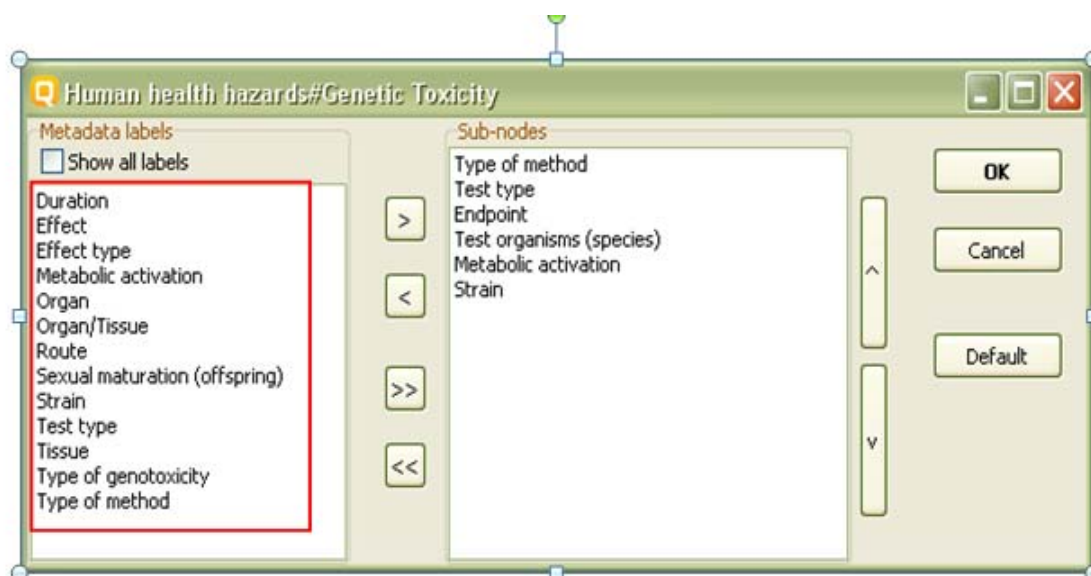
These are fields for metadata such as Duration, Organ, Tissue, Route of administration etc., which are not mandatory for the import:

*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 al | 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 f | 456 | h | | | Reproduc | Adult | Freshwater | | 26 | 8.1 | 317 | | 1 |
| EC 50 | Pimephales f | 456 | h | | | Reproduc | Adult | Freshwater | | 26 | 8.1 | 317 | | 1 |
| EC 50 | Pimephales f | 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 aztei | 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.

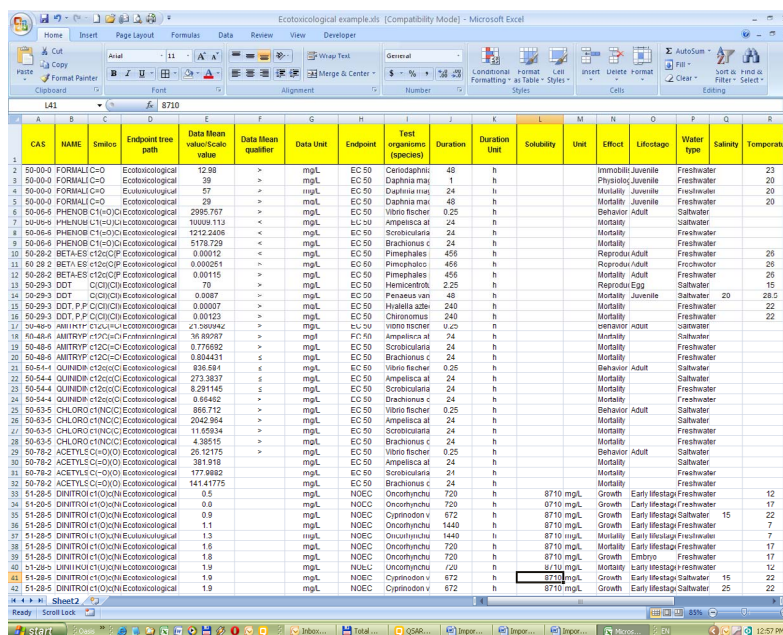
Appendix II: Import example for a database with ecotoxicological information

 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.

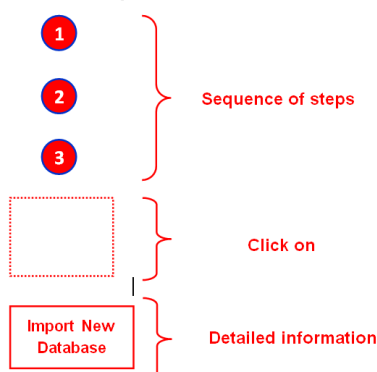
The destination for example files is [Install folder]\Examples

The default path is: C:\Program Files\QSAR Toolbox\QSAR Toolbox

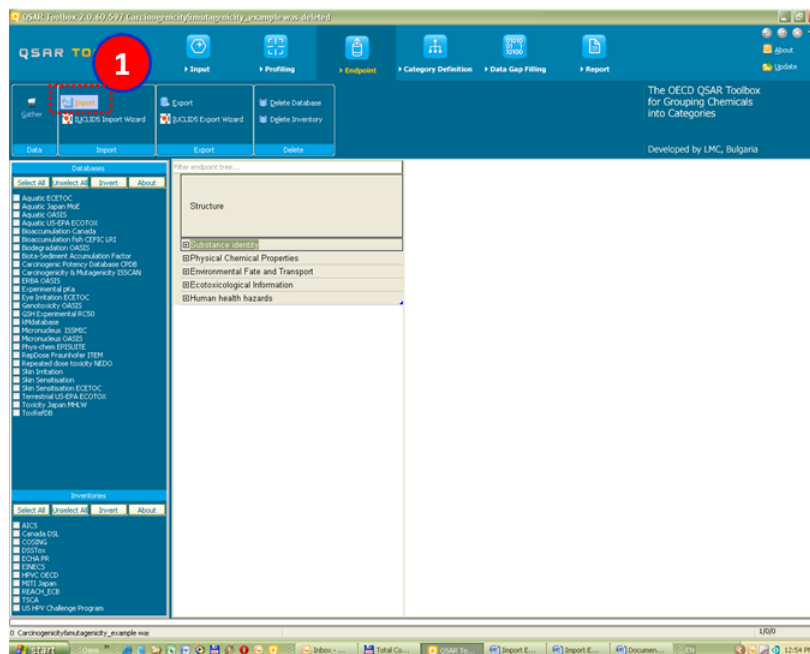
2.1\Examples\Ecotoxicological example.xls



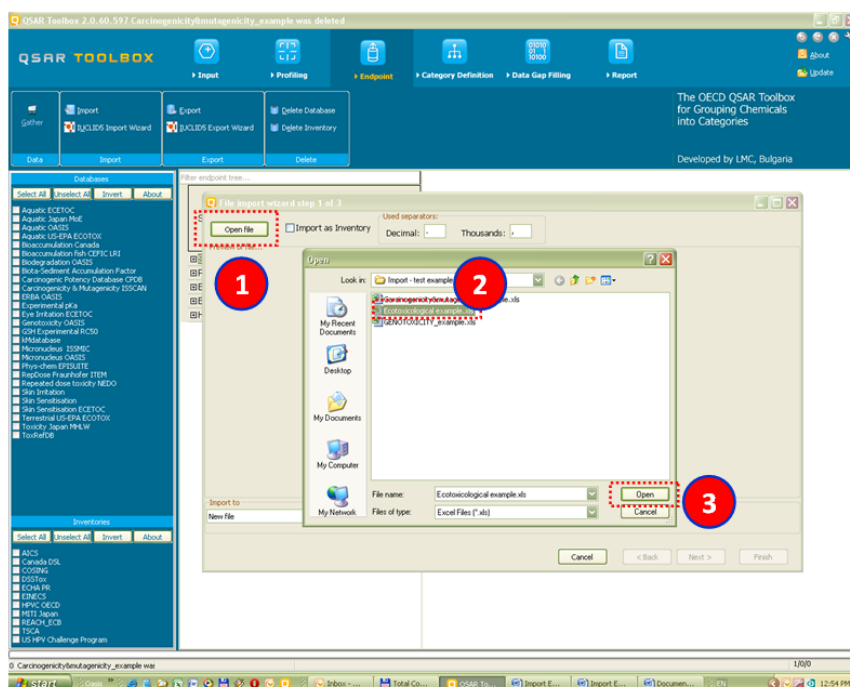
Legend:



Import New Database



Open example file



File is opened

File import wizard step 1 of 3

Open file ☐ Import as Inventory

Used separators:
Decimal: Thousands:

Preview of file D:\Transfer\Import - test example\Ecotoxicological example.xls

| CAS | NAME | Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qu |
|---------|--------------------|---|--|-----------------------------|--------------|
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Tox12.98 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Tox139 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Tox157 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Tox129 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox12995.767 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox10009.113 | < | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox1212.2406 | < | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox15178.729 | < | |
| 50-28-2 | BETA-ESTRADIOL, 17 | c12c(C{P+}3C{P+})(C{P-}4C{P-})(C{P-}Ecotoxicological Information#Aquatic Tox10.00012 | < | | |
| 50-28-2 | BETA-ESTRADIOL, 17 | c12c(C{P+}3C{P+})(C{P-}4C{P-})(C{P-}Ecotoxicological Information#Aquatic Tox10.000251 | > | | |
| 50-28-2 | BETA-ESTRADIOL, 17 | c12c(C{P+}3C{P+})(C{P-}4C{P-})(C{P-}Ecotoxicological Information#Aquatic Tox10.00115 | > | | |
| 50-29-3 | DDT | C(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1 | Ecotoxicological Information#Aquatic Tox170 | > | |
| 50-29-3 | DDT | C(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1 | Ecotoxicological Information#Aquatic Tox10.0087 | > | |
| 50-29-3 | DDT, P,P' | C(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1 | Ecotoxicological Information#Aquatic Tox17e-005 | > | |
| 50-29-3 | DDT, P,P' | C(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1 | Ecotoxicological Information#Aquatic Tox10.00123 | > | |
| 50-48-6 | AMITRYPTYLIN | c12C(=CCCN(C)C)c3c(cccc3)CCc1ccc2 | Ecotoxicological Information#Aquatic Tox121.580942 | > | |
| 50-48-6 | AMITRYPTYLIN | c12C(=CCCN(C)C)c3c(cccc3)CCc1ccc2 | Ecotoxicological Information#Aquatic Tox136.89287 | > | |
| 50-48-6 | AMITRYPTYLIN | c12C(=CCCN(C)C)c3c(cccc3)CCc1ccc2 | Ecotoxicological Information#Aquatic Tox10.776692 | > | |
| 50-48-6 | AMITRYPTYLIN | c12C(=CCCN(C)C)c3c(cccc3)CCc1ccc2 | Ecotoxicological Information#Aquatic Tox10.804431 | < | |

Import to
New File ☐ Database title Ecotoxicological example

Cancel < Back **Next >** Finish

Import to: The user has to choose whether to import the file as a new database or whether to add the data to a database already existing in the Toolbox.

Database title : Ecotoxicological example.
Note: the user could change the name

⚠ 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

File import wizard step 2 of 3

File layout:
☒ Vertical
☐ Horizontal **1**

☒ I have a header row [What do different layouts mean?](#)

Define new region

CAS
 Chemical name
 SMILES
 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.

| CAS | NAME | Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qua |
|---------|--------------------|--|--|-----------------------------|---------------|
| CAS-0 | FORMALDEHYDE | SMILES | Ecotoxicological Information#Aquatic Toxi12.98 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi39 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi57 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi29 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi2995.767 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi10009.113 | < | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi1212.2406 | < | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi5178.729 | < | |
| 50-28-2 | BETA-ESTRADIOL, 17 | -12c(C{P+}3C{P+}(C{P-}4C{P-}(C{C{P- | Ecotoxicological Information#Aquatic Toxi0.00012 | < | |
| 50-28-2 | BETA-ESTRADIOL, 17 | -12c(C{P+}3C{P+}(C{P-}4C{P-}(C{C{P- | Ecotoxicological Information#Aquatic Toxi0.000251 | > | |
| 50-28-2 | BETA-ESTRADIOL, 17 | -12c(C{P+}3C{P+}(C{P-}4C{P-}(C{C{P- | Ecotoxicological Information#Aquatic Toxi0.00115 | > | |
| 50-29-3 | DDT | C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1 | Ecotoxicological Information#Aquatic Toxi70 | > | |
| 50-29-3 | DDT | C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1 | Ecotoxicological Information#Aquatic Toxi0.0087 | > | |
| 50-29-3 | DDT, P,P'- | C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1 | Ecotoxicological Information#Aquatic Toxi7e-005 | > | |
| 50-29-3 | DDT, P,P'- | C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1 | Ecotoxicological Information#Aquatic Toxi0.00123 | > | |
| 50-48-6 | AMITRYPTYLIN | -12C(=CCCN(C)C)C3c(cccc3)CCc1cccc2 | Ecotoxicological Information#Aquatic Toxi21.580942 | > | |
| 50-48-6 | AMITRYPTYLIN | -12C(=CCCN(C)C)C3c(cccc3)CCc1cccc2 | Ecotoxicological Information#Aquatic Toxi36.89287 | > | |
| 50-48-6 | AMITRYPTYLIN | -12C(=CCCN(C)C)C3c(cccc3)CCc1cccc2 | Ecotoxicological Information#Aquatic Toxi0.776692 | > | |

Cancel < Back **Next >** Finish **2**

Select: CAS

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

CAS **2**
 Chemical name
 SMILES
 Endpoint tree path

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

☐ is value add

Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

| CAS | NAME | Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qua |
|---------|---------------|------------------------------------|--|-----------------------------|---------------|
| CAS-0 | FORMALDEHYDE | SMILES | Ecotoxicological Information#Aquatic Toxi12.98 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi39 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi57 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi29 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi2995.767 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi10009.113 | < | |

Cancel < Back **Next >** Finish **1**

Select: *Chemical name*

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:
 CAS
 Chemical name **2**
 SMILES
 Endpoint tree path

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
☐ is value

| CAS | NAME | Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qua |
|---------|---------------|------------------------------------|--|-----------------------------|---------------|
| CAS-0 | Chemical name | SMILES | Ecotoxicological Information#Aquatic Toxi12.98 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi39 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi57 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi29 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi2995.767 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi10000.113 | > | |

Cancel < Back Next > Finish

Select: *SMILES*

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:
 CAS
 Chemical name
 SMILES **2**
 Endpoint tree path
 Data
 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
☐ is value

| CAS | NAME | Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qua |
|---------|---------------|------------------------------------|--|-----------------------------|---------------|
| CAS-0 | Chemical name | SMILES | Ecotoxicological Information#Aquatic Toxi12.98 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi39 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi57 | > | |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Toxi29 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi2995.767 | > | |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Toxi10000.113 | > | |

Cancel < Back Next > Finish

Select : Endpoint tree path

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 (2)
 Data
 Undefined

Scales editor: Select one or more columns from the grid below and then assign the selection to a region by choosing from the left hand side radio buttons.

Metadata:
☐ is value

| CAS | NAME | Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qua |
|---------|---------------|------------------------------------|--|-----------------------------|---------------|
| 50-00-0 | FORMALDEHYDE | C=O | Endpoint tree path | 12.98 | > |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Tox | 39 | > |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Tox | 57 | > |
| 50-00-0 | FORMALDEHYDE | C=O | Ecotoxicological Information#Aquatic Tox | 29 | > |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox | 2995.767 | > |
| 50-06-6 | PHENOBARBITAL | C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox | 112 | > |

Cancel < Back Next > Finish

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

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 (2)
 Data
 Undefined

Define value:
☐ Scale ☐ Low qualifier ☐ Upper value
☐ Mean qualifier ☐ Low value ☐ Unit
☒ Mean value/Scale value ☐ 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 left hand side radio buttons.

Metadata:
☐ is value

| Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qualifier | Data Unit | Endpoint Test organisms |
|------------------------------------|--|-----------------------------|---------------------|-----------|----------------------------|
| SMILES | Endpoint tree path | Data Mean value/Scale value | | | |
| C=O | Ecotoxicological Information#Aquatic Tox | 39 | | mg/L | EC 50 Ceriodaphnia affinis |
| C=O | Ecotoxicological Information#Aquatic Tox | 57 | | mg/L | EC 50 Daphnia magna |
| C=O | Ecotoxicological Information#Aquatic Tox | 29 | | mg/L | EC 50 Daphnia magna |
| C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox | 2995.767 | | mg/L | EC 50 Vibrio fischeri |
| C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox | 112 | | mm/L | EC 50 Annelina shubba |

Cancel < Back Next > Finish

Select: DATA Mean qualifier

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
☒ Mean qualifier
☐ Mean value/Scale value
☐ Low qualifier
☐ Low value
☐ Upper value
☐ Unit
☐ 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
☐ is value add

| Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qualifier | Data Unit | Endpoint | Test organisms |
|------------------------------------|--|-----------------------------|---------------------|-----------|------------------|----------------------|
| SMILES | Endpoint tree path | Data Mean value/Scale value | Data Mean qualifier | Data Unit | EC 50 | Ceriodaphnia affinis |
| C=O | Ecotoxicological Information#Aquatic Tox | 39 | mg/L | EC 50 | Daphnia magna | |
| C=O | Ecotoxicological Information#Aquatic Tox | 57 | mg/L | EC 50 | Daphnia magna | |
| C=O | Ecotoxicological Information#Aquatic Tox | 29 | mg/L | EC 50 | Daphnia magna | |
| C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox | 2995.767 | mg/L | EC 50 | Vibrio fischeri | |
| C1=CC=C(C=C1)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox | 10000.112 | mg/L | EC 50 | Amniontes abdita | |

Cancel < Back Next > Finish

Select: DATA Unit

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
☐ Mean qualifier
☐ Mean value/Scale value
☐ Low qualifier
☐ Low value
☒ Upper value
☒ Unit
☐ 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
☐ is value add

| Smiles | Endpoint tree path | Data Mean value/Scale value | Data Mean qualifier | Data Unit | Endpoint | Test organisms |
|------------------------------------|--|-----------------------------|---------------------|-----------|------------------|----------------------|
| SMILES | Endpoint tree path | Data Mean value/Scale value | Data Mean qualifier | Data Unit | EC 50 | Ceriodaphnia affinis |
| C=O | Ecotoxicological Information#Aquatic Tox | 39 | mg/L | EC 50 | Daphnia magna | |
| C=O | Ecotoxicological Information#Aquatic Tox | 57 | mg/L | EC 50 | Daphnia magna | |
| C=O | Ecotoxicological Information#Aquatic Tox | 29 | mg/L | EC 50 | Daphnia magna | |
| C1(=O)C(c2ccccc2)(CC)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox | 2995.767 | mg/L | EC 50 | Vibrio fischeri | |
| C1=CC=C(C=C1)C(=O)NC(=O)N1 | Ecotoxicological Information#Aquatic Tox | 10000.112 | mg/L | EC 50 | Amniontes abdita | |

Cancel < Back Next > Finish

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

Add test Duration data

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
☐ Mean qualifier
☐ Mean
☐ Low qualifier
☐ Low value
☐ Upper value
☒ Unit
☐ 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
 Duration
 Effect
 Effect additional
 Effect details
 Effect type
 Elimination constant - k2
 Elimination phase duration
 Elimination > 5xT50
 Embryotoxic / teratogenic effects
 Endpoint

is value ☐ add

| Data | Mean qualifier | Data Unit | Endpoint | Test organisms (species) | Duration | Duration Unit | Solubility | Unit | Effect | Lifestage | Water type | Salinity | Temp |
|------|---------------------|-----------|----------|--------------------------|----------|---------------|------------|------|----------------|-----------|------------|----------|------|
| > | Data.Mean qualifier | Data.Unit | EC 50 | Ceriodaphnia affinis | 48 | h | | | Immobilisation | Juvenile | Freshwater | | 23 |
| > | | mg/L | EC 50 | Daphnia magna | 1 | h | | | Physiology | Juvenile | Freshwater | | 20 |
| > | | mg/L | EC 50 | Daphnia magna | 24 | h | | | Mortality | Juvenile | Freshwater | | 20 |
| > | | mg/L | EC 50 | Daphnia magna | 48 | h | | | Mortality | Juvenile | Freshwater | | 20 |
| > | | mg/L | EC 50 | Vibrio fischeri | 0.25 | h | | | Behavior | Adult | Saltwater | | |
| > | | mg/L | EC 50 | Amalica shulka | 74 | h | | | Mortality | | Saltwater | | |

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?](#)

☐ 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 value
☐ 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
 Duration
 Effect
 Effect additional
 Effect details
 Effect type
 Elimination constant - k2
 Elimination phase duration
 Elimination>5xT50
 Embryotoxic / teratogenic effects
 Endpoint

Define value:
☐ Scale
☐ Upper qualifier
☐ Mean qualifier
☐ Upper value
☒ Mean value/Scale value
☐ Low qualifier
☐ Undefined
☐ Low value

☒ is value add

| Data | Mean qualifier | Data Unit | Endpoint | Test organisms (species) | Duration | Mean value/Scale value | Duration Unit | Solubility | Unit | Effect | Lifestage | V |
|------|----------------|-----------|----------|--------------------------|----------|------------------------|---------------|------------|------|----------------|-----------|---|
| > | | mg/L | EC 50 | Ceriodaphnia affinis | 48 | | h | | | Immobilisation | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 1 | | h | | | Physiology | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 24 | | h | | | Mortality | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 48 | | h | | | Mortality | Juvenile | F |
| > | | mg/L | EC 50 | Vibrio fischeri | 0.25 | | h | | | Behavior | Adult | S |
| > | | mg/L | EC 50 | Amalicia shubia | 24 | | h | | | Mortality | Juvenile | F |

Cancel < Back Next > Finish

Add test "Duration unit"

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 value
☐ 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
 Dry Weight Percent
 Duration
 Effect
 Effect additional
 Effect details
 Effect type
 Elimination constant - k2
 Elimination phase duration
 Elimination>5xT50
 Embryotoxic / teratogenic effects

Define value:
☐ Scale
☐ Upper qualifier
☐ Mean qualifier
☐ Upper value
☒ Mean value/Scale value
☐ Low qualifier
☐ Undefined
☐ Low value

☒ is value add

| Data | Mean qualifier | Data Unit | Endpoint | Test organisms (species) | Duration | Mean value/Scale value | Duration Unit | Solubility | Unit | Effect | Lifestage | V |
|------|----------------|-----------|----------|--------------------------|----------|------------------------|---------------|------------|------|----------------|-----------|---|
| > | | mg/L | EC 50 | Ceriodaphnia affinis | 48 | | h | | | Immobilisation | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 1 | | h | | | Physiology | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 24 | | h | | | Mortality | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 48 | | h | | | Mortality | Juvenile | F |
| > | | mg/L | EC 50 | Vibrio fischeri | 0.25 | | h | | | Behavior | Adult | S |
| > | | mg/L | EC 50 | Amalicia shubia | 24 | | h | | | Mortality | Juvenile | F |

Cancel < Back Next > Finish

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
☐ Low value
☐ Mean value/Scale value
☐ Upper qualifier
☐ Upper value
☒ Unit
☐ Undefined

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

Define value
☐ Scale
☐ Upper qualifier
☐ Mean qualifier
☐ Upper value
☐ Mean value/Scale value
☐ Unit
☐ Low qualifier
☒ Undefined
☐ Low value

is value add

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.

| 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 | F |
| > | | mg/L | EC 50 | Daphnia magna | 1 | | | h | | | Physiology | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 24 | | | h | | | Mortality | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 48 | | | h | | | Mortality | Juvenile | F |
| > | | mg/L | EC 50 | Vibrio fischeri | 0.25 | | | h | | | Behavior | Adult | F |
| > | | mg/L | EC 50 | Amelara shiba | 24 | | | h | | | Mortality | | F |

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?](#)

☐ Private data

Define new region

SMILES
 Endpoint tree path
 Data
 Undefined

Define value
☐ Scale
☐ Low qualifier
☐ Low value
☐ Mean value/Scale value
☐ Upper qualifier
☒ Unit
☐ Undefined

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

Define value
☐ Scale
☐ Upper qualifier
☐ Mean qualifier
☐ Upper value
☐ Mean value/Scale value
☐ Unit
☐ Low qualifier
☒ Undefined
☐ Low value

is value Solubility add

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.

| 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 | F |
| > | | mg/L | EC 50 | Daphnia magna | 1 | | | h | | | Physiology | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 24 | | | h | | | Mortality | Juvenile | F |
| > | | mg/L | EC 50 | Daphnia magna | 48 | | | h | | | Mortality | Juvenile | F |
| > | | mg/L | EC 50 | Vibrio fischeri | 0.25 | | | h | | | Behavior | Adult | F |
| > | | mg/L | EC 50 | Amelara shiba | 24 | | | h | | | Mortality | | F |

Cancel < Back Next > Finish

Define "Solubility", click "add"

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
☐ Mean qualifier
☐ Mean value/Scale value
☐ Low value
☐ Upper value
☒ Unit
☐ 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 | F |
| > | | ng/L | EC 50 | Daphnia magna | 1 | | | h | | | Physiology | Juvenile | F |
| > | | ng/L | EC 50 | Daphnia magna | 24 | | | h | | | Mortality | Juvenile | F |
| > | | ng/L | EC 50 | Daphnia magna | 48 | | | h | | | Mortality | Juvenile | F |
| > | | ng/L | EC 50 | Vibrio fischeri | 0.25 | | | h | | | Behavior | Adult | F |
| > | | ng/L | EC 50 | Amalica shubia | 24 | | | h | | | Mortality | Adult | F |

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?](#)

☐ Private data

Define new region

SMILES
 Endpoint tree path
 Data
 Undefined

Define value
☐ Scale
☐ Low qualifier
☐ Mean qualifier
☐ Mean value/Scale value
☐ Low value
☐ Upper value
☒ Unit
☐ 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

8

7

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 | Effect | |
|------|----------------|-----------|----------|--------------------------|----------|------------------------|----------|------|------------|------------------------|------|--------|--|
| Data | Mean qualifier | Data Unit | EC 50 | Ceriodaphnia affinis | 48 | | | h | | | | Imm | |
| > | | ng/L | EC 50 | Daphnia magna | 1 | | | h | | | | Phys | |
| > | | ng/L | EC 50 | Daphnia magna | 24 | | | h | | | | Mort | |
| > | | ng/L | EC 50 | Daphnia magna | 48 | | | h | | | | Mort | |
| > | | ng/L | EC 50 | Vibrio fischeri | 0.25 | | | h | | | | Beha | |
| > | | ng/L | EC 50 | Amalica shubia | 24 | | | h | | | | Mort | |

6

Cancel < Back Next > Finish

Select "Unit" of defined "Solubility" parameter

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 value ☐ 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 flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Solubility
 Undefined

Define value
☐ Scale ☐ Upper qualifier ☒ is value Solubility
☐ Mean qualifier ☐ Upper value
☐ Mean value/Scale value ☒ Unit
☐ Low qualifier ☐ Undefined
☐ Low value

| Endpoint | Test organisms (species) | Duration | Mean value/Scale value | Duration | Unit | Solubility | Mean value/Scale value | Solubility | Unit | Effect | Lifestage |
|----------|--------------------------|----------|------------------------|----------|------|------------|------------------------|------------|-----------|----------------|-----------|
| EC 50 | Ceriodaphnia affinis | 48 | | | h | | | | | Immobilisation | Juvenile |
| EC 50 | Daphnia magna | 1 | | | h | | | | | Physiology | Juvenile |
| EC 50 | Daphnia magna | 24 | | | h | | | | Mortality | Juvenile | |
| EC 50 | Daphnia magna | 48 | | | h | | | | Mortality | Juvenile | |
| EC 50 | Vibrio fischeri | 0.25 | | | h | | | | Behavior | Adult | |
| EC 50 | Amelara shubia | 24 | | | h | | | | Mortality | | |

Cancel < Back Next > Finish

Scroll bar

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 value ☐ 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 flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Solubility
 Undefined

Define value
☐ Scale ☐ Upper qualifier ☒ is value Solubility
☐ Mean qualifier ☐ Upper value
☐ Mean value/Scale value ☒ Unit
☐ Low qualifier ☐ Undefined
☐ Low value

| Effect | Lifestage | Water type | Salinity | Temperature | pH | Water alkalinity | Water Hardness | DATA QUALITY | Author | Year |
|----------------|-----------|------------|----------|-------------|----|------------------|----------------|--------------|----------------------|------|
| Immobilisation | Juvenile | Freshwater | | 23 | | | | 2.2 | WARNE AND SCHIFKO | 1999 |
| Physiology | Juvenile | Freshwater | | 20 | | | | 3 | JANSSEN AND PERSOONE | 1993 |
| Mortality | Juvenile | Freshwater | | 20 | | | | 3 | JANSSEN AND PERSOONE | 1993 |
| Mortality | Juvenile | Freshwater | | 20 | | | | 3 | JANSSEN AND PERSOONE | 1993 |
| Behavior | Adult | Saltwater | | | | | | 2.2 | Calleja | 1994 |

Cancel < Back Next > Finish

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

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 value ☐ 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 flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Solubility
 Undefined

Define value
☐ Scale ☐ Upper qualifier
☐ Mean qualifier ☐ Upper value
☐ Mean value/Scale ☒ Unit
☐ Low qualifier ☐ Undefined
☐ Low value

☒ is value Solubility

| Author | Year | Title | Reference source | Comment |
|----------------------|------|-------|------------------|---|
| WARNE AND SCHIFKO | 1999 | | | |
| JANSSEN AND PERSOONE | 1993 | | | End point is fluorescence od Daphnia with |
| JANSSEN AND PERSOONE | 1993 | | | |
| JANSSEN AND PERSOONE | 1993 | | | |
| Calleja | 1994 | | | |

Cancel < Back Next > **1** Finish

Click on "Finish" button

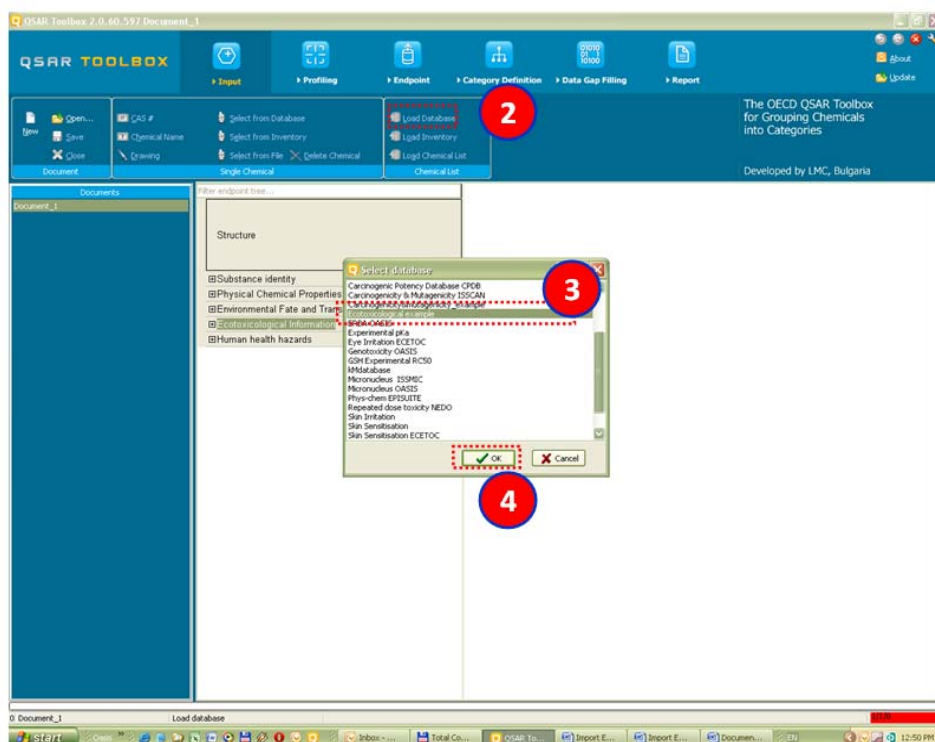
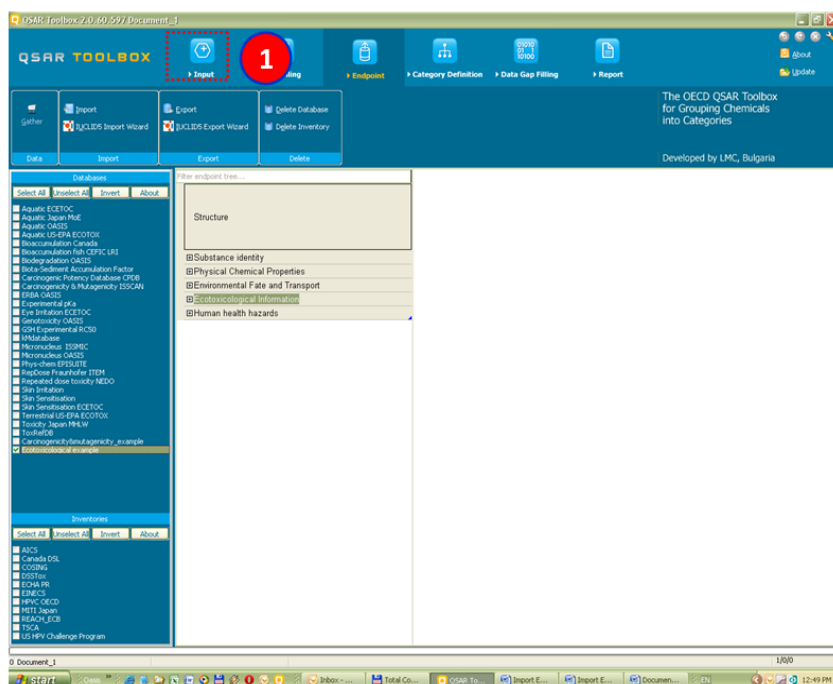
File import wizard step 3 of 3

| Author | Year | Title | Reference source | Comment |
|---|------|---|------------------------------------|--|
| WARNE AND SCHIFKO | 1999 | | | |
| JANSSEN AND PERSOONE | 1993 | | | End point is fluorescence od Daphnia with |
| JANSSEN AND PERSOONE | 1993 | | | |
| JANSSEN AND PERSOONE | 1993 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Kramer VJ, Miles-Richardson S, Pierens SL | 1998 | Reproductive impairment and induction of Aquat Toxicol 40:335-360 | | End point egg production (female). |
| Kramer VJ, Miles-Richardson S, Pierens SL | 1998 | Reproductive impairment and induction of Aquat Toxicol 40:335-360 | | End point inhibition of vitellogenin in male |
| Kramer VJ, Miles-Richardson S, Pierens SL | 1998 | Reproductive impairment and induction of Aquat Toxicol 40:335-360 | | Male fish only. |
| WYNBERG | 1989 | | | Egg refers to sperm. Sperm exposed for 1 |
| REYES | 1996 | | | |
| Phipps GL, Mattson VR, Ankley GT | 1995 | Relative sensitivity of three freshwater b | Arch Env Contam Toxicol 28:281-286 | |
| Phipps GL, Mattson VR, Ankley GT | 1995 | Relative sensitivity of three freshwater b | Arch Env Contam Toxicol 28:281-286 | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |
| Calleja | 1994 | | | |

Cancel < Back Next > **1** Finish



Load imported database



[illegible]

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



The example 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

| CAS | ChemName | Smiles | Endpoint tree path | Scale | Data Mean value/Scale value | Data Unit | Endpoint | Type of method |
|-------------|---|-------------------------------------|-------------------------------------|----------------------------|-----------------------------|-----------|-------------------------|----------------|
| 92177-18-8 | Nitrozo-2-oxopropylamine | NC(=O)C(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 15973-39-9 | 4-Nitro-5-oxo-1,2,3,4-tetrahydronaphthalene | C1=CC(=C2C(=C1)C(=O)N=O)C2=CC=CC=C2 | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 76881-18-4 | 1-Nitro-3,4,5-trimethoxybenzene | COC1=C(C(OC)=C(C(OC)=C1)N=O) | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 105-09-9 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 51179-11-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 71785-67-7 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 114382-83-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 10595-26-6 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 66587-10-3 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 114279-28-2 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 101016-48-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 25081-31-6 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Equival | | Summary carcinogenicity | |
| 29921-49-9 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 70416-19-7 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 59884-51-5 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 17-9 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 69658-91-9 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 15219-30-1 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 44647-91-2 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 4215-16-8 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 56247-3 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 7516-26-9 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 81795-97-5 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 26541-51-6 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 23292-30-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 59-43-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 2444-63-3 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 23062-74-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 115-80-1 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Equival | | Summary carcinogenicity | |
| 64221-21-1 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 71799-59-5 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 65-89-1 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Equival | | Summary carcinogenicity | |
| 22105-20-0 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 3098-92-2 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 14688-28-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 116558-85-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Equival | | Summary carcinogenicity | |
| 89837-35-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 6462-71-7 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 102-77-2 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 149-28-1 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 87690-02-0 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 2227-09-2 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Equival | | Summary carcinogenicity | |
| 92-84-2 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 103-75-0 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 106-45-2 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 90-49-1 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |
| 105650-23-4 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Positive | | Summary carcinogenicity | |
| 56393-22-7 | Nitrosodiazolide | C1=NC(=O)N=O | Human health hazardsCarcinogenicity | Carcinogenicity (I) (RSC4) | Negative | | Summary carcinogenicity | |

1

2

3

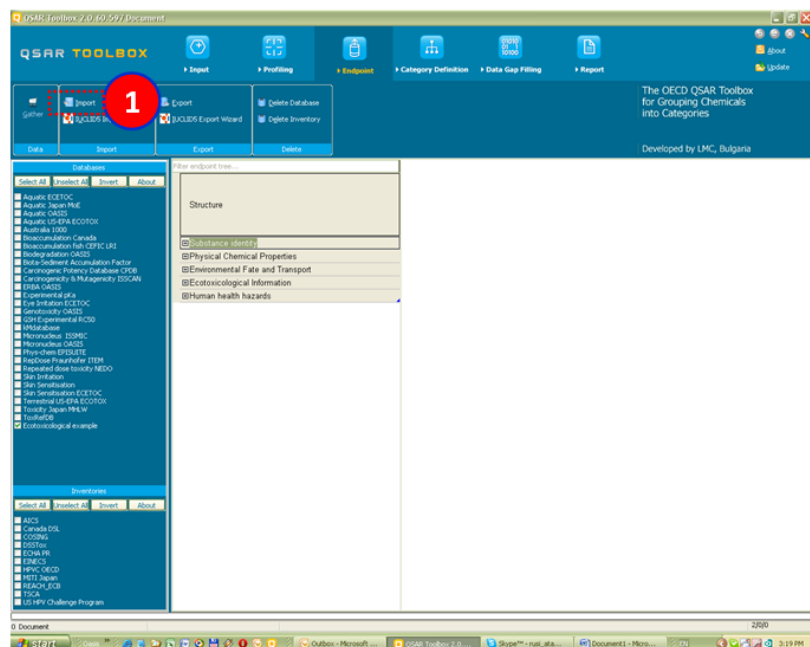
Sequence of steps

Click on

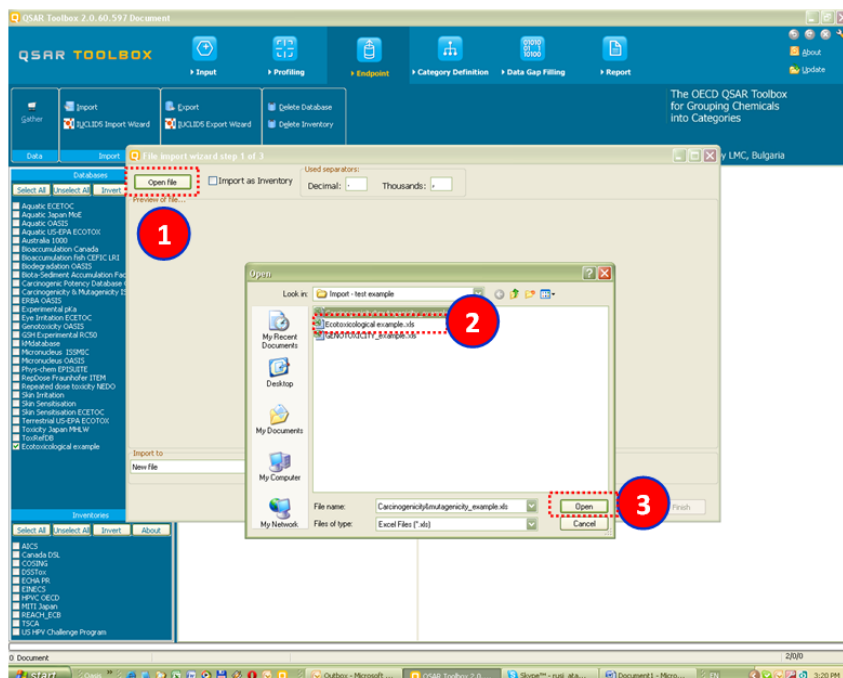
Import New Database

Detailed information

Import New Database



Open example file



File is open

File import wizard step 1 of 3

Used separators:
 ☐ Import as Inventory
 Decimal: Thousands:

Preview of file D:\Transfer\Import - test example\Carcinogenicity\mutagenicity_example.xls

| CAS | ChemName | Smiles | Endpoint tree path | Scale | Data Mea |
|-------------|--|--|--------------------------------------|----------------------------|----------|
| 92177-49-6 | Nitroso-2-oxopropylethanolamine | <chem>N(CC(C)=O)(CCO)N=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 15973-99-6 | di(N-Nitroso)-perhydropyrimidine | <chem>C1CCN(CN1N=O)N=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 75881-18-4 | 1-Nitroso-3,4,5-trimethylpiperazine | <chem>C1C(N(C(CN1N=O)C)C)C</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 625-89-8 | N-Nitrosobis(2,2,2-trifluoroethyl) amine | <chem>N(N(CC(F)(F)F)CC(F)(F)F)=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 51715-17-4 | Nitroschloridiazepoxide | <chem>c1(C2c3c(ccc(C)C)N=C(N(C)N=O)CN=2</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 73785-40-7 | N-Nitrosocimetidine | <chem>O=NN(C)C(=N(C#N)NCCSCC1=C(N=CN1)</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 114282-83-6 | N-Nitrosodithiazine | <chem>N1(CSCSC1)N=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 10595-95-6 | Nitrosoethylmethylamine | <chem>CN(CC)N=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 55557-02-3 | N-Nitrosoguvacoline | <chem>OC(=O)C1=CCCN(C1)N=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 42579-28-2 | 1-Nitrosohydantoin | <chem>C1(NC(CN1N=O)=O)=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 30310-80-6 | Nitrosohydroxyproline | <chem>C(=O)O(C)C(CCN1N=O)O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 25081-31-6 | Nitrosiminodiacetic acid | <chem>N(N(CC(O)=O)CC(O)=O)=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Equivoca |
| 26921-68-6 | N-Nitrosomethyl-(2-hydroxyethyl) amine | <chem>CN(CCO)N=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 70415-59-7 | N-Nitrosomethyl-(3-hydroxypropyl) amine | <chem>CN(CCCO)N=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 55984-51-5 | N-Nitrosomethyl-(2-oxopropyl) amine | <chem>CN(CC(C)=O)N=O</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 9 | N-Nitrosomethyl-(2-tosyloxyethyl) amine | <chem>NC(COS(=O)(=O)C1C=CC(C)=CC=1)CN</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 69658-91-9 | 3-Nitrosomethylaminopyridine | <chem>C1=CC=C(C(=N1)N(N=O)C</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 16219-99-1 | 4-Nitrosomethylaminopyridine | <chem>C1=CC(=CC=N1)N(N=O)C</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 55557-03-4 | Nitrosomethylphenidate | <chem>C1=CC=C(C(C(=O)OC)C2N(N=O)CCCC2</chem> | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |

Import to:
 Database title:

Import to: The user has to choose whether to import the file as a new database or whether to add the data to a database already existing in the Toolbox.

Database title:
Carcinogenicity&mutagenicity_example
 Note: the user could change the name

⚠ 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

File import wizard step 2 of 3

File layout
☒ Vertical
☐ Horizontal 1
☒ I have a header row [What do different layouts mean?](#)

Define new region

CAS
 Chemical name
 SMILES
 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.

| CAS | ChemName | Smiles | Endpoint tree path | Scale | Data Mean |
|-------------|--|-----------------------------------|--------------------------------------|----------------------------|-----------|
| 92177-49-6 | Nitroso-2-oxopropylethanolamine | SMILES=O(CCO)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 15973-99-6 | di(N-Nitroso)-perhydropyrimidine | C1CCN(CN1N=O)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 75881-18-4 | 1-Nitroso-3,4,5-trimethylpiperazine | C1C(N(C(CN1N=O)C)C)C | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 625-89-8 | N-Nitrosobis(2,2,2-trifluoroethyl) amine | WN(C(C(F)(F)F)CC(F)(F)F)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 51715-17-4 | Nitrosochloridiazepoxide | C1(C2c3c(ccc(C)C)N=C(N(C)N=O)CN=2 | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 73785-40-7 | N-Nitrosocimetidine | O=NN/C(=N/C#N)NCCSCC1=C(N=CN1 | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 114282-83-6 | N-Nitrosodithiazine | N1(CSCSC1)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 10595-95-6 | Nitrosoethylmethylaniline | CN(CC)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 55557-02-3 | N-Nitrosoguvacoline | OC(=O)C1=CCCN(C1)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 42579-28-2 | 1-Nitrosopyridine | C1(NC(CN1N=O)=O)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 30310-80-6 | Nitrosohydroxyproline | C(=O)O(C)C1CC(CN1N=O)O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 25081-31-6 | Nitrosiminodiacetic acid | N(N(C(C(=O)O)CC(C(=O)O)=O)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Equivocal |
| 26921-68-6 | N-Nitrosomethyl-(2-hydroxyethyl) amine | CN(CCO)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 70415-59-7 | N-Nitrosomethyl-(3-hydroxypropyl) amine | N(N(CCCO)C)O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 55984-51-5 | N-Nitrosomethyl-(2-oxopropyl)amine | CN(C(C)O)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 9 | N-Nitrosomethyl-(2-tosyloxyethyl) amine | NC(COS(=O)(=O)C1C=CC(C)=CC=1)CN | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 69658-91-9 | 3-Nitrosomethylaminopyridine | C1=CC=C(C(=N1)N(N=O)C | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 16219-99-1 | 4-Nitrosomethylaminopyridine | C1=CC(=CC(=N1)N(N=O)C | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |

Cancel < Back Next > Finish 2

Select : CAS

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

CAS 2
 Chemical name
 SMILES
 Endpoint tree path

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

☐ is value

add

Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

| CAS | ChemName | Smiles | Endpoint tree path | Scale | Data Mean |
|------------|--|-----------------------------------|--------------------------------------|----------------------------|-----------|
| CAS7-49-6 | Nitroso-2-oxopropylethanolamine | SMILES=O(CCO)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 15973-99-6 | di(N-Nitroso)-perhydropyrimidine | C1CCN(CN1N=O)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 75881-18-4 | 1-Nitroso-3,4,5-trimethylpiperazine | C1C(N(C(CN1N=O)C)C)C | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 625-89-8 | N-Nitrosobis(2,2,2-trifluoroethyl) amine | WN(C(C(F)(F)F)CC(F)(F)F)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 51715-17-4 | Nitrosochloridiazepoxide | C1(C2c3c(ccc(C)C)N=C(N(C)N=O)CN=2 | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 73785-40-7 | N-Nitrosocimetidine | O=NN/C(=N/C#N)NCCSCC1=C(N=CN1 | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |

1

Cancel < Back Next > Finish

Select : *Chemical name*

Q 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

CAS
Chemical name
SMILES
Endpoint tree path

2 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

☐ Is value add

| CAS | ChemName | Smiles | Endpoint tree path | Scale | Data Measure |
|------------|--------------------------------|------------------------------------|--------------------------------------|----------------------------|--------------|
| 7-49-6 | ethanolamine | O=CCO)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 15973-99-6 | (N-Nitroso)-perhydropyrimidine | C1CCN(CN1N=O)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 75881-18-4 | N-Nitroso-3,4,5-trimethylpi | C1C(N(C(CN1N=O)C)C)C | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 525-89-8 | N-Nitrosobis(2,2,2-trifluoro | N(N(CC(F)(F)F)CC(F)(F)F)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 51715-17-4 | Nitrosochlordiazepoxide | C1C2c3c(ccc(Cl)c3)N=C(N(C=N=O)CN=2 | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 3305-40-7 | N,N-Dimethyl-N-nitrosoglycine | CN(C)CNC(=O)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |

< Back Next > Finish

Select : SMILES

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

CAS
 Chemical name
 SMILES
 Endpoint tree path

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.

☐ is value

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

| CAS | ChemName | Smiles | Endpoint tree path | Scale | Data Measurement |
|------------|--|-----------------------------------|--------------------------------------|----------------------------|------------------|
| 457-49-6 | Chemical nameylethanolamine | SMILES=O)(CCO)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 15973-99-6 | 4-Nitroso-3,4,5-trimethylpiperazine | C1CCN(CN1N=O)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 75881-18-4 | 1-Nitroso-3,4,5-trimethylpiperazine | C1C(N(CCN1N=O)C)C | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 525-89-8 | 4-Nitrosobis(2,2,2-trifluoroethyl) amine | N(C(C(F)(F)F)C(F)(F)F)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 51715-17-4 | Nitroschloridiazepoxide | C1(C2c3c(ccc(C)C3)N=C(N(CN=O)CN=2 | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 52500-46-7 | 4-Nitrosobis(2,2,2-trifluoroethyl) amine | N(C(C(F)(F)F)C(F)(F)F)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |

Buttons: Cancel, < Back, Next >, Finish

Select : Endpoint tree path

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

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

☐ is value add

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.

| CAS | ChemName | Smiles | Endpoint tree path | Scale | Data Mean |
|------------|--|-----------------------------------|--------------------------------------|----------------------------|-----------|
| 74-49-6 | Chemical nameylethanamine | SMILES=O(CCO)N=O | Endpoint tree path#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 15973-99-6 | di(N-Nitroso)-perhydropyrimidine | C1CCN(CN1N=O)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 75881-18-4 | 1-Nitroso-3,4,5-trimethylpiperazine | C1C(N(C(CN1N=O)C)C)C | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 525-89-8 | N-Nitrosobis(2,2,2-trifluoroethyl) amine | N(N(C(C(F)(F)F)CC(F)(F)F)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 51715-17-4 | Nitroschloridiazepoxide | -1(C2c3c(ccc(C)C)N=C(N(C)N=O)CN=2 | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |

Cancel < Back Next > Finish

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

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

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

☐ is value add

Define value
☒ Scale
☐ Low qualifier
☐ Upper value
☐ Mean qualifier
☐ Low value
☐ Unit
☐ Mean value/Scale val
☐ Upper qualifier
☐ Undefined

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.

| CAS | ChemName | Smiles | Endpoint tree path | Scale | Data Mean |
|------------|--|-----------------------------------|--------------------------------------|----------------------------|-----------|
| 74-49-6 | Chemical nameylethanamine | SMILES=O(CCO)N=O | Endpoint tree path#Carcinogenicity | Data Scale by I (ISSCAN) | Positive |
| 15973-99-6 | di(N-Nitroso)-perhydropyrimidine | C1CCN(CN1N=O)N=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 75881-18-4 | 1-Nitroso-3,4,5-trimethylpiperazine | C1C(N(C(CN1N=O)C)C)C | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive |
| 525-89-8 | N-Nitrosobis(2,2,2-trifluoroethyl) amine | N(N(C(C(F)(F)F)CC(F)(F)F)=O | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |
| 51715-17-4 | Nitroschloridiazepoxide | -1(C2c3c(ccc(C)C)N=C(N(C)N=O)CN=2 | Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative |

Finish

The Scale Carcinogenicity I (ISSCAN) has been defined in advance. According to this scale chemicals from the database are classified as "Positive" and "Negative". This is the default scale.

Note : Scale editor

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

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

☐ is value add

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.

| CAS | Chemical name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale v |
|--------|---------------------------------------|------------------------------------|---------------------------------------|-----------------|-------------------------|
| 1: A50 | Chemical name ULFONATE | SMILES:*(=O)=O | Endpoint tree path#Genetic Toxicity | Gene mutation I | Positive |
| 52737 | DICHLORVOS | C(Cl)(Cl)=COP(=O)(OC)OC | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 53923 | Phenoxybenzamine_hydrochloride [USAN] | 1(CN(+)(.Cl(-))C(C)Coc2ccccc2)CCCl | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 54675 | Diethyl_Sulfate | C(C)OS(=O)(=O)OCC | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56273 | METHYL_METHANESULFONATE | COS(C(=O)=O)=O | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 66251 | Isotretinoin | CC1=CC=CC=C(C=C1)C(=O)OCC | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |

Cancel < Back Next > Finish

Note : Scale definition

Scales definition...

Scales list Scale conversions

Scale list

New

Name Carcinogenicity I (ISSCAN)

Type Ordinal

Families

Carcinogenicity

Scale members

High Positive
Equivocal
Negative

Low

Scale description

Save & Close

Close

1

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

Select : DATA Main Value/Scale value

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
☒ Mean value/Scale value
☐ Low qualifier
☐ Upper value
☐ Unit
☐ Undefined

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

Endpoint tree path

| Endpoint tree path | Scale | Data Mean value/Scale value | Data Unit | Endpoint | Type of method | Type of |
|--------------------------------------|----------------------------|-----------------------------|-----------|-------------------------|----------------|---------|
| Endpoint tree path#Carcinogenicity | Scale | Mean value/Scale value | | Summary carcinogenicity | | |
| Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive | | Summary carcinogenicity | | |
| Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive | | Summary carcinogenicity | | |
| Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative | | Summary carcinogenicity | | |
| Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative | | Summary carcinogenicity | | |

Cancel < Back Next > Finish

Select : DATA Unit

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
☐ Mean value/Scale value
☐ Low qualifier
☐ Upper value
☒ Unit
☐ Undefined

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

Endpoint tree path

| Endpoint tree path | Scale | Data Mean value/Scale value | Data Unit | Endpoint | Type of method | Type of |
|--------------------------------------|----------------------------|-----------------------------|-----------|-------------------------|----------------|---------|
| Endpoint tree path#Carcinogenicity | Scale | Mean value/Scale value | Data Unit | Summary carcinogenicity | | |
| Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive | | Summary carcinogenicity | | |
| Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Positive | | Summary carcinogenicity | | |
| Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative | | Summary carcinogenicity | | |
| Human health hazards#Carcinogenicity | Carcinogenicity I (ISSCAN) | Negative | | Summary carcinogenicity | | |

Cancel < Back Next > Finish



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

Scroll bar

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
☐ Mean qualifier
☐ Mean value/Scale val
☐ Low qualifier
☐ Low value
☐ Upper qualifier
☐ Upper value
☒ Unit
☐ 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
☐ is value

| Type of method | Type of genotoxicity | Test type | Test organisms (species) | Sexual maturation (offspring) | Route | Comment |
|----------------|----------------------|-----------|--------------------------|-------------------------------|-------|-------------------------|
| | | | | | other | Summary carcinogenicit; |
| | | | | | other | Summary carcinogenicit; |
| | | | | | other | Summary carcinogenicit; |
| | | | | | other | Summary carcinogenicit; |
| | | | | | other | Summary carcinogenicit; |
| | | | | | other | Summary carcinogenicit; |

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?](#)

☐ Private data

Define new region

SMILES
 Endpoint tree path
 Data
 Undefined

Define value
☐ Scale
☐ Mean qualifier
☐ Mean value/Scale value
☐ Low qualifier
☐ Low value
☐ Upper qualifier
☐ Upper value
☒ Unit
☐ 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.

☐ is value

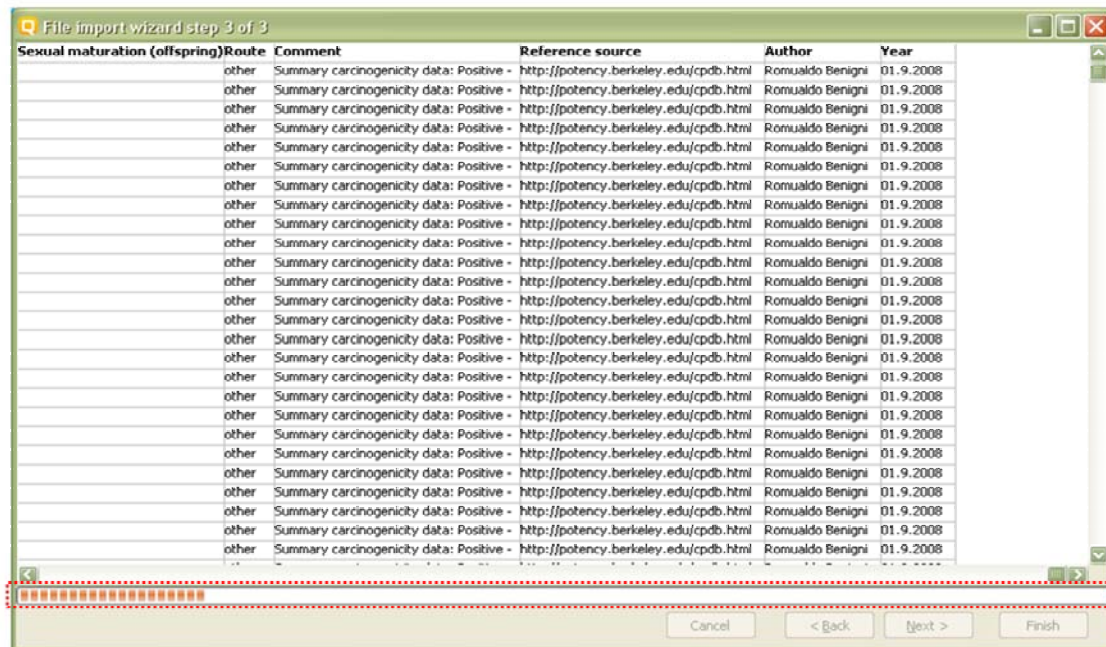
Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

| Sexual maturation (offspring)Route | Comment | Reference source | Author | Year |
|------------------------------------|--|---------------------------------------|------------------|-----------|
| other | Summary carcinogenicity data: Positive - | http://potency.berkeley.edu/cpdb.html | Romualdo Benigni | 01.9.2008 |
| other | Summary carcinogenicity data: Positive - | http://potency.berkeley.edu/cpdb.html | Romualdo Benigni | 01.9.2008 |
| other | Summary carcinogenicity data: Positive - | http://potency.berkeley.edu/cpdb.html | Romualdo Benigni | 01.9.2008 |
| other | Summary carcinogenicity data: Positive - | http://potency.berkeley.edu/cpdb.html | Romualdo Benigni | 01.9.2008 |
| other | Summary carcinogenicity data: Positive - | http://potency.berkeley.edu/cpdb.html | Romualdo Benigni | 01.9.2008 |

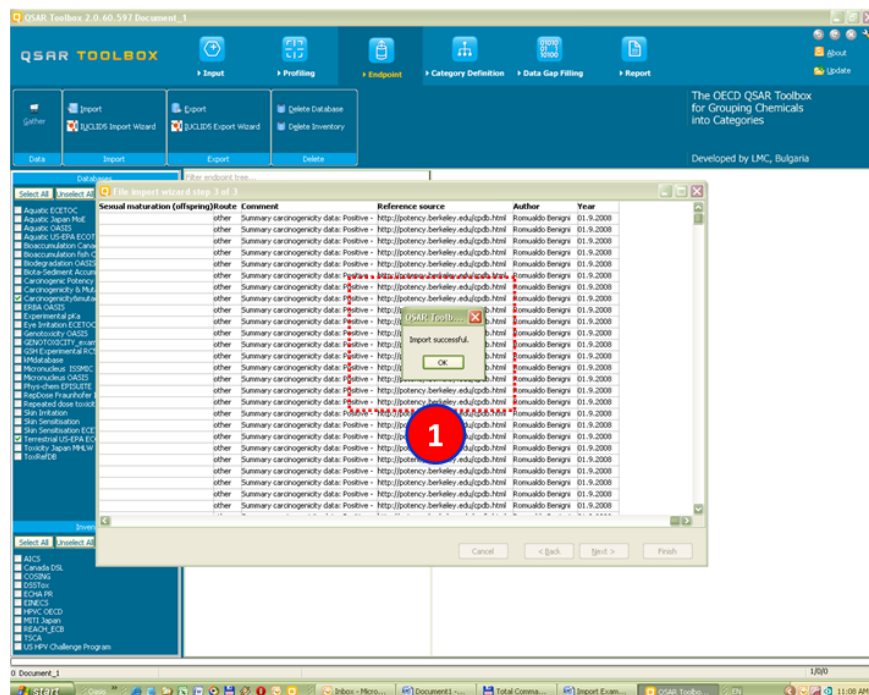
Cancel < Back Next > Finish

[illegible]

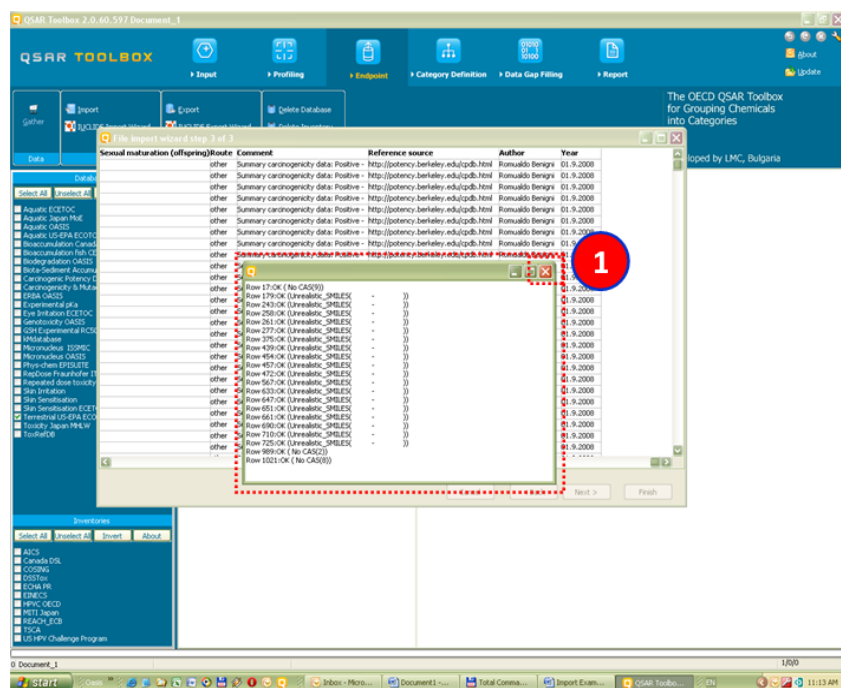
Database is being imported: Progress bar.



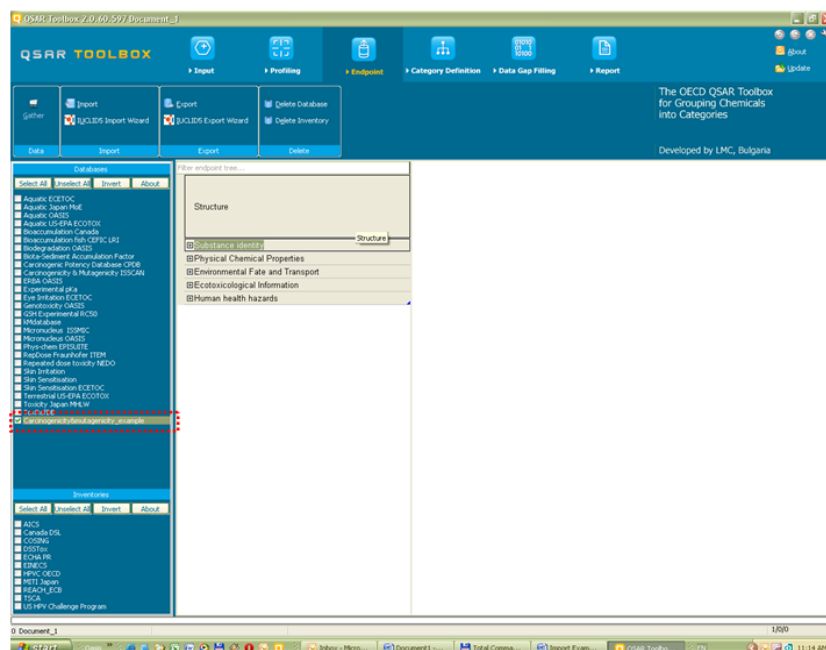
Database is imported successfully. Click "OK".




Error message log file



Imported database

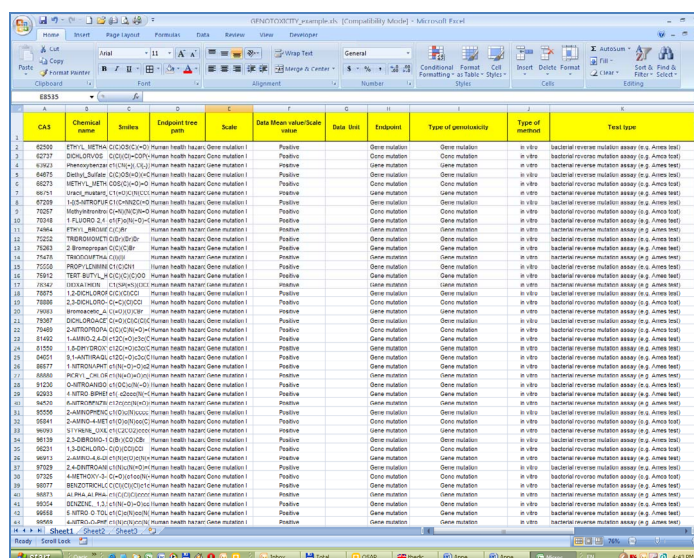


Appendix IV: Import example for database with Human health hazards Information

 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



| CAS | Chemical name | Studies | Endpoint time point | Scale | Data Mean value/Scale value | Data unit | Evidence | Type of genotoxicity | Type of method | Test type |
|-------|-------------------------|---------------------|---------------------|----------|-----------------------------|-----------|---------------|----------------------|----------------|---|
| 62592 | ETHYL METHYL CARBAMATE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 62777 | DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 43923 | Phenylketonamide | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 64875 | Butyltin Sulfide | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 68273 | METHYL METHYL CARBAMATE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 69751 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 67239 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 76287 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 70348 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 74944 | ETHYL METHYL CARBAMATE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 75252 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 76283 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 76425 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 75526 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 75912 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 10447 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 76875 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 76886 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 76903 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 76987 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 76949 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 81482 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 81505 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 84051 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86577 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86680 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 81226 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 82823 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 84539 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 85056 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 85841 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86953 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86139 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86231 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86917 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 87329 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 87325 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86977 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86973 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 85054 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86618 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |
| 86959 | 1,2-DICHLORIDE | Human health hazard | Gene mutation | Positive | | | Gene mutation | Gene mutation | In vitro | biochemical-reverse mutation assay (e.g. Ames test) |

1

2

3

Sequence of steps

Click on

Import New Database

Detailed information

[illegible]

The screenshot shows the QSRAR TOOLBOX software interface. The top menu bar includes 'File', 'Edit', 'View', 'Tools', 'Help', 'About', and 'Update'. The main window has a sidebar with 'Databases' and 'Inventory' sections. The 'Import' button is highlighted in the top bar. The 'Open' dialog box is open, showing the file 'GENOTOXITY_example.xls' selected. Red dashed boxes and blue circles with numbers 1, 2, and 3 highlight the 'Open File' button, the selected file, and the 'Open' button respectively.

File is open

File import wizard step 1 of 3

Used separators:
☐ Open file ☐ Import as Inventory
 Decimal: Thousands:

Preview of file D:\Transfer\Import - test example\GENOTOXICITY_example.xls

| CAS | Chemical name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale |
|-------|---|--|---------------------------------------|-----------------|-----------------------|
| 62500 | ETHYL METHANESULFONATE | C(C)OS(CX=O)=O | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 62737 | DICHLORVOS | C(Cl)(Cl)=COP(=O)(OC)OC | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 63923 | Phenoxybenzamine_hydrochloride_[USAN] | C1(CN(+)C1)(Cl)(Cl)C(C)OCc2ccccc2)CCCl | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 64675 | Diethyl_Sulfate | C(C)OS(=O)(=O)OCC | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 66273 | METHYL METHANESULFONATE | COS(CX=O)=O | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 66751 | Uracil_mustard_[USAN] | C1(=O)C(N(CCC)CCC)=CNC(=O)N1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 67209 | 1-[(5-NITROFURFURYLIDENE)AMINO]HYDRAZINE | C1(C=NN2C(=O)NC(=O)C2)=CC=C(N1)C(=O)N | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 70257 | Methylnitronitrosoguanidine | C(=N)(N(C)N=O)NN(=O)=O | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 70348 | 1-FLUORO-2,4-DINITROBENZENE | c1(F)c(N(=O)=O)c(cc(N(=O)=O)=O)cc1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 74964 | ETHYL BROMIDE | C(C)Br | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75252 | TRIBROMOMETHANE | C(Br)(Br)Br | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75263 | 2-Bromopropane | C(C)(C)Br | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75478 | TRITODOMETHANE | C(I)(I)I | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75558 | PROPYLENIMINE | C1(C)CN1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75912 | TERT-BUTYL HYDROPEROXIDE | C(C)(C)(C)OO | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 78342 | DIOXATHION | C1(SP(=S)(OCC)OCC)C(SP(=S)(OCC)OCC)C1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 78875 | 1,2-DICHLOROPROPANE;_1,2-Dichloro- <i>propan-1,2-diol</i> | C(C)(Cl)CCl | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 78886 | 2,3-DICHLORO-1-PROPENE | C(=C)(Cl)CCl | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 79083 | Bromoacetic_Acid | C(=O)(O)CBr | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |

Import to
☐ New file ☒ Database title GENOTOXICITY_example

Cancel < Back **Next >** Finish

Import to: The user has to choose whether to import the file as a new database or whether to add the data to a database already existing in the Toolbox.

Database title : GENOTOXICITY_example
 Note: the user could change the name

⚠ 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

File import wizard step 2 of 3

File layout
☒ Vertical
☐ Horizontal
☒ I have a header row

Define new region

CAS
 Chemical name
SMILES
 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.

[What do different layouts mean?](#)

| CAS | Chemical name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale v |
|-------|---|---|---------------------------------------|-----------------|-------------------------|
| 52450 | ETHYL_METHANESULFONATE | SMILES :C(=O)=O | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 52737 | DICHLORVOS | C(Cl)(Cl)=COP(=O)(O)COC | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 53923 | Phenoxybenzamine_hydrochloride_[USAN] | C1(CN(+)(X.Cl(-))C(C)COC2ccccc2)CCCC1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 54675 | Diethyl_Sulfate | C(C)OS(=O)(=O)OCC | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56273 | METHYL_METHANESULFONATE | COS(C)=O=O | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56751 | Uracil_mustard_[USAN] | C1=(O)C(N(CCC)CCC)=CNC(=O)N1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 57209 | 1-[(S-NITROFURFURYLIDENE)AMINO]HYDRAZINE | C1C(=NN2C(=O)NC(=O)C2)=CC=C(N(=N)C1=O)N | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 70257 | Methylnitrosoguanidine | C(=N)N(C)N=O | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 70348 | 1-FLUORO-2,4-DINITROBENZENE | C1(F)(C(N(=O)=O)cc(N(=O)=O)cc1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 74964 | ETHYL_BROMIDE | C(C)Br | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75252 | TRIBROMOMETHANE | C(Br)(Br)Br | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75263 | 2-Bromopropane | C(C)C)Br | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75478 | TRIOMOMETHANE | C(I)(I)I | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75558 | PROPYLENIMINE | C1C(C)CN1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 75912 | TERT-BUTYL_HYDROPEROXIDE | C(C)(C)OO | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 78342 | DIOXATHION | C1(SP(=S)(OCC)OCC)C(SP(=S)(OCC)OCC)S1 | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 78875 | 2,2-DICHLOROPROPANE; "1,2-Dichloro-2-methylpropane" | C(C)(C)C(Cl)C(Cl) | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 78886 | 2,3-DICHLORO-1-PROPENE | C=C(C)C(Cl)C(Cl) | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |

Navigation: < Back Next > Finish

Select : CAS

File import wizard step 2 of 3

File layout
☒ Vertical
☐ Horizontal
☒ I have a header row

☐ Private data

Default column region

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.

☐ is value [] add

| CAS | name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale v |
|-------|-------------------------------------|---|---------------------------------------|-----------------|-------------------------|
| 52737 | DICHLORVOS | <chem>ClC(Cl)=COP(=O)(OC)OC</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 53923 | Phenoxybenzamine_hydrochloride_USAN | <chem>c1cn(+)(c(-))c(C)c(Coc2ccccc2)CCC1</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 54675 | Diethyl_Sulfate | <chem>C(C)OS(=O)(=O)OCC</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56273 | METHYL_METHANESULFONATE | <chem>COS(C)=O=O</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56273 | 1-benzyl-mustard (USAN) | <chem>ClC1CNCCCCCCCC1N</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |

Select : Chemical name

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

CAS
 Chemical name
 SMILES
 Endpoint tree path

Metadata
☐ is value

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.

| CAS | Chemical name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale v |
|-------|--------------------------------|---|---------------------------------------|-----------------|-------------------------|
| 52737 | DICHLORVOS | <chem>C(Cl)(Cl)=COP(=O)(OC)OC</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 53923 | Phenoxybenzamine_hydrochloride | <chem>C1(CN(+)C1)C(C)COC2CCCC2CC(C)C</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 54675 | Diethyl_Sulfate | <chem>C(C)OS(=O)(=O)OCC</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56273 | METHYL_METHANESULFONATE | <chem>COS(C)(=O)=O</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |

Cancel < Back Next > Finish

Select : SMILES

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

CAS
 Chemical name
 SMILES
 Endpoint tree path

Metadata
☐ is value

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.

| CAS | Chemical name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale v |
|-------|-------------------------------------|---|---------------------------------------|-----------------|-------------------------|
| 52737 | DICHLORVOS | <chem>C(Cl)(Cl)=COP(=O)(OC)OC</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 53923 | Phenoxybenzamine_hydrochloride_USAN | <chem>C1(CN(+)C1)C(C)COC2CCCC2CC(C)C</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 54675 | Diethyl_Sulfate | <chem>C(C)OS(=O)(=O)OCC</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56273 | METHYL_METHANESULFONATE | <chem>COS(C)(=O)=O</chem> | Human health hazards#Genetic Toxicity | Gene mutation I | Positive |

Cancel < Back Next > Finish

Select : DATA Scale

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 value ☐ 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.

☐ Is value add

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

| CAS | Chemical name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale v |
|-------|---------------------------------------|---|---------------------------------------|-----------------|-------------------------|
| 52737 | DICHLORVOS | <chem>C(Cl)(Cl)=COP(=O)(OC)OC</chem> | human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 53923 | Phenoxybenzamine_hydrochloride_[USAN] | <chem>C1(CN(+)C1C(C)C(C)C2CCCC2)CCCl</chem> | human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 54675 | Diethyl_Sulfate | <chem>CCOS(=O)(=O)OCC</chem> | human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56273 | METHYL_METHANESULFONATE | <chem>COS(C)(=O)=O</chem> | human health hazards#Genetic Toxicity | Gene mutation I | Positive |

Cancel < Back Next > Finish

Select : Endpoint tree path

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 value ☐ 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.

☐ Is value add

Metadata
 Water alkalinity
 Water flow
 Water Hardness
 Water media type
 Water type
 WaterType
 Weekly exposure (days/ week)
 Wet_Dry
 Year
 Undefined

| CAS | Chemical name | Smiles | Endpoint tree path | Scale | Data Mean value/Scale v |
|-------|---------------------------------------|---|---------------------------------------|-----------------|-------------------------|
| 52737 | DICHLORVOS | <chem>C(Cl)(Cl)=COP(=O)(OC)OC</chem> | human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 53923 | Phenoxybenzamine_hydrochloride_[USAN] | <chem>C1(CN(+)C1C(C)C(C)C2CCCC2)CCCl</chem> | human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 54675 | Diethyl_Sulfate | <chem>CCOS(=O)(=O)OCC</chem> | human health hazards#Genetic Toxicity | Gene mutation I | Positive |
| 56273 | METHYL_METHANESULFONATE | <chem>COS(C)(=O)=O</chem> | human health hazards#Genetic Toxicity | Gene mutation I | Positive |

Cancel < Back Next > Finish

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 Main Value/Scale value

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: **2** Data

Define value: ☐ Scale ☐ Low qualifier ☐ Upper value ☒ Mean value/Scale value ☐ Mean qualifier ☐ Low value ☐ Upper qualifier ☐ Undefined **3**

Metadata: Water alkalinity, Water flow, Water Hardness, Water media type, Water type, WaterType, Weekly exposure (days/ week), Wet_Dry, Year, Undefined

Endpoint tree path: Genetic Toxicity, Human health hazards#Genetic Toxicity, Gene mutation I, Positive, Gene mutation I, Positive, Gene mutation I, Positive, Gene mutation I, Positive, Gene mutation I, Positive

| Scale | Data Unit | Endpoint | Type of genotoxicity | Type of method | Test type |
|-----------------|--------------------|---------------|----------------------|----------------|------------------|
| Data Scale | 1 Data Unit | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |

Cancel < Back Next > Finish

Select : DATA Unit

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: **2** Data

Define value: ☐ Scale ☐ Low qualifier ☐ Upper value ☒ Mean value/Scale value ☐ Mean qualifier ☐ Low value ☐ Upper qualifier ☐ Undefined **3**

Metadata: Water alkalinity, Water flow, Water Hardness, Water media type, Water type, WaterType, Weekly exposure (days/ week), Wet_Dry, Year, Undefined

Endpoint tree path: Genetic Toxicity, Human health hazards#Genetic Toxicity, Gene mutation I, Positive, Gene mutation I, Positive, Gene mutation I, Positive, Gene mutation I, Positive, Gene mutation I, Positive

| Scale | Data Unit | Endpoint | Type of genotoxicity | Type of method | Test type |
|-----------------|--------------------|---------------|----------------------|----------------|------------------|
| Data Scale | 1 Data Unit | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |
| Gene mutation I | Positive | Gene mutation | Gene mutation | in vitro | bacterial revers |

Cancel < Back Next > Finish



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

Scroll bar

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
☐ Mean qualifier
☐ Mean value/Scale value
☐ Low qualifier
☐ Low value
☐ Upper qualifier
☐ Upper value
☒ Unit
☐ 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
☐ is value add

| Endpoint | Type of genotoxicity | Type of method | Test type | Test organisms (species) | Strain | Species/strain | Metabolic activation |
|---------------|----------------------|----------------|--|--------------------------|--------|----------------|----------------------|
| Gene mutation | Gene mutation | in vitro | bacterial reverse mutation assay (e.g. Ames) | Salmonella typhimurium | TA 100 | | without S9 |
| Gene mutation | Gene mutation | in vitro | bacterial reverse mutation assay (e.g. Ames) | Salmonella typhimurium | TA 100 | | without S9 |
| Gene mutation | Gene mutation | in vitro | bacterial reverse mutation assay (e.g. Ames) | Salmonella typhimurium | TA 100 | | without S9 |
| Gene mutation | Gene mutation | in vitro | bacterial reverse mutation assay (e.g. Ames) | Salmonella typhimurium | TA 100 | | without S9 |
| Gene mutation | Gene mutation | in vitro | bacterial reverse mutation assay (e.g. Ames) | Salmonella typhimurium | TA 100 | | without S9 |

Cancel < Back Next > Finish

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

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
☐ Mean qualifier
☐ Mean value/Scale value
☐ Low qualifier
☐ Low value
☐ Upper qualifier
☐ Upper value
☒ Unit
☐ Undefined

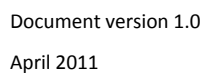
Scales editor
 Select one or more columns from the grid below and then assign the selection to a region by choosing from the lefthand side radio buttons.

Metadata
☐ is value add

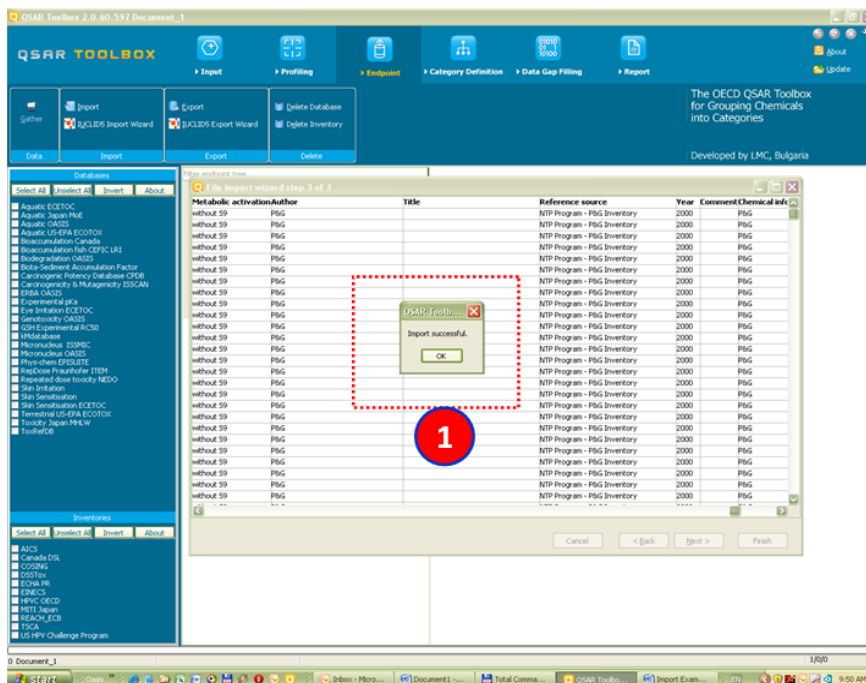
| Author | Title | Reference source | Year | Comment | Chemical info |
|--------|-------|-----------------------------|------|---------|---------------|
| P&G | | NTP Program - P&G Inventory | 2000 | | P&G |
| P&G | | NTP Program - P&G Inventory | 2000 | | P&G |
| P&G | | NTP Program - P&G Inventory | 2000 | | P&G |
| P&G | | NTP Program - P&G Inventory | 2000 | | P&G |
| P&G | | NTP Program - P&G Inventory | 2000 | | P&G |

Cancel < Back Next > Finish

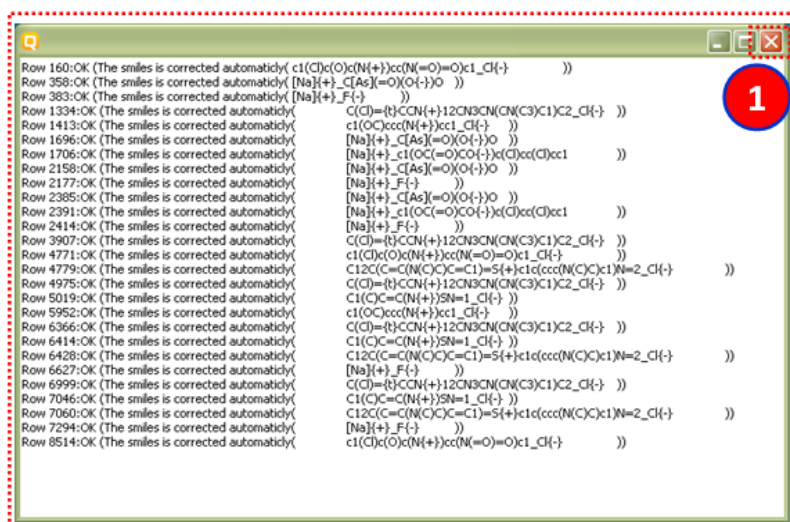
Click on “*Finish*” button



Database is imported successfully. Click "OK".



Error message log file



OECD

2, rue André Pascal
75775 Paris Cedex 16
France

Tel.: +33 1 45 24 82 00

Fax: +33 1 45 24 85 00

ehscont@oecd.org