QSAR TOOLBOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

OECD QSAR Toolbox v.4.1

Tutorial of how to Import/Export a custom database and Import/Export IUCLID

Outlook

- **Aim**
- Definition of Database/Inventory
- Import
- Export

Aim

This is a step-by-step presentation designed to take the user of Toolbox through the process of importing/exporting of custom databases/inventories.

Outlook

- Aim
- **Definition of Database and Inventory**
- Import
- Export

Definition of database and inventory

- A database is a collection of structures accompanied with experimental data.

- An inventory is a collection of structures without experimental data.

Outlook

- Aim
- Definition of Database and Inventory
- **Import:**
  - ❖ Import of database
    - ➢ Vertical import
    - ➢ Horizontal import
  - ❖ Import of inventory
  - ❖ Import via IUCLID
- Export Data matrix

Import of database: Types of import

- **Vertical import:**
  It is appropriate for a set of chemicals with consistent experimental data and the same supporting information (e.g. endpoint, test organism, test condition, author etc.).
- **Horizontal import:**
  It is appropriate for a set of chemicals with different types of experimental data accompanied with supporting information (endpoints, test condition, test organism, author etc).

Outlook

- Aim
- Definition of Database and Inventory
- **Import:**
  - **Import of database**
    - **Vertical import**
    - Horizontal import
  - Import of inventory
  - Import via IUCLID
- Export Data matrix

Import of database: Vertical import

- Vertical import layout contains two main sections: substance information (1) and experimental data (2);
- Each column (2) defines data points for a single experiment.
- The imported file can be in *xlsx* or *tsv* format.

CAS #	NAME	SMILES	Experiment 1	Experiment 2	...	Experiment M
CAS 1	NAME 1	SMILES 1	Value 1.1	Value 2.1	...	Value M.1
CAS 2	NAME 2	SMILES 2	Value 1.2	Value 2.2	...	Value M.2
CAS 3	NAME 3	SMILES 3	Value 1.3	Value 2.3	...	Value M.3
...	...	...	...	...	...	...
CAS N	NAME N	SMILES N	Value 1.N	Value 2.N	...	Value M.N

1

2

Import of database: Vertical import

- In this tutorial an example of vertical import of a database containing experimental information about Biochemical oxygen demand (BOD) and Bacterial reversed mutation assay (Ames) is shown.
- The excel file (*Vertical import_ BOD and Ames.xlsx*) is depicted below and it could be found: *C:\Program Files (x86)\Common Files\QSAR Toolbox 4\Config\Examples*

	A	B	C	D	E
1	CAS	NAME	Smiles	BOD	Ames
2	60-34-4	METHYLHYDRAZINE	CNN	0.2	Positive
3	50-29-3	DICHLORO_DIPHENYL_TRICHL	C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(	7.1	Negative
4	50-32-8	BENZOPYRENE;3,4-";_BENZOI	c12c3c4c(c5c(cc4ccc3ccc1)cccc5)c	60.7	Negative
5	50-33-9	PHENYLBUTAZONE	C1(=O)C(CCCC)C(=O)N(c2ccccc2)	0.09	Negative
6	148-82-3	MELPHALAN	C(=O)(O)C(N)Cc1ccc(N(CCCl)CCC	5	Positive
7	154-93-8	carmustine	C(=O)(N(CCCl)N=O)NCCCl	0.09	Positive
8	61785-57-7	Benzofurazan,_4-(1-aziridiny	C1(N(=O)=O)C2C(C(N3CC3)=CC=1	1.63	Positive
9	62-75-9	N-NITROSODIMETHYLAMINE	CN(C)N=O	80	Positive
10	91-59-8	2-NAPHTHYLAMINE	c12c(cc(N)cc1)cccc2	25	Positive
11	96-09-3	STYRENE_OXIDE	c1(C2CO2)ccccc1	0.01	Positive
12	107-13-1	2-propenenitrile	C(#N)C=C	2	Positive
13	51-79-6	URETHANE	C(N)(=O)OCC	1.8	Negative
14	53-96-3	2-ACETYLAMINOFLUORENE	c12-c3c(cc(NC(C)=O)cc3)Cc1cccc2	6.2	Negative
15	54-11-5	Pyridine,_3-(1-methyl-2-pyrr	c1(C2CCCN2C)cccnc1	75	Negative
16	54-42-2	idoxuridine	C1(=O)C(I)=CN(C2CC(O)C(CO)O2	0.09	Negative
17	55-38-9	FENTHION	c1(SC)c(C)cc(OP(=S)(OC)OC)cc1	1.8	Negative
18	55-48-1	atropine_sulphate	C(=O)(C(c1ccccc1)CO)OC1CC2CC(	4.5	Negative
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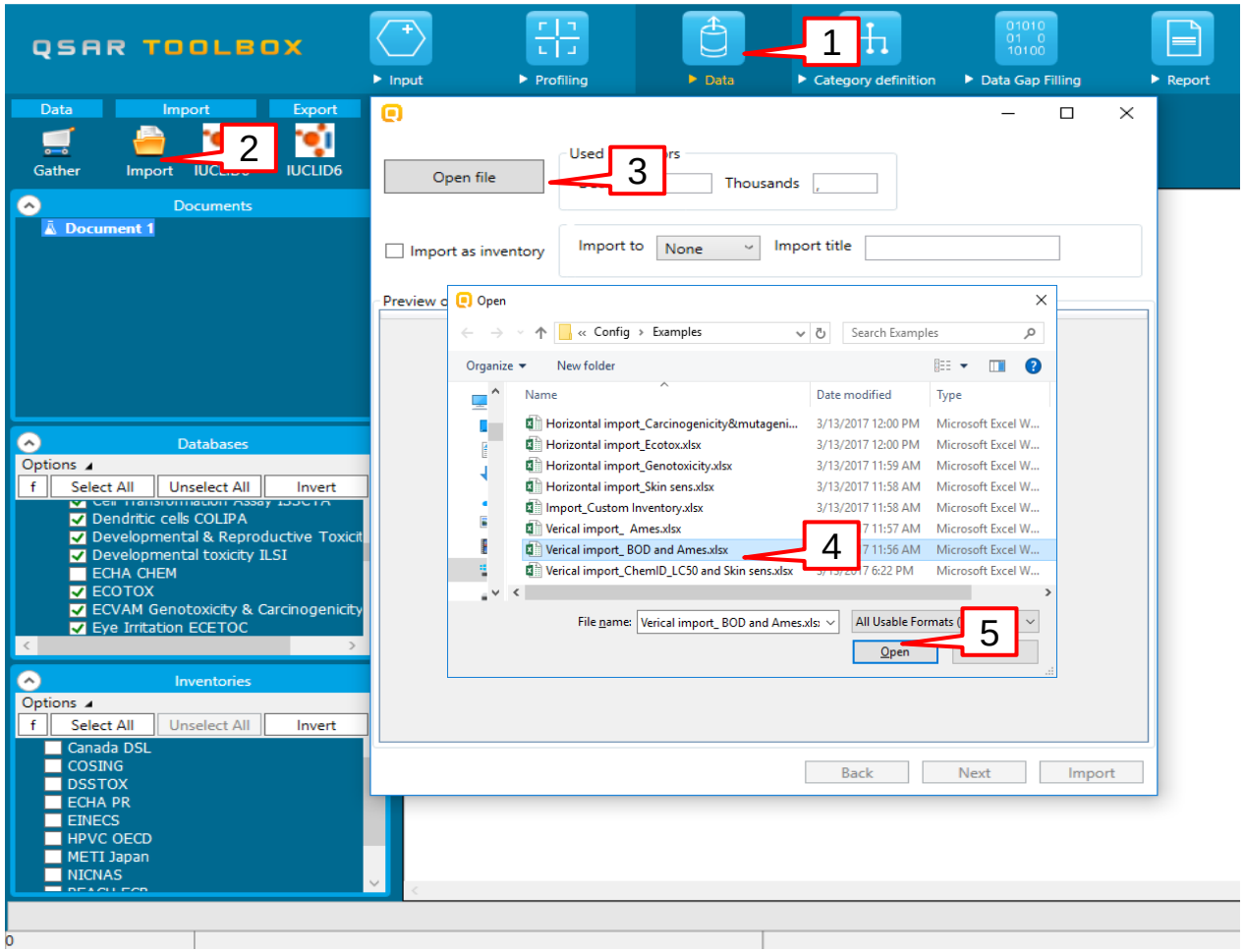
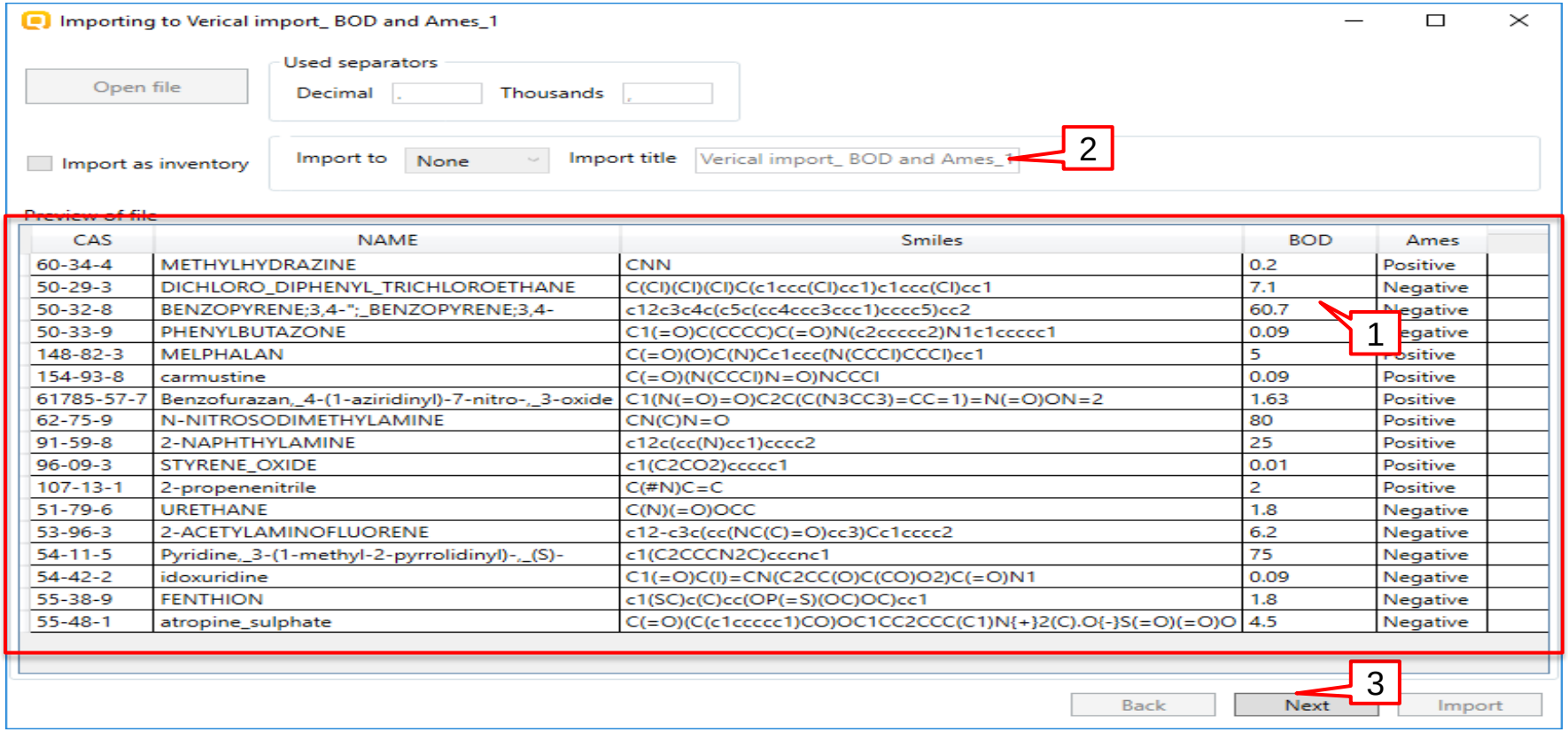
Import of database: Vertical import

1. Go to *Data* panel (1);
2. Click on *Import* (2);
3. Click on *Open file* (3);
4. Select the file (*Verical import_ BOD and Ames.xlsx*)(4);
5. Click on *Open* (5).



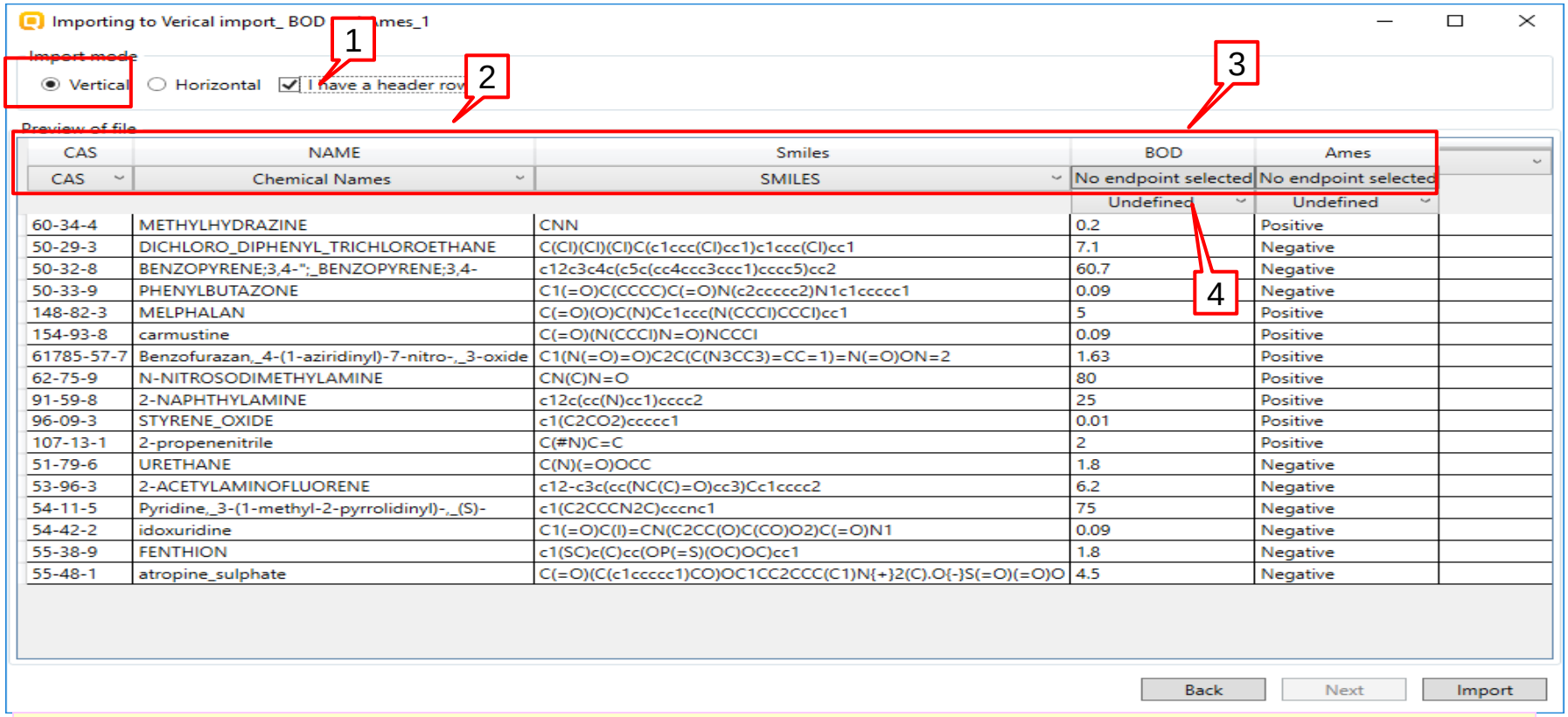
Import of database: Vertical import



CAS	NAME	Smiles	BOD	Ames
60-34-4	METHYLHYDRAZINE	CNN	0.2	Positive
50-29-3	DICHLORO_DIPHENYL_TRICHLOROETHANE	C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1	7.1	Negative
50-32-8	BENZOPYRENE;3,4-";_BENZOPYRENE;3,4-	c12c3c4c(c5c(cc4ccc3ccc1)cccc5)cc2	60.7	Negative
50-33-9	PHENYLBUTAZONE	C1(=O)C(CCCC)C(=O)N(c2ccccc2)N1c1ccccc1	0.09	egative
148-82-3	MELPHALAN	C(=O)(O)C(N)Cc1ccc(N(CCCl)CCCl)cc1	5	ositive
154-93-8	carmustine	C(=O)(N(CCCl)N=O)NCCCl	0.09	Positive
61785-57-7	Benzofurazan,_4-(1-aziridinyl)-7-nitro-,_3-oxide	C1(N(=O)=O)C2C(C(N3CC3)=CC=1)=N(=O)ON=2	1.63	Positive
62-75-9	N-NITROSODIMETHYLAMINE	CN(C)N=O	80	Positive
91-59-8	2-NAPHTHYLAMINE	c12c(cc(N)cc1)cccc2	25	Positive
96-09-3	STYRENE_OXIDE	c1(C2CO2)ccccc1	0.01	Positive
107-13-1	2-propenenitrile	C(#N)C=C	2	Positive
51-79-6	URETHANE	C(N)(=O)OCC	1.8	Negative
53-96-3	2-ACETYLAMINOFLUORENE	c12-c3c(cc(NC(C)=O)cc3)Cc1cccc2	6.2	Negative
54-11-5	Pyridine,_3-(1-methyl-2-pyrrolidinyl)-,_(S)-	c1(C2CCCN2C)cccnc1	75	Negative
54-42-2	idoxuridine	C1(=O)C(I)=CN(C2CC(O)C(CO)O2)C(=O)N1	0.09	Negative
55-38-9	FENTHION	c1(SC)c(C)cc(OP(=S)(OC)OC)cc1	1.8	Negative
55-48-1	atropine_sulphate	C(=O)(C(c1ccccc1)CO)OC1CC2CCC(C1)N{+}2(C).O{-}S(=O)(=O)O	4.5	Negative

1. A preview of the imported file is shown (1); 2. The title of the imported file is also included; 3. Click on *Next* (2);

Import of database: Vertical import

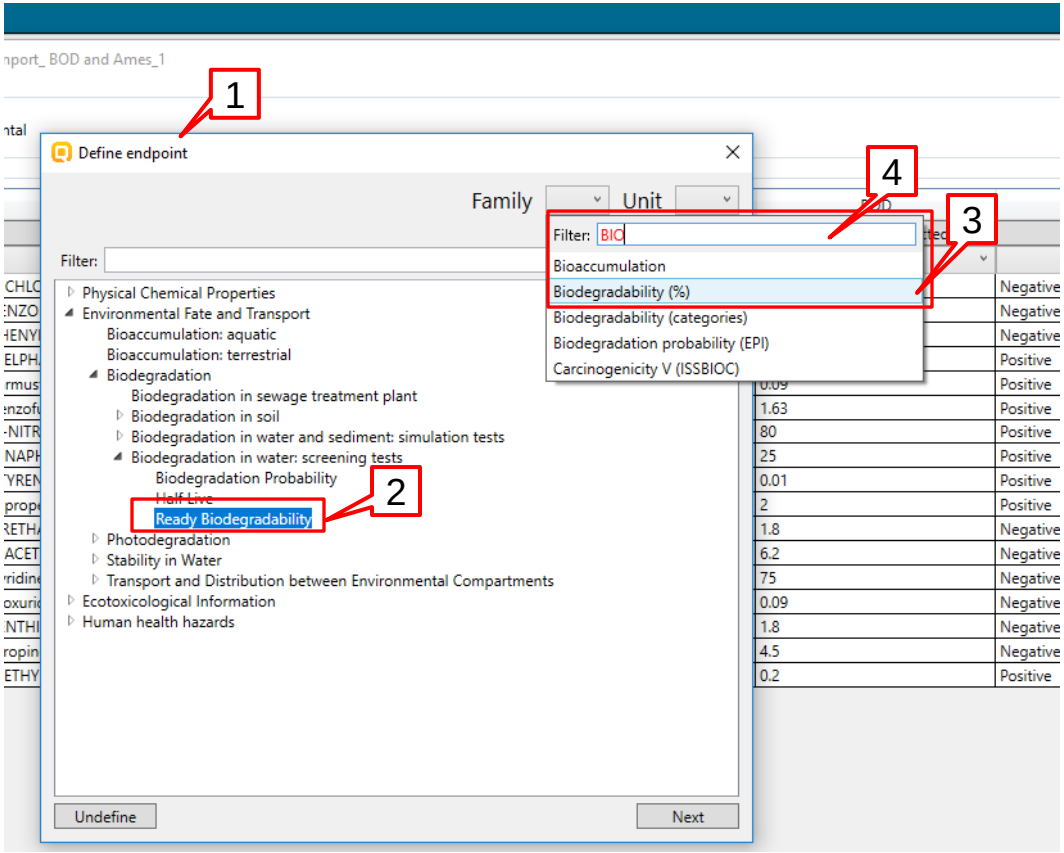


CAS	NAME	Smiles	BOD	Ames
CAS	Chemical Names	SMILES	No endpoint selected	No endpoint selected
			Undefined	Undefined
60-34-4	METHYLHYDRAZINE	CNN	0.2	Positive
50-29-3	DICHLORO_DIPHENYL_TRICHLOROETHANE	C(Cl)(Cl)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1	7.1	Negative
50-32-8	BENZOPYRENE;3,4-";_BENZOPYRENE;3,4-	c12c3c4c(c5c(cc4ccc3ccc1)cccc5)cc2	60.7	Negative
50-33-9	PHENYLBUTAZONE	C1(=O)C(CCCC)C(=O)N(c2ccccc2)N1c1ccccc1	0.09	Negative
148-82-3	MELPHALAN	C(=O)(O)C(N)Cc1ccc(N(CCCl)CCCl)cc1	5	Positive
154-93-8	carmustine	C(=O)(N(CCCl)N=O)NCCCl	0.09	Positive
61785-57-7	Benzofurazan,_4-(1-aziridinyl)-7-nitro-,_3-oxide	C1(N(=O)=O)C2C(C(N3CC3)=CC=1)=N(=O)ON=2	1.63	Positive
62-75-9	N-NITROSODIMETHYLAMINE	CN(C)N=O	80	Positive
91-59-8	2-NAPHTHYLAMINE	c12c(cc(N)cc1)cccc2	25	Positive
96-09-3	STYRENE_OXIDE	c1(C2CO2)ccccc1	0.01	Positive
107-13-1	2-propenenitrile	C(#N)C=C	2	Positive
51-79-6	URETHANE	C(N)(=O)OCC	1.8	Negative
53-96-3	2-ACETYLAMINOFLUORENE	c12-c3c(cc(NC(C)=O)cc3)Cc1cccc2	6.2	Negative
54-11-5	Pyridine,_3-(1-methyl-2-pyrrolidinyl)-,_(S)-	c1(C2CCCN2C)cccnc1	75	Negative
54-42-2	idoxuridine	C1(=O)C(I)=CN(C2CC(O)C(CO)O2)C(=O)N1	0.09	Negative
55-38-9	FENTHION	c1(SC)c(C)cc(OP(=S)(OC)OC)cc1	1.8	Negative
55-48-1	atropine_sulphate	C(=O)(C(c1ccccc1)CO)OC1CC2CCC(C1)N{+}2(C).O{-}S(=O)(=O)O	4.5	Negative

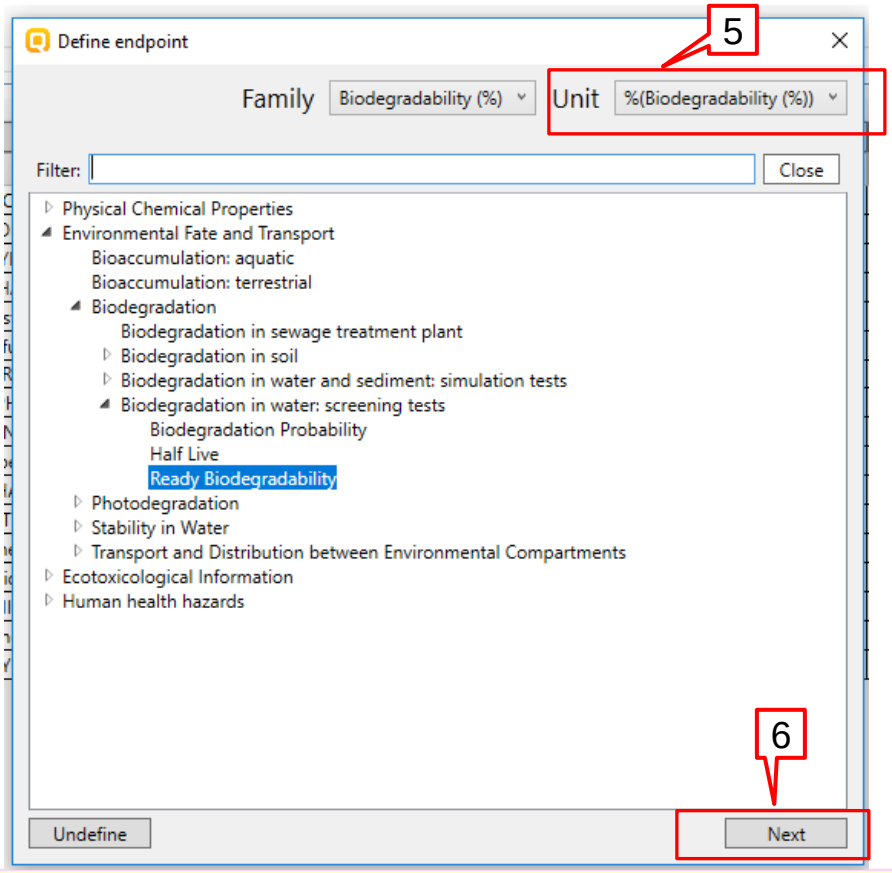
1. Select *Vertical* radio button (1).
2. Header row (2)
3. Define the relevant endpoints associated with BOD (Biological oxygen demand) and Ames (Bacterial reverse mutation assay) (2) by clicking individually on each *No endpoint* selected button under the endpoints names. (4)

Import of database: Vertical import

*For **BOD**:*
Define endpoint window is displayed (1).
Select Ready Biodegradability (2) from the endpoint tree, then select the family (Biodegradability %) (3) by using the filter options (4).



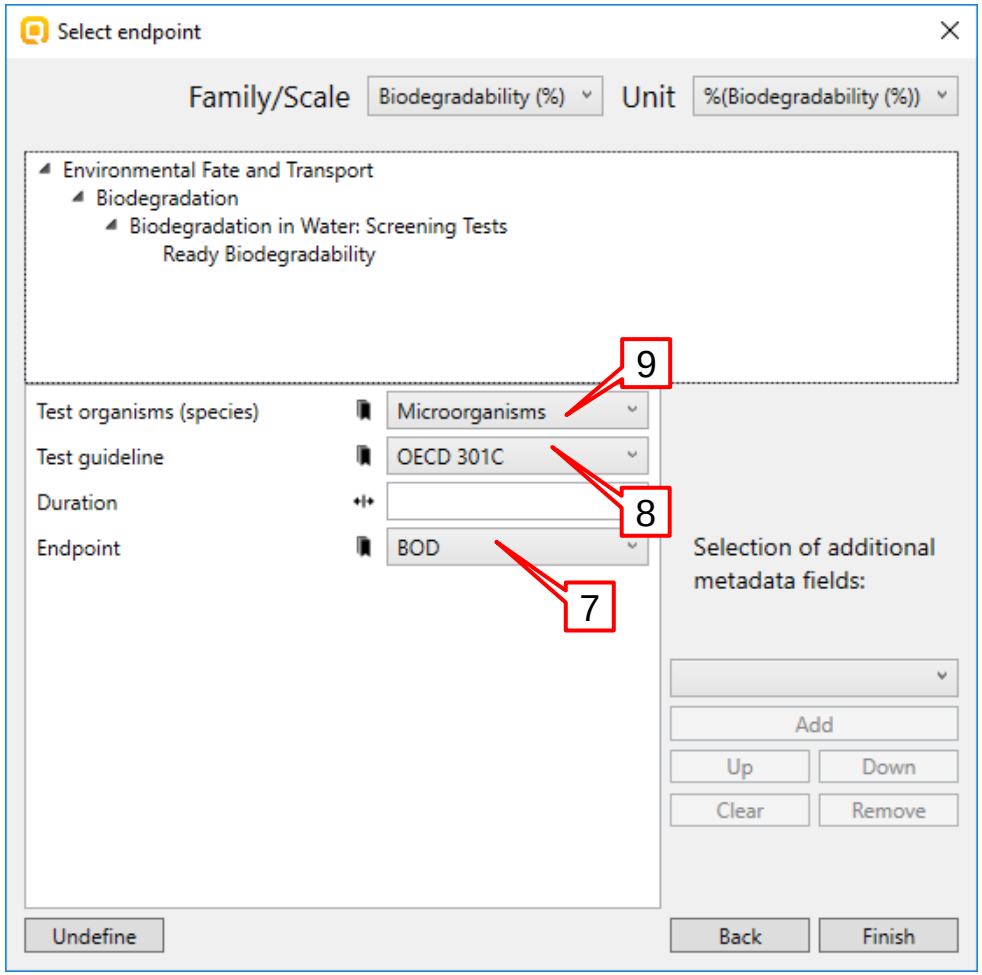
Import of database: Vertical import



For BOD:

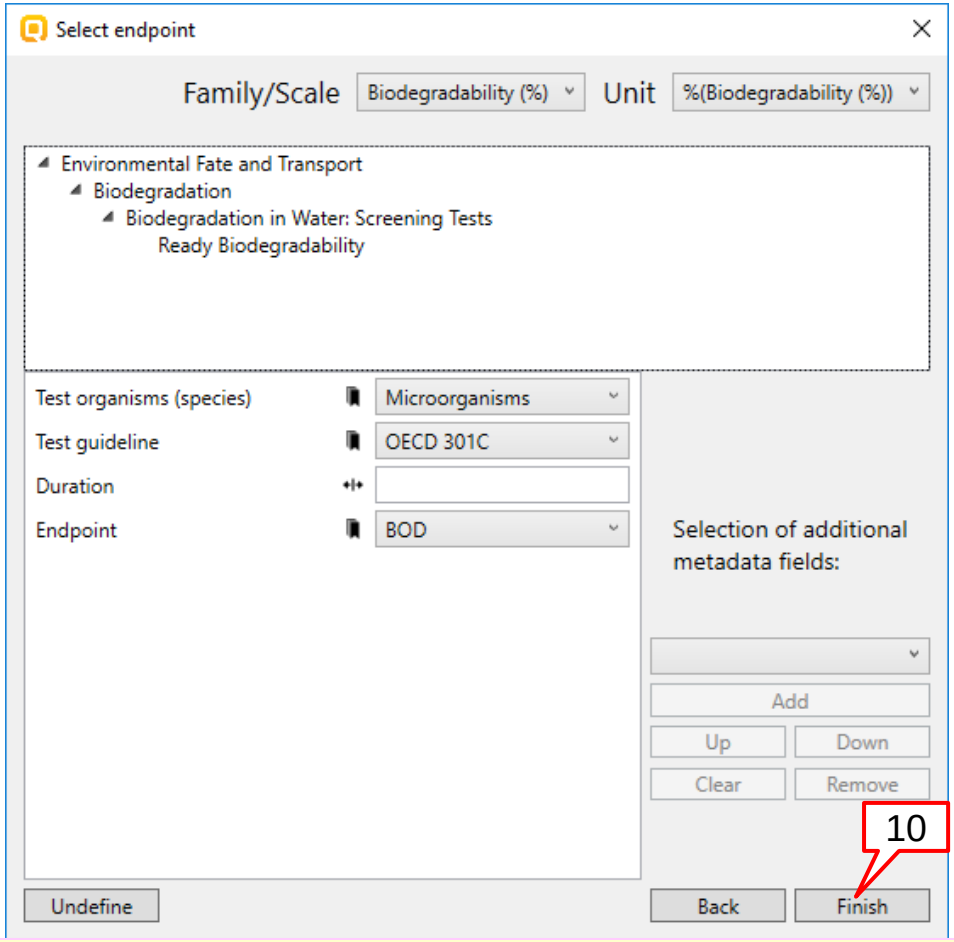
Then select the unit from the drop-down menu (% Biodegradability(%))(5) and then to press Next (6).

Import of database: Vertical import



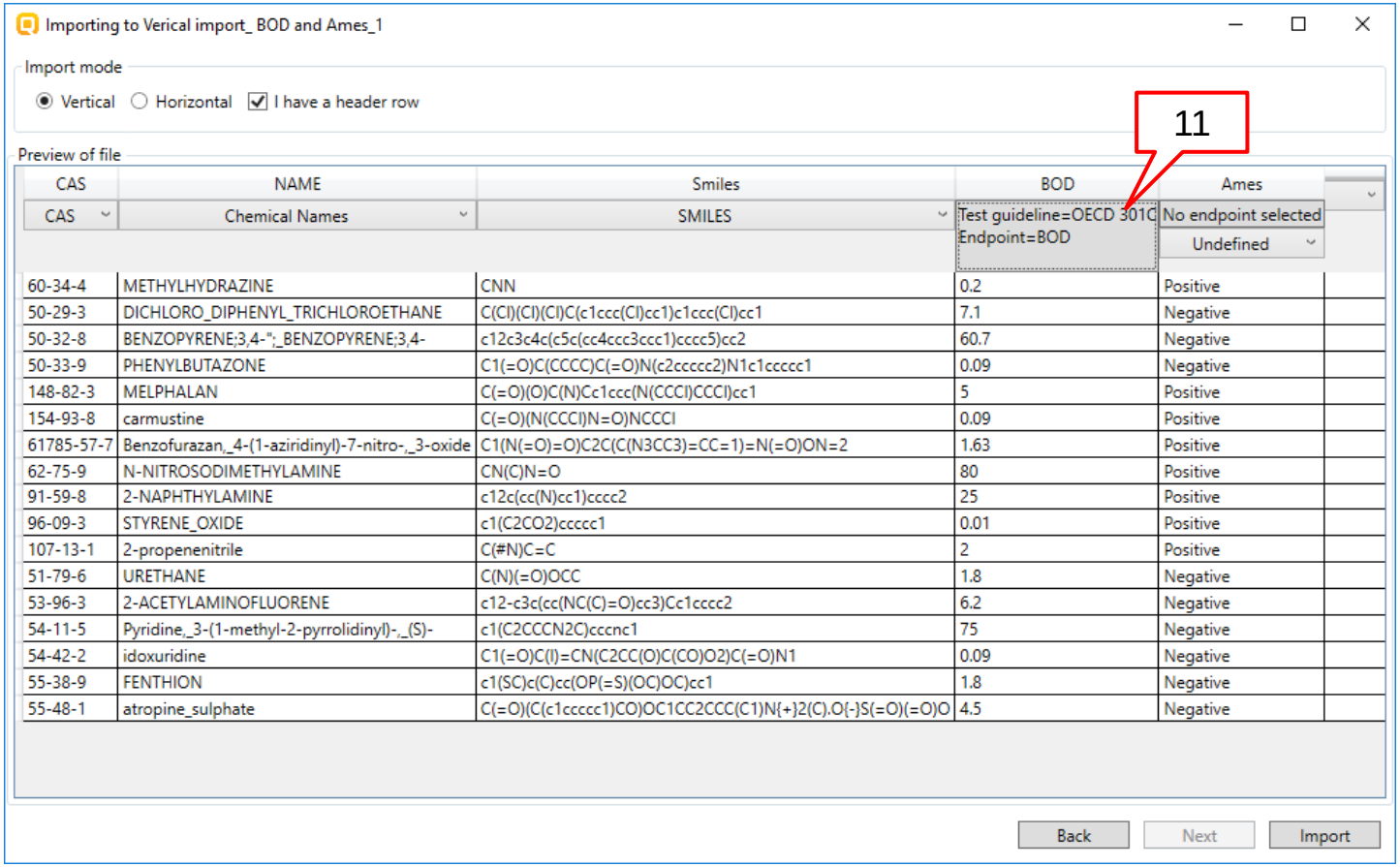
*For **BOD***: Select BOD endpoint (7) from the drop-down menu. Then from the drop-down menu associated with test guideline select OECD301C (8) and test organism (species): select Microorganisms (9).

Import of database: Vertical import



*For **BOD***: Once all the data fields are filled , press *Finish* (10).

Import of database: Vertical import

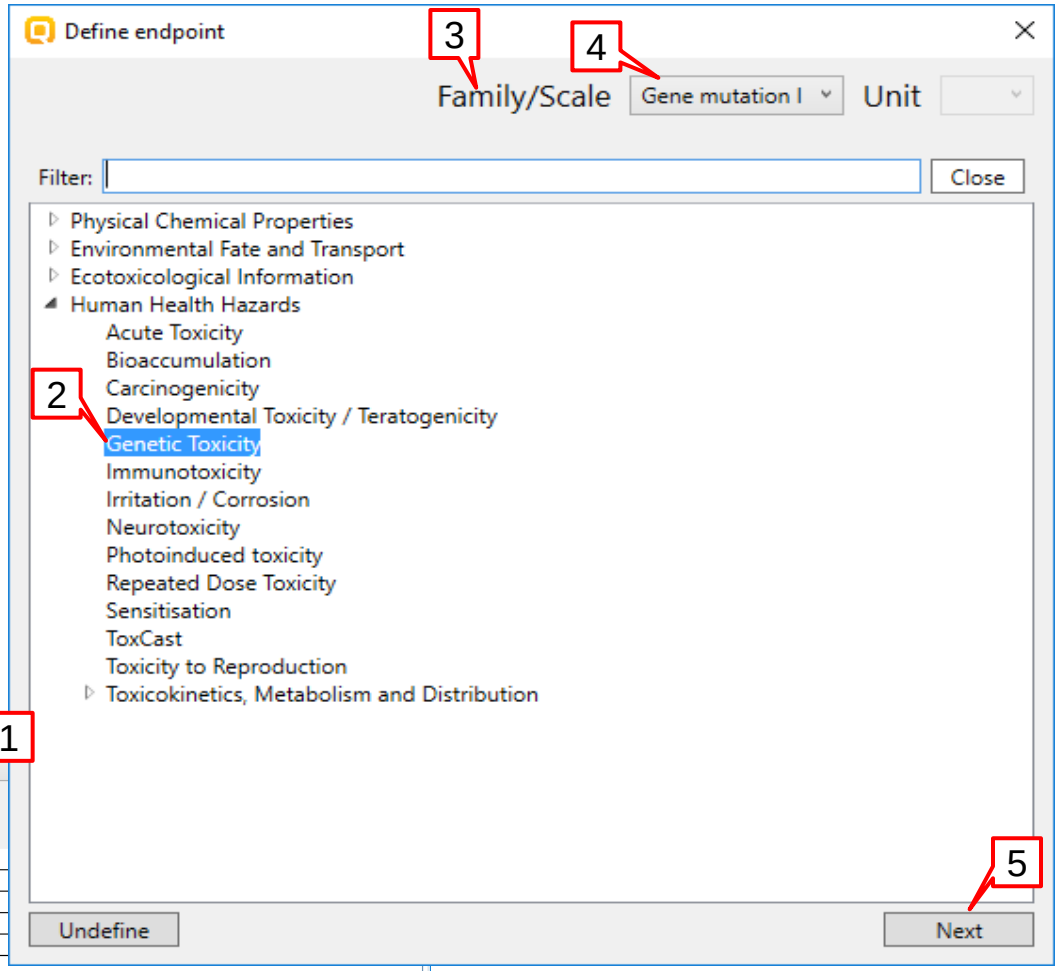


*For **BOD***: The edited fields are displayed in the main table (11).

Import of database: Vertical import

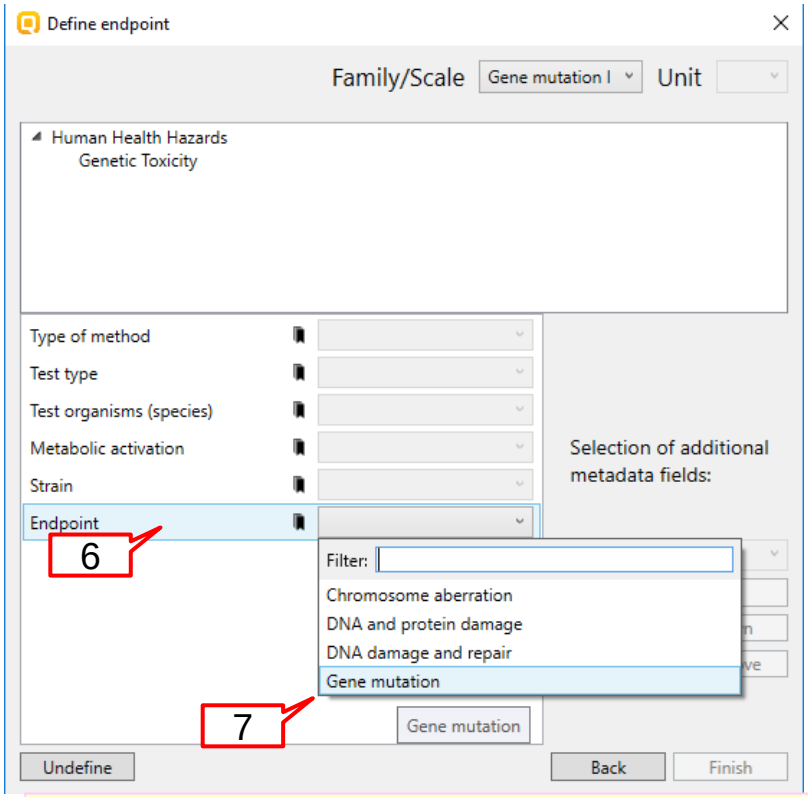
*For **Ames***:

1. Click on *No endpoint selected* (1);
2. Expand the tree and select Genetic toxicity (2).
3. From the drop-down menu of Family(3) select Gene mutation I (4), which could be found by using the implemented filter.
4. Click on *Next* (5)



Smiles	BOD	Ames
SMILES	Test organisms (species)=Microorganisms Test guideline=OECD 301C Endpoint=BOD	No endpoint selected Undefined
	0.2	Positive
)(Cl)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1	7.1	Negative
4c(c5c(cc4ccc3ccc1)cccc5)cc2	60.7	Negative
C(CCCC)C(=O)N(c2ccccc2)N1c1ccccc1	0.09	Negative
O)C(N)Cc1ccc(N(CCCl)CCCl)cc1	5	Positive
N(CCCl)N=O)NCCCl	0.09	Positive
O)=O)C2C(C(N3CC3)=CC=1)=N(=O)ON=2	1.63	Positive
=O	80	Positive

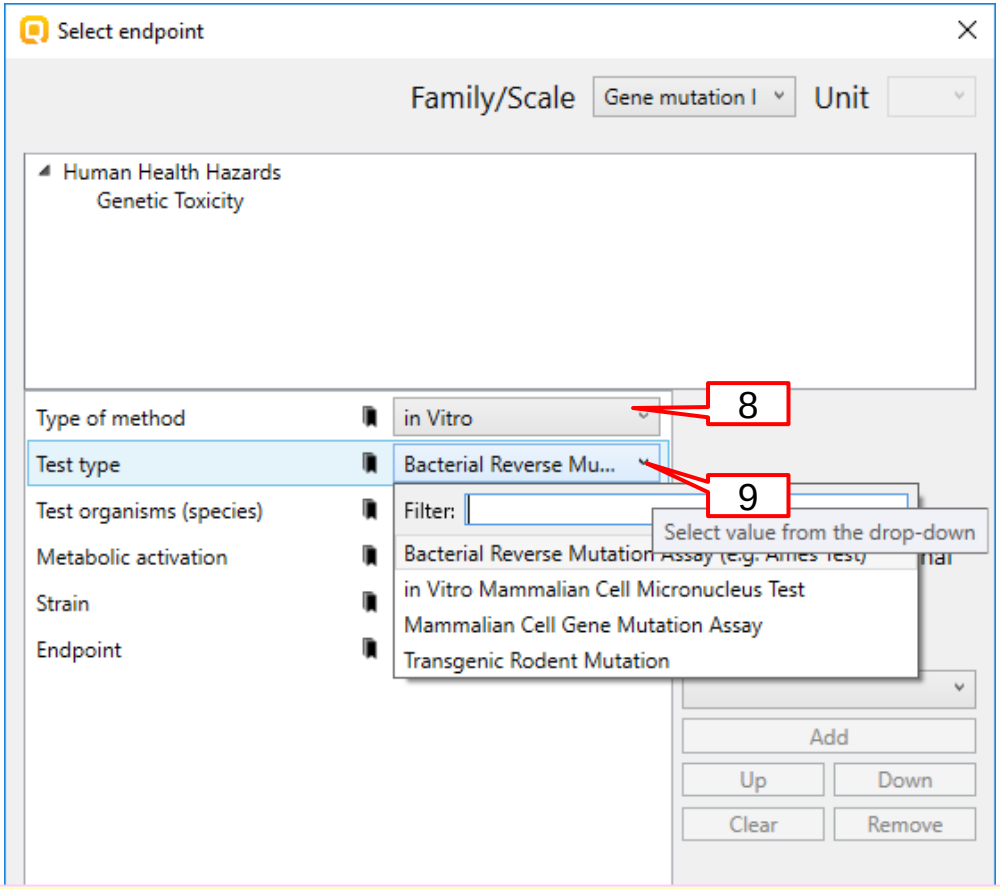
Import of database: Vertical import



*For **Ames***:

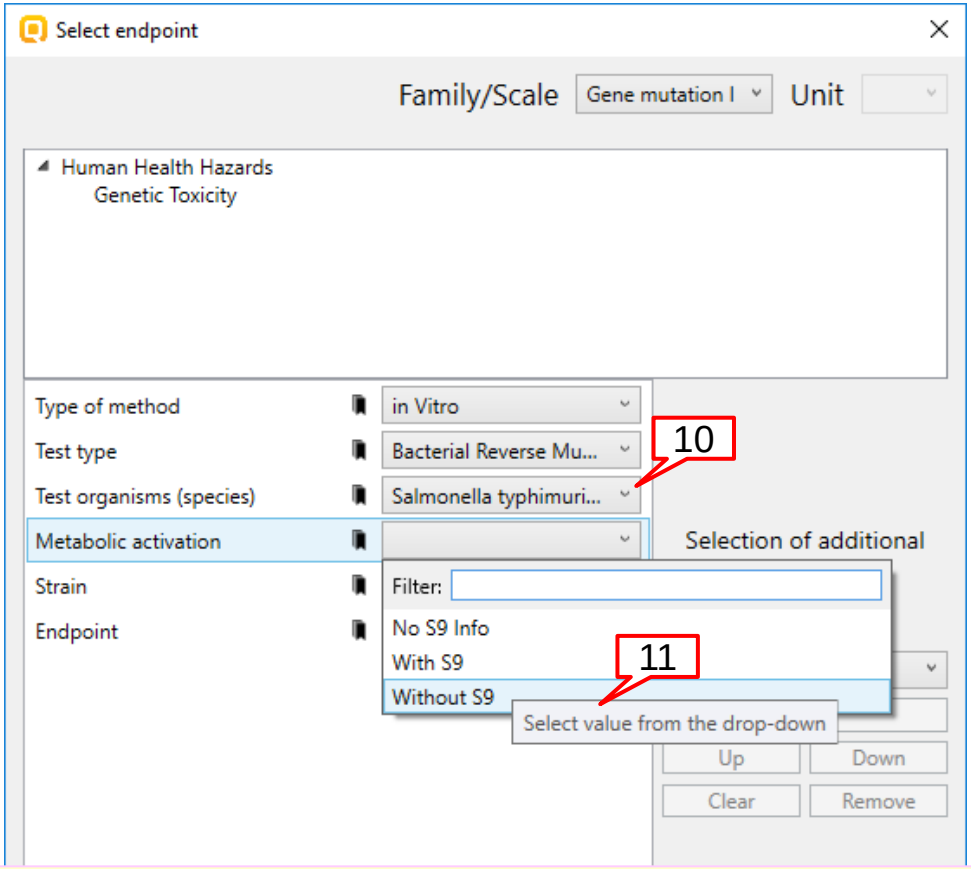
1. Select *Endpoint*(6) – Gene mutation(7).

Import of database: Vertical import



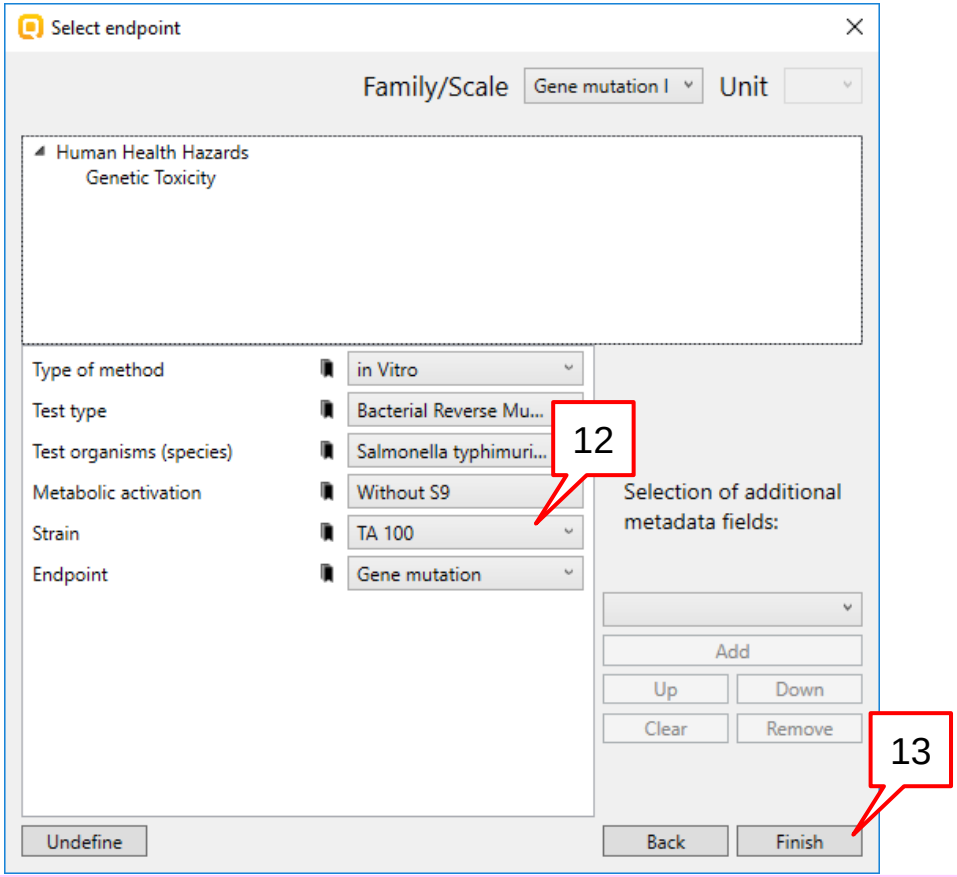
*For **Ames***:
From the drop-down menu of *Type of method*, select In vitro and from *Test type* filed select : Bacterial reverse Mutation assays (e.g. Ames test) (9).

Import of database: Vertical import



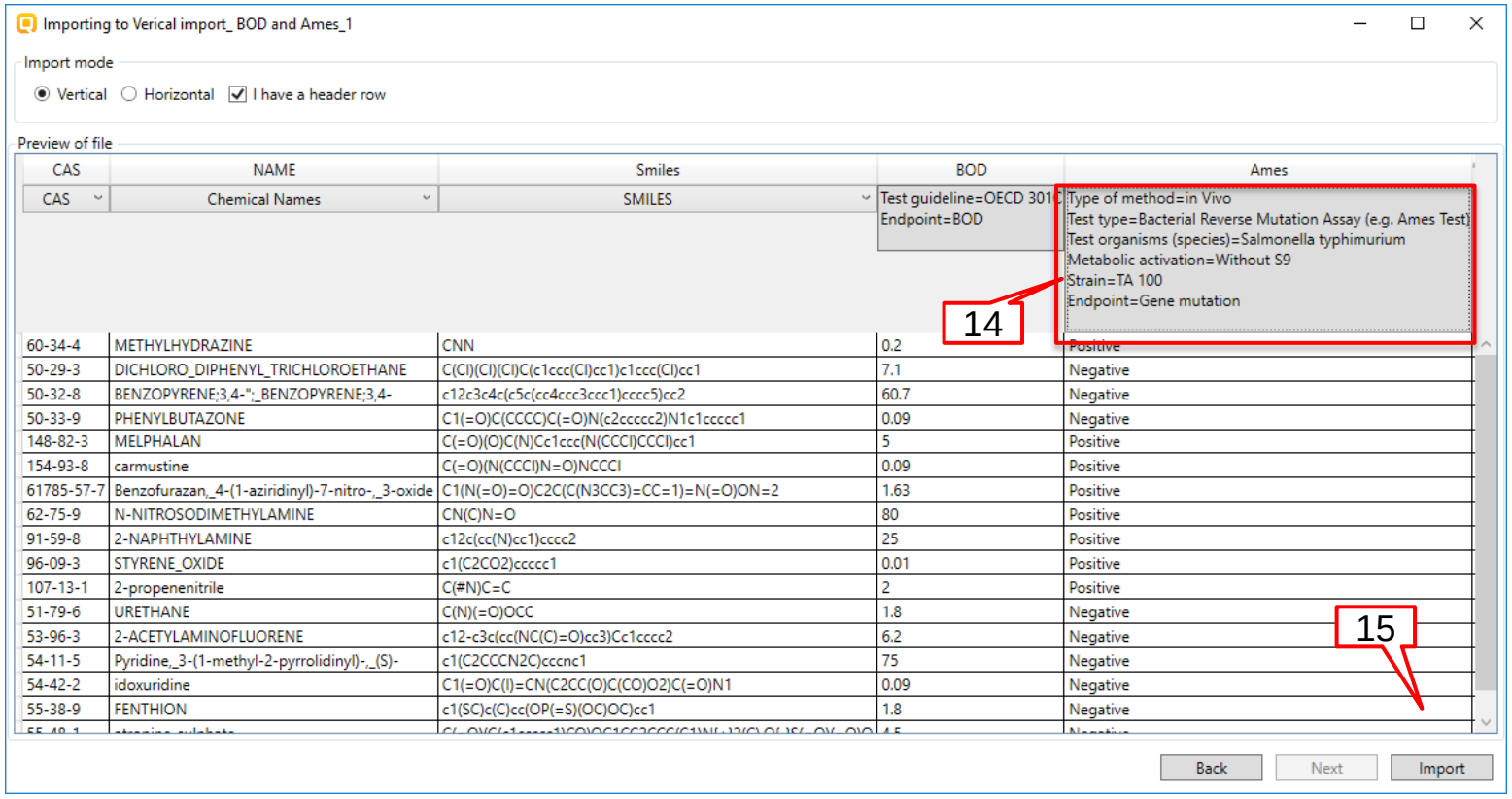
*For **Ames***:
Select *Test organism (species)*: Salmonella typhimurium (10) and for *Metabolic activation* and click on Without S9 (11).

Import of database: Vertical import



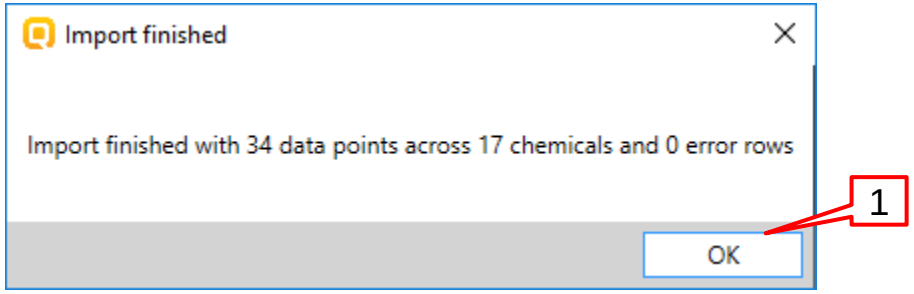
*For **Ames***:
Select Strain: TA 100 (12) for instance and then click Finish (13).

Import of database: Vertical import



*For **Ames***: The edited fields are displayed in the main table (14).
Finally, click on *Import* (15).

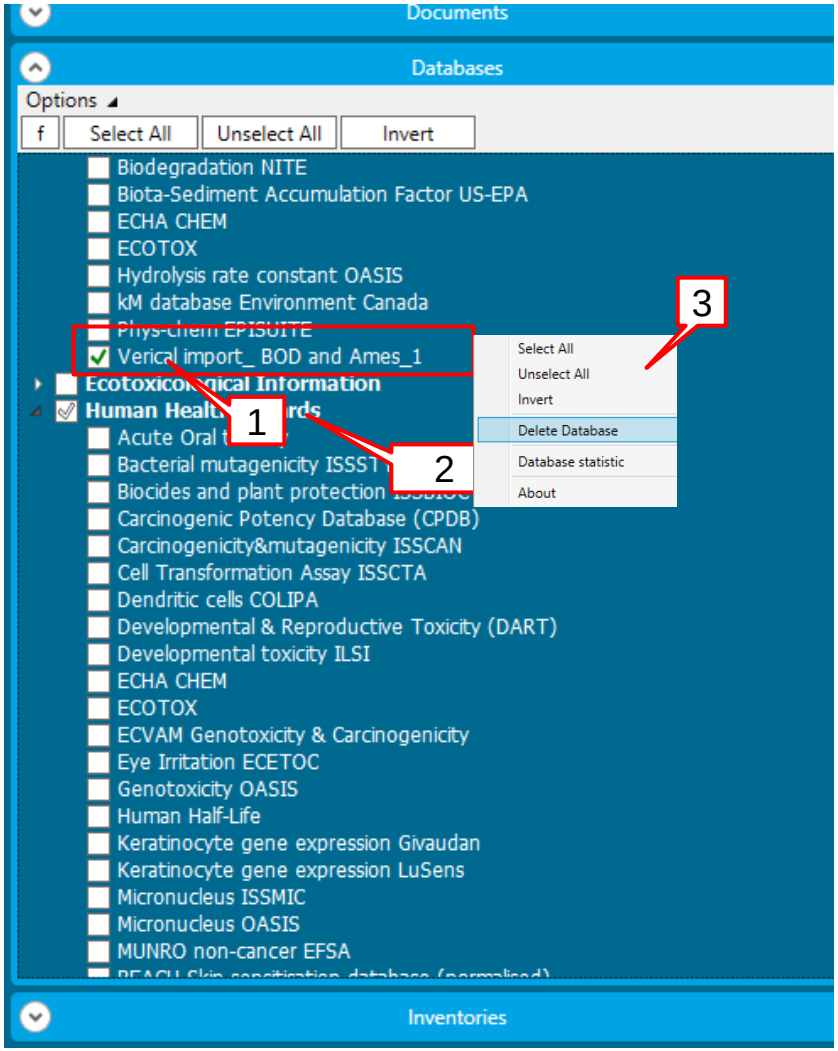
Import of database: Vertical import



- The import process could take a couple of minutes;
- An informative message is displayed when it is completed;
- Click on *OK* (1).

Import of database: Vertical import

- The new database is displayed in the Databases panel (1) in the *Environmental fate and transport* group and in the *Human health hazard group* (2).
- Right-click menu (3) is implemented where you can see the database statistics or delete the database.



Outlook

- Aim
- Definition of Database and Inventory
- **Import:**
  - **Import of database**
    - Vertical import
    - **Horizontal import**
  - Import of inventory
  - Import via IUCLID
- Export Data matrix

Import of database: Horizontal import

- In this tutorial an example of horizontal import of a database containing experimental information related to genotoxicity is shown.
- The excel file (Horizontal import_Genotoxicity.xlsx) is depicted below and it could be found: C:\Program Files (x86)\Common Files\QSAR Toolbox 4\Config\Examples

F1 Data Mean value/Scale value

	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	Data Mean value/Scale value	Endpoint	Type of genotoxicity	Type of method	Test type	Metabolic activation	Test organisms (species)	Strain	Source of methabolic system	Author	Title	Year	Chemical info
2	Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	with S9	Salmonella typhimurium	TA 100	rat	U.S. Environ	The Salmonella typhimuri	1996	US_GTox
3	Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	without S9	Salmonella typhimurium	TA 100		U.S. Environ	The Salmonella typhimuri	1996	US_GTox
4	Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	with S9	Salmonella typhimurium	TA 100	rat	U.S. Environ	The Salmonella typhimuri	1996	US_GTox
5	Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	without S9	Salmonella typhimurium	TA 100		U.S. Environ	The Salmonella typhimuri	1996	US_GTox
6	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	with S9	Salmonella typhimurium	TA 98	hamster	National Car	Short-Term Testing Progra	2000	NCI-STTP
7	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	without S9	Salmonella typhimurium	TA 98		National Car	Short-Term Testing Progra	2000	NCI-STTP
8	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	with S9	Salmonella typhimurium	TA 1535	mouse	U.S. Environ	The Salmonella typhimuri	1996	US_GTox
9	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	without S9	Salmonella typhimurium	TA 1535		U.S. Environ	The Salmonella typhimuri	1996	US_GTox
10	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	with S9	Salmonella typhimurium	TA 1537	rat	U.S. Environ	The Salmonella typhimuri	1996	US_GTox
11	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse muta	without S9	Salmonella typhimurium	TA 1535		U.S. Environ	The Salmonella typhimuri	1996	US_GTox
12	Positive	Gene mutation	Gene mutation	in vitro	alian cell gene mutation assay		Mouse Lymphoma cells			Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
13	Positive	Gene mutation	Gene mutation	in vitro	alian cell gene mutation assay		Mouse Lymphoma cells			Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
14	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chromosome aberra		Chinese Hamster	chinese hams		Japan Minist	Japan Ministry of Health L		
15	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chromosome aberra		Chinese Hamster	chinese hams		Japan Minist	Japan Ministry of Health L		
16	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chromosome aberra		Chinese Hamster	chinese hams		Japan Minist	Japan Ministry of Health L		
17	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chromosome aberra		Chinese Hamster	chinese hams		Japan Minist	Japan Ministry of Health L		
18	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chi	with S9			rat	LSIC	Japan-Danish EPA Inventc	2000	
19	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chi	without S9				Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
20	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chi	with S9			rat	LSIC	Japan-Danish EPA Inventc	2000	
21	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chi	without S9				Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
22	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chi	with S9			rat	LSIC	Japan-Danish EPA Inventc	2000	
23	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chi	without S9				Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
24	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chi	with S9			rat	LSIC	Japan-Danish EPA Inventc	2000	
25	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chi	without S9				Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
26	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test					Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
27	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test					Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
28	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test					Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
29	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test					Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
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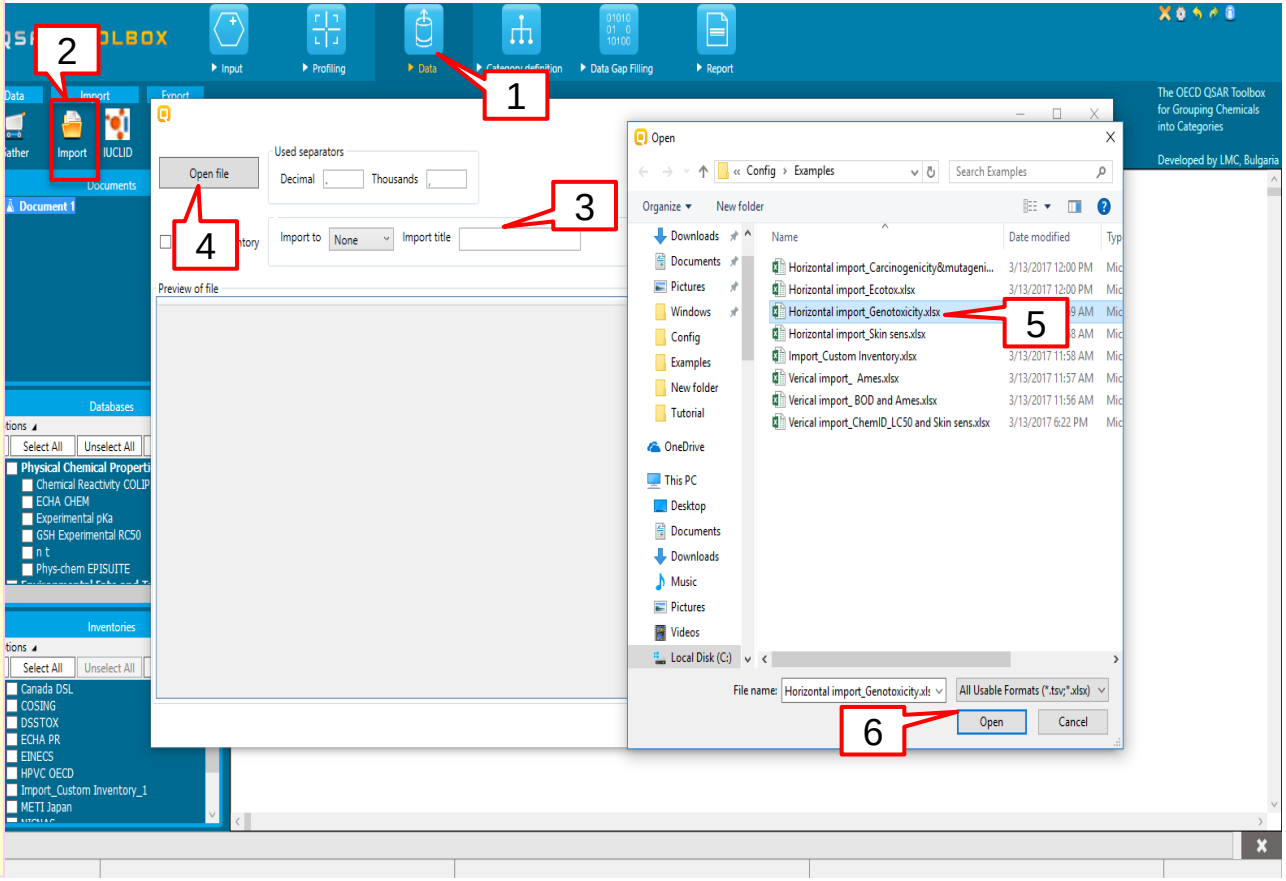
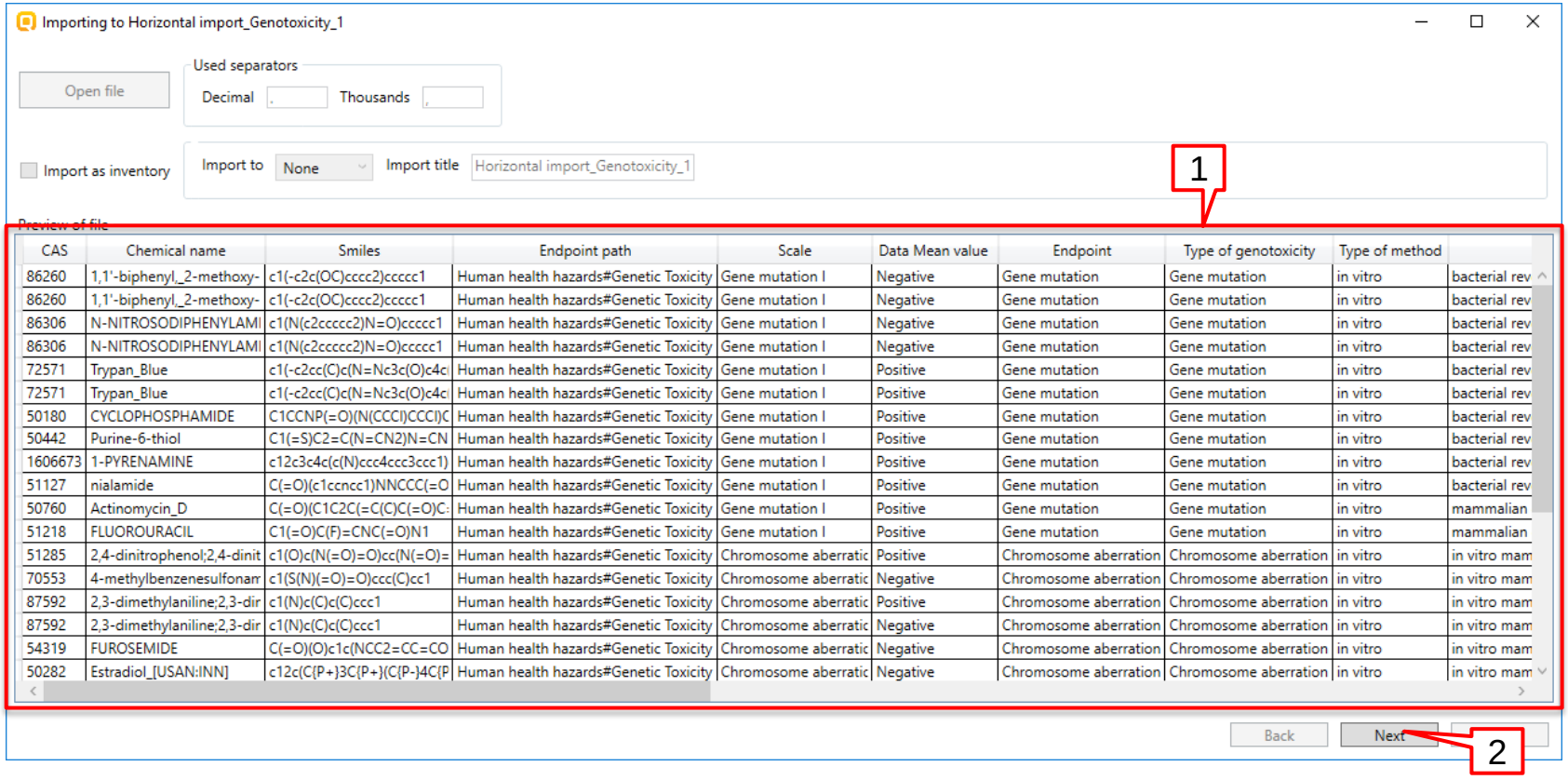
Import of database: Horizontal import

1. Go to *Data* panel (1);
2. Click on *Import* (2);
3. Type in the name of the database as you would want it to be displayed in Toolbox (3). Otherwise the name of the file will be used as the name of the database.
4. Click on *Open file* (4);
5. Select the file (Horizontal import_genotoxicity.*xlsx*)(5);
6. Click on *Open* (6).

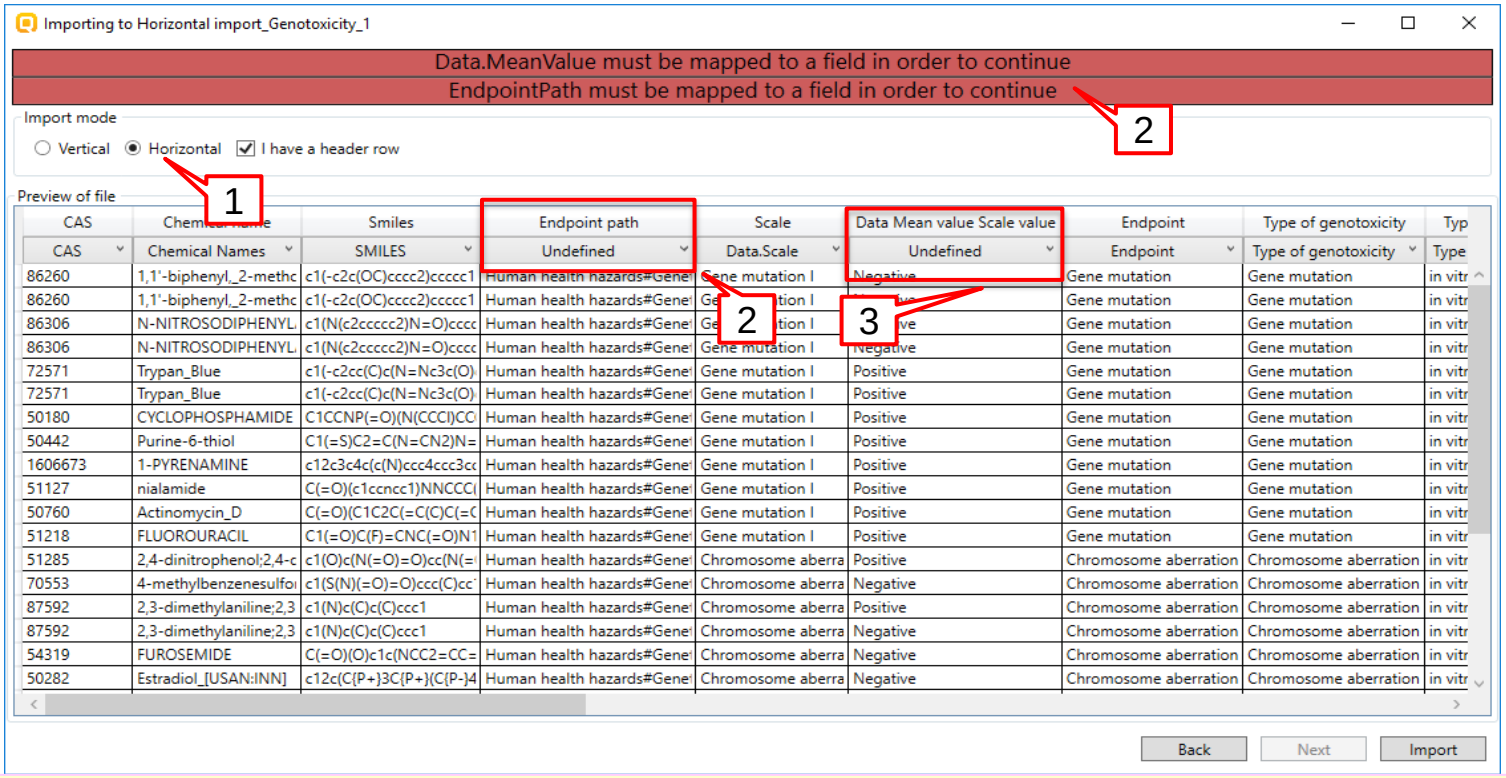


Import of database: Horizontal import



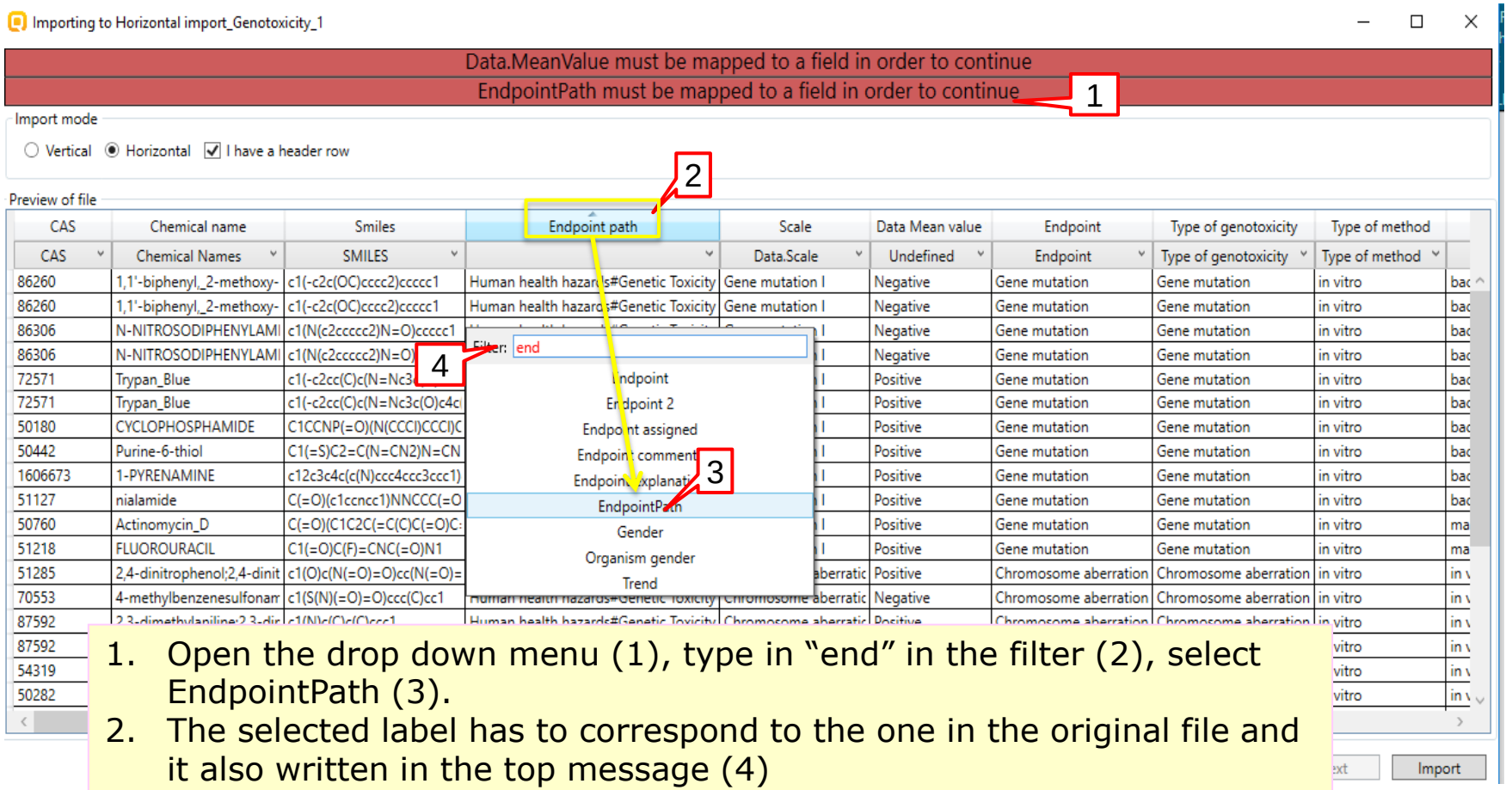
1. A preview of the imported file is shown (1); 2. Click on *Next* (2);

Import of database: Horizontal import



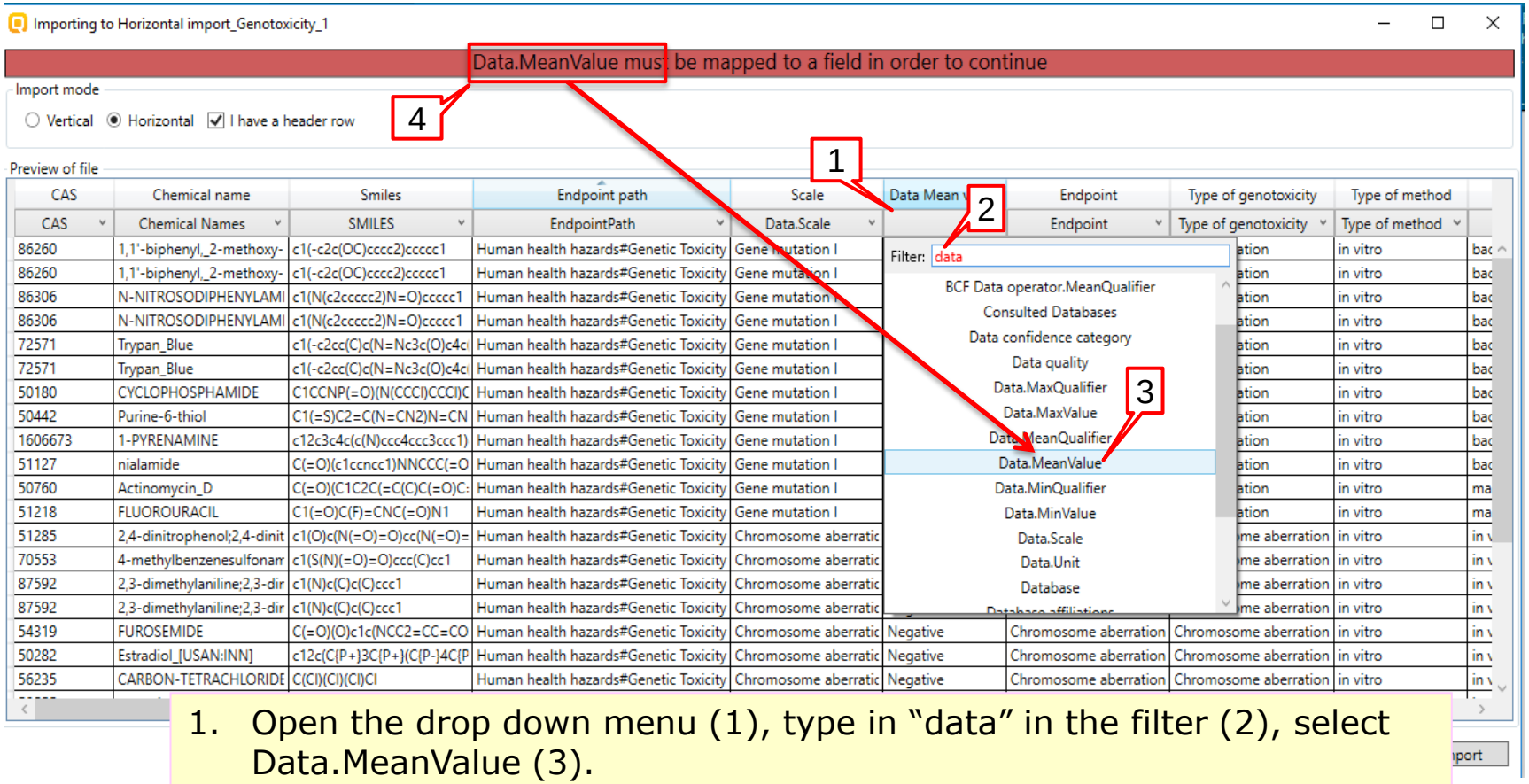
- Select *Horizontal* radio button (1)
- When there are fields from the original file which cannot be mapped to the labels existing in Toolbox , burgundy colored messages are displayed on the top (2) and Undefined is written below the data which is not mapped (3).

Import of database: Horizontal import



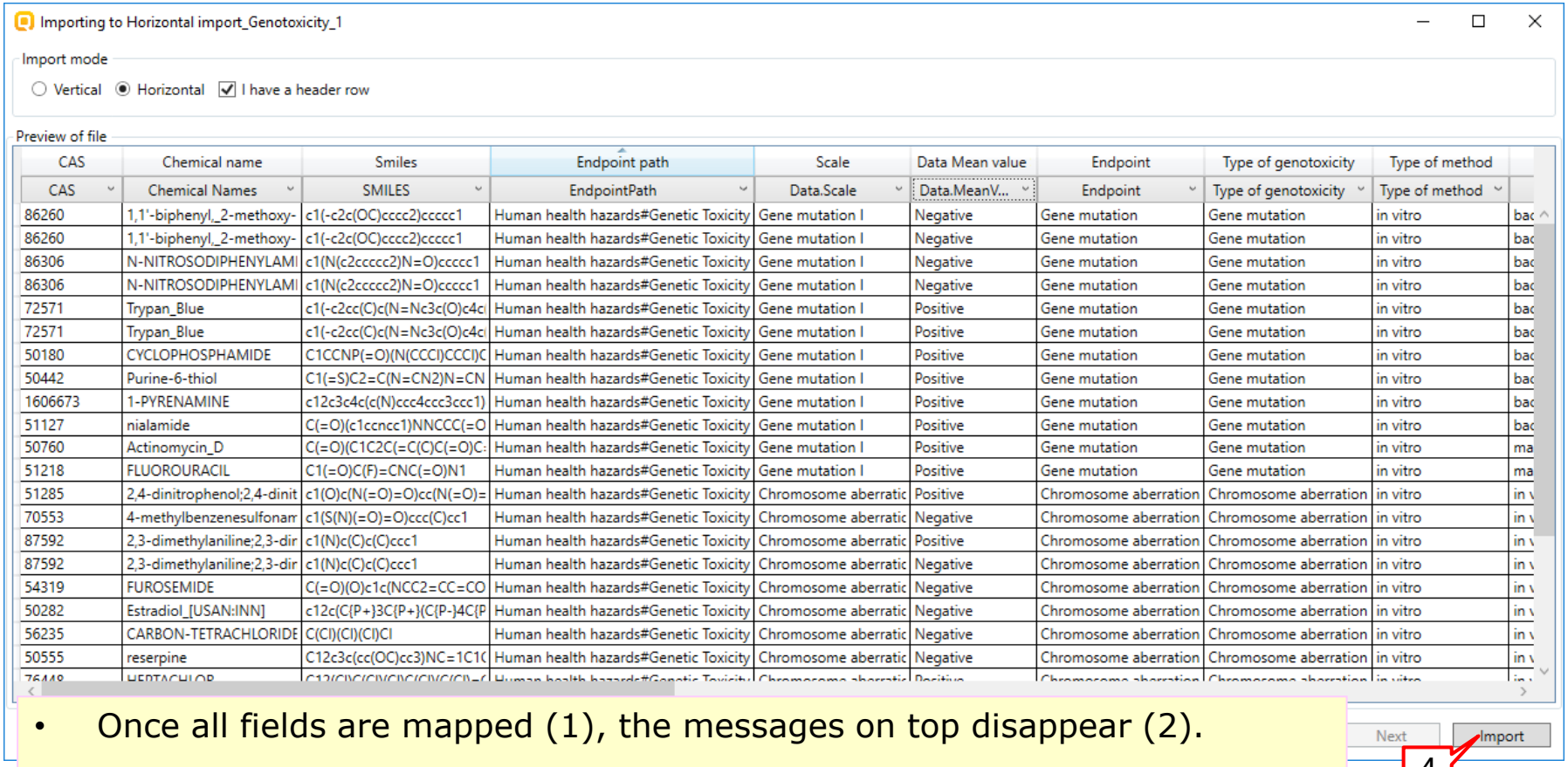
1. Open the drop down menu (1), type in “end” in the filter (2), select EndpointPath (3).
2. The selected label has to correspond to the one in the original file and it also written in the top message (4)

Import of database: Horizontal import



1. Open the drop down menu (1), type in "data" in the filter (2), select Data.MeanValue (3).
2. The selected label has to correspond to the one in the original file and it also written in the top message (4).

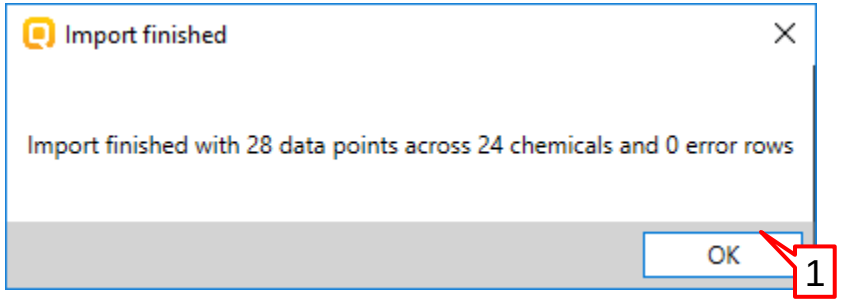
Import of database: Horizontal import



CAS	Chemical name	Smiles	Endpoint path	Scale	Data Mean value	Endpoint	Type of genotoxicity	Type of method
CAS	Chemical Names	SMILES	EndpointPath	Data.Scale	Data.MeanV...	Endpoint	Type of genotoxicity	Type of method
86260	1,1'-biphenyl,_2-methoxy-	c1(-c2c(OC)cccc2)ccccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86260	1,1'-biphenyl,_2-methoxy-	c1(-c2c(OC)cccc2)ccccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86306	N-NITROSODIPHENYLAMI	c1(N(c2ccccc2)N=O)ccccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86306	N-NITROSODIPHENYLAMI	c1(N(c2ccccc2)N=O)ccccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCCl)CCCl)C	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
50442	Purine-6-thiol	C1(=S)C2=C(N=CN2)N=CN	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
1606673	1-PYRENAMINE	c12c3c4c(c(N)ccc4ccc3ccc1)	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
51127	nialamide	C(=O)(c1ccncc1)NNCCC(=O	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
50760	Actinomycin_D	C(=O)(C1C2C(=C(C)C(=O)C:	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
51218	FLUOROURACIL	C1(=O)C(F)=CNC(=O)N1	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
51285	2,4-dinitrophenol;2,4-dinit	c1(O)c(N(=O)=O)cc(N(=O)=	Human health hazards#Genetic Toxicity	Chromosome aberratic	Positive	Chromosome aberration	Chromosome aberration	in vitro
70553	4-methylbenzenesulfonam	c1(S(N)(=O)=O)ccc(C)cc1	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
87592	2,3-dimethylaniline;2,3-dir	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic Toxicity	Chromosome aberratic	Positive	Chromosome aberration	Chromosome aberration	in vitro
87592	2,3-dimethylaniline;2,3-dir	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
54319	FUROSEMIDE	C(=O)(O)c1c(NCC2=CC=CO	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
50282	Estradiol_[USAN:INN]	c12c(C{P+}3C{P+}(C{P-}4C{P	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
56235	CARBON-TETRACHLORIDE	C(Cl)(Cl)(Cl)Cl	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
50555	reserpine	C12c3c(cc(OC)cc3)NC=1C1(	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro

- Once all fields are mapped (1), the messages on top disappear (2).
- You can use the scrollbar (3) to check all columns, their titles and content.
- Click on *Import* (4)

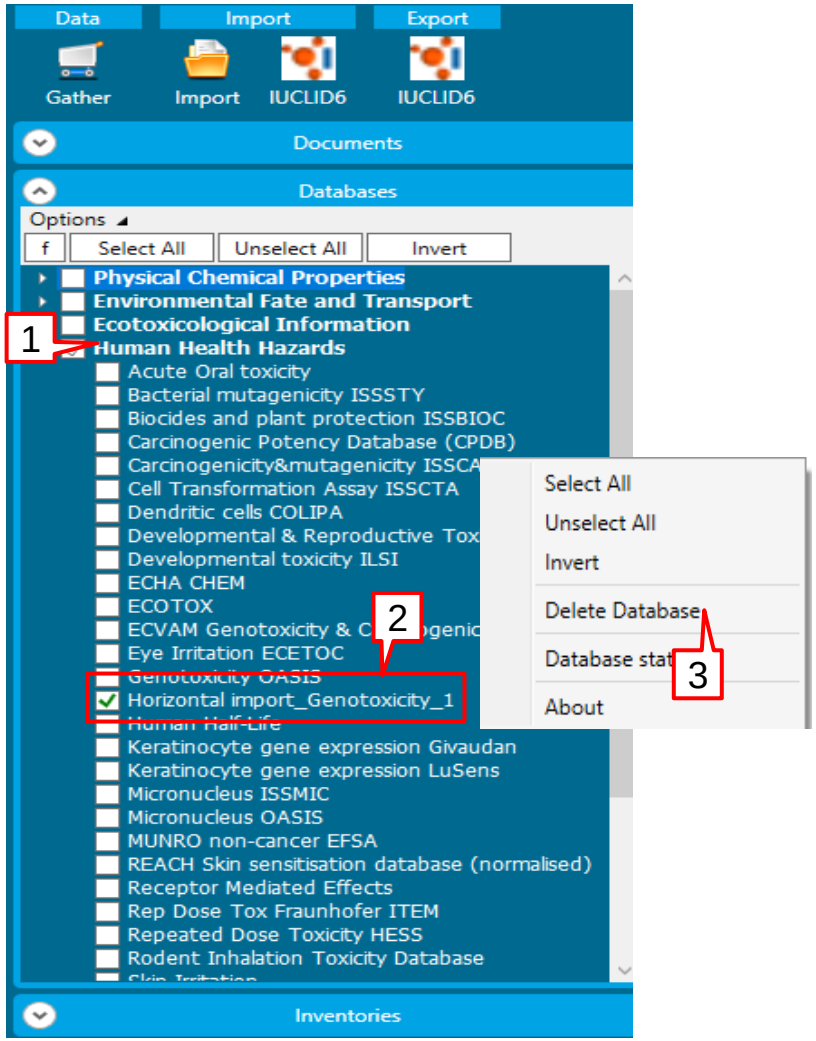
Import of database: Horizontal import



- The import process could take a couple of minutes;
- An informative message is displayed when it is completed;
- Click on *OK* (1).

Import of database: Horizontal import

- The new database is displayed in the Databases panel (1) in the *Human health hazard* group (2).
- Right-click menu (3) is implemented where you can see the database statistics or delete the database.
- The software automatically adds a numeration in the name ("1" in this example) in case the same database is imported for the second time.



Outlook

- Aim
- Definition of Database and Inventory
- **Import of database:**
  - Vertical import
  - Horizontal import
  - **Supporting information**
- Import of inventory
- Export Data matrix

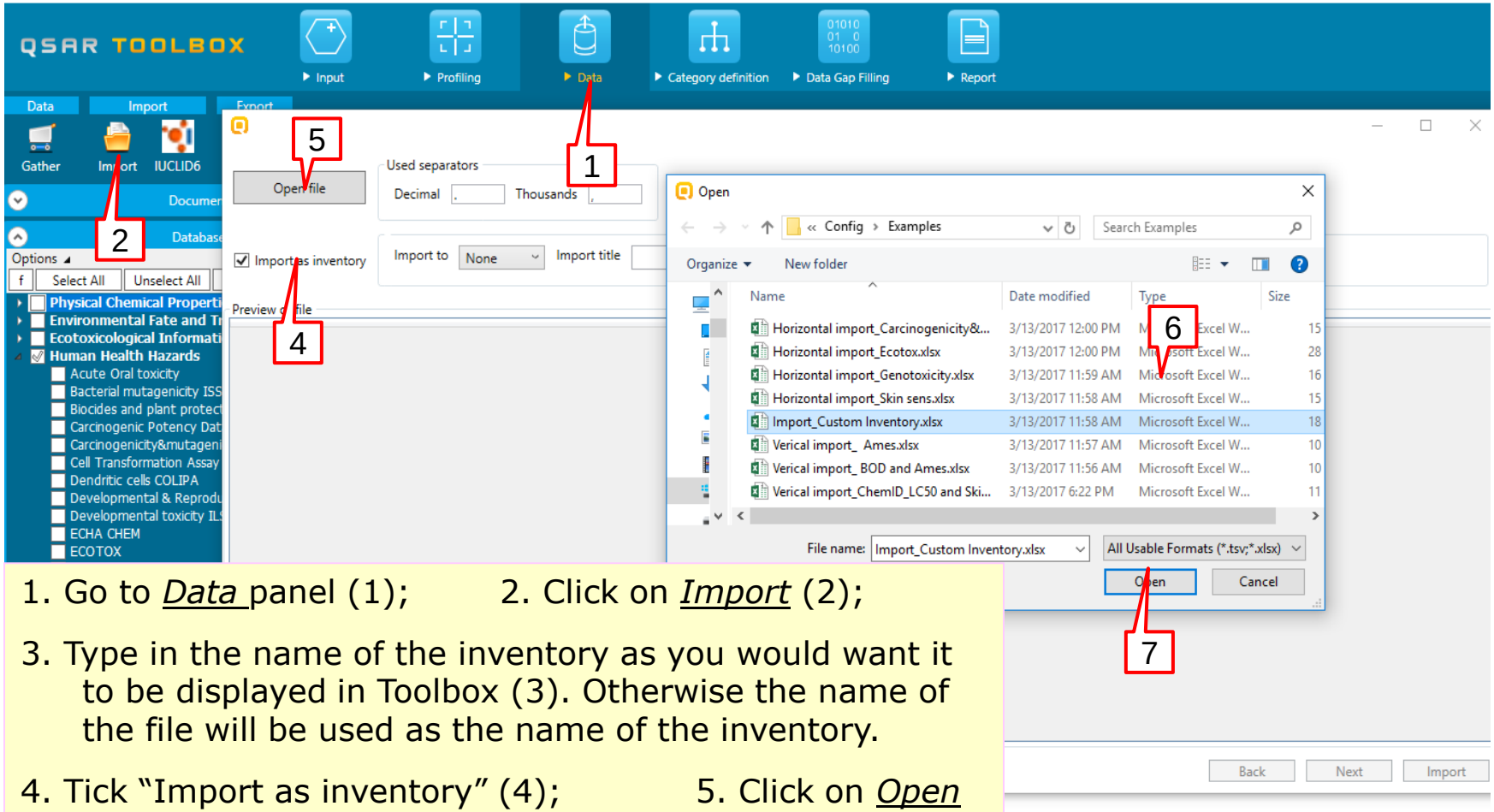
Supporting information

- A table of the most important endpoints implemented in Toolbox could be found in *F1 Help: D.3.4.4. Supporting Information*.
- The information in the table aims to facilitate the users' work when importing new databases.

Outlook

- Aim
- Definition of Database and Inventory
- **Import:**
  - ❖ Import of database
    - ➢ Vertical import
    - ➢ Horizontal import
  - ❖ **Import of inventory**
  - ❖ Import via IUCLID
- Export Data matrix

Import of inventory



1. Go to *Data* panel (1); 2. Click on *Import* (2);

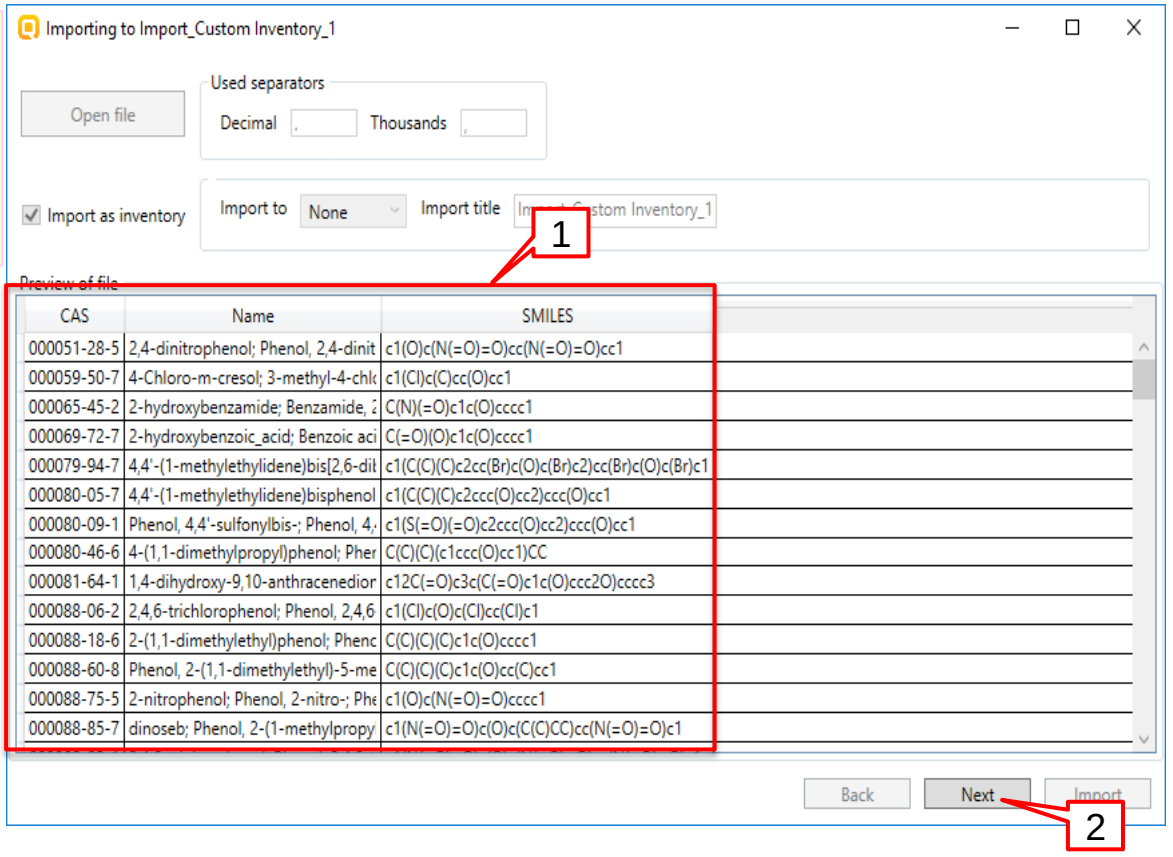
3. Type in the name of the inventory as you would want it to be displayed in Toolbox (3). Otherwise the name of the file will be used as the name of the inventory.

4. Tick "Import as inventory" (4); 5. Click on *Open file* (5);

6. Select the file (Import_Custom Inventory.xlsx)(6); 7. Click on *Open* (7).

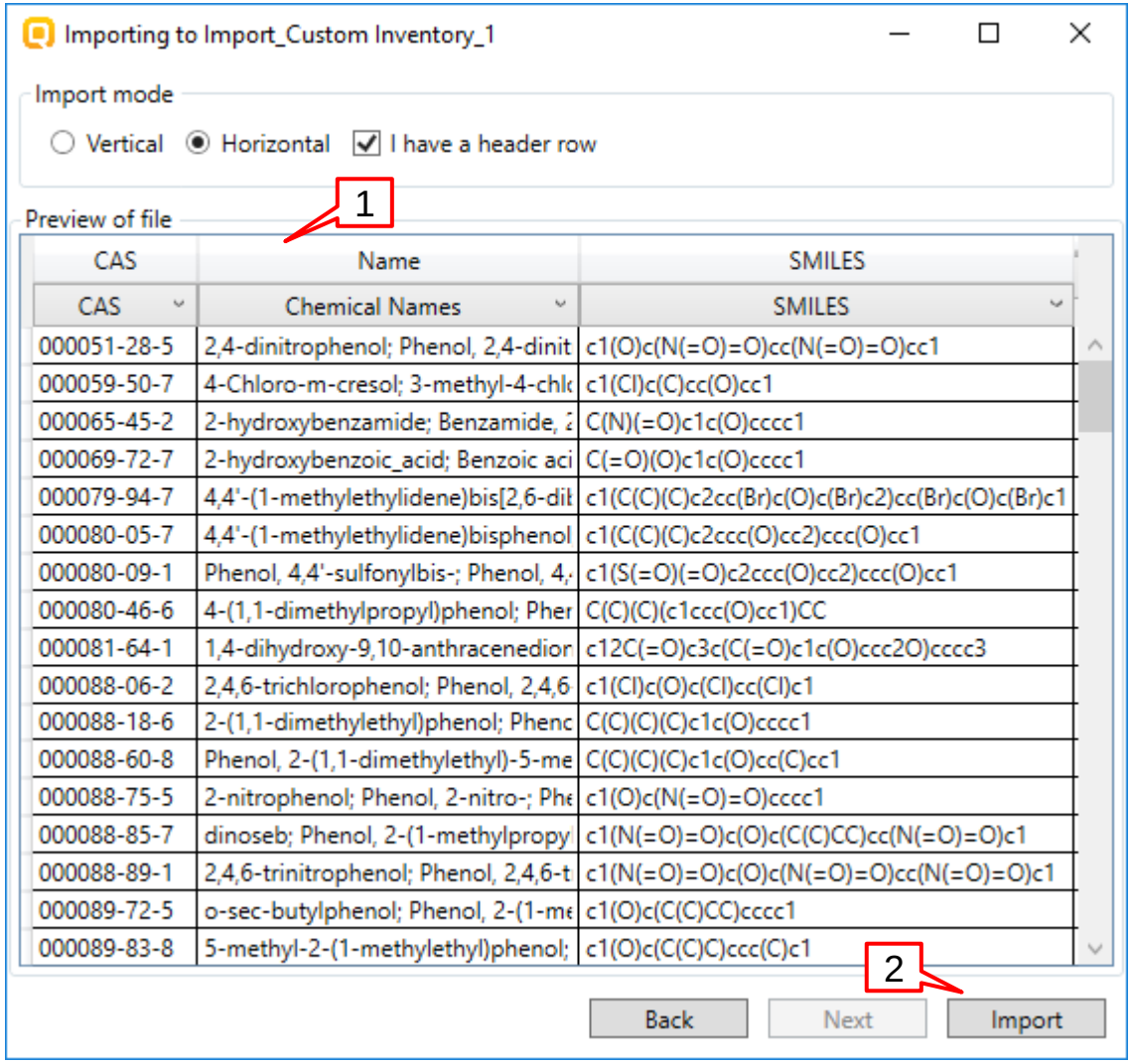
Import of inventory

1. A preview of the imported file is shown (1);
2. Click on *Next* (2);

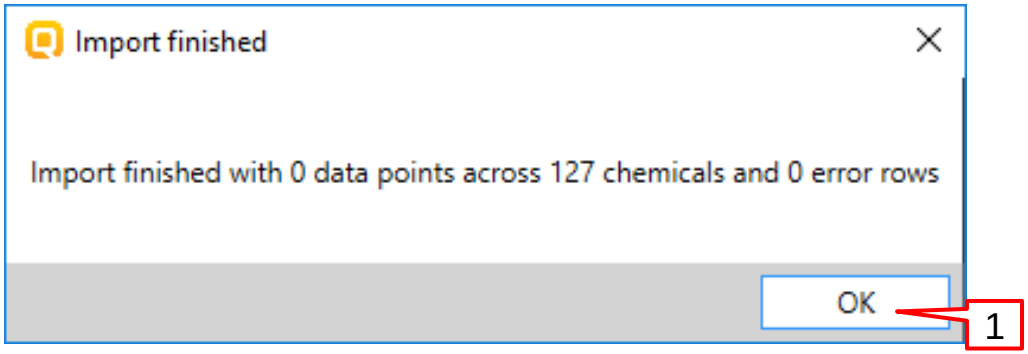


Import of inventory

1. On the second top row are displayed the chemical identifiers as they are going to be shown in Toolbox(1);
2. Click on *Import*(2);



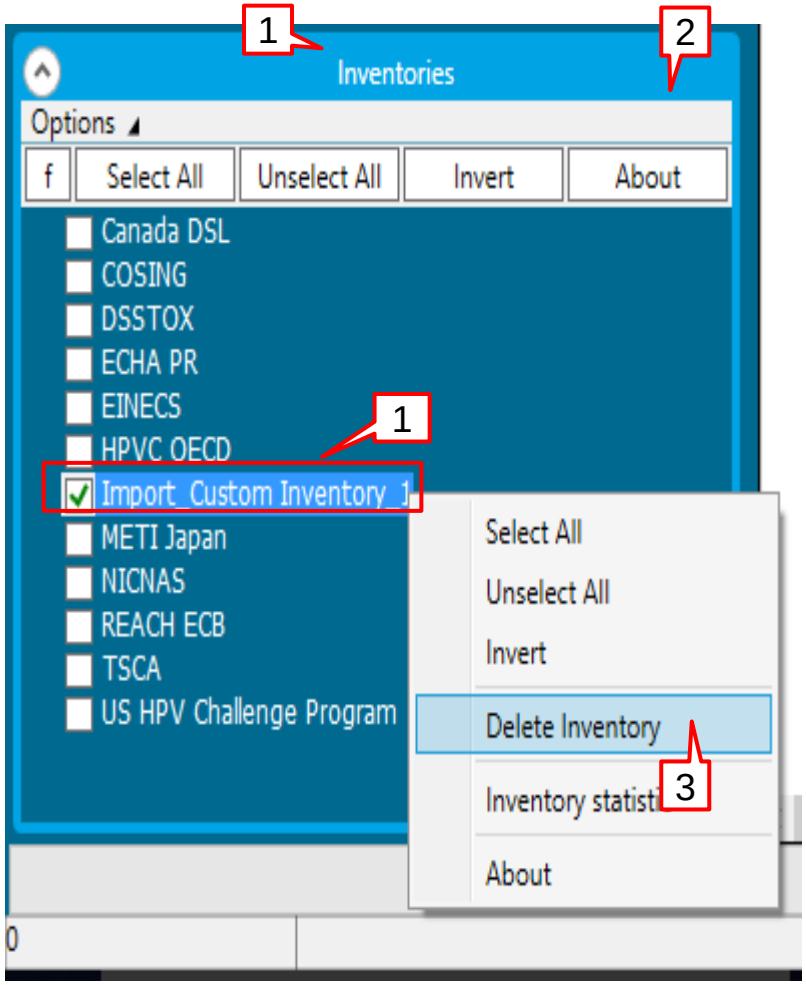
Import of inventory



- The import process could take a couple of minutes;
- An informative message is displayed when it is completed;
- Click on *OK* (1).

Import of inventory

- The new inventory (1) is displayed in the Inventories panel (2).
- Right-click menu (3) is implemented where you can or delete the inventory.
- The software automatically adds a numeration in the name ("1" in this example) in case the same database is imported for the second time.

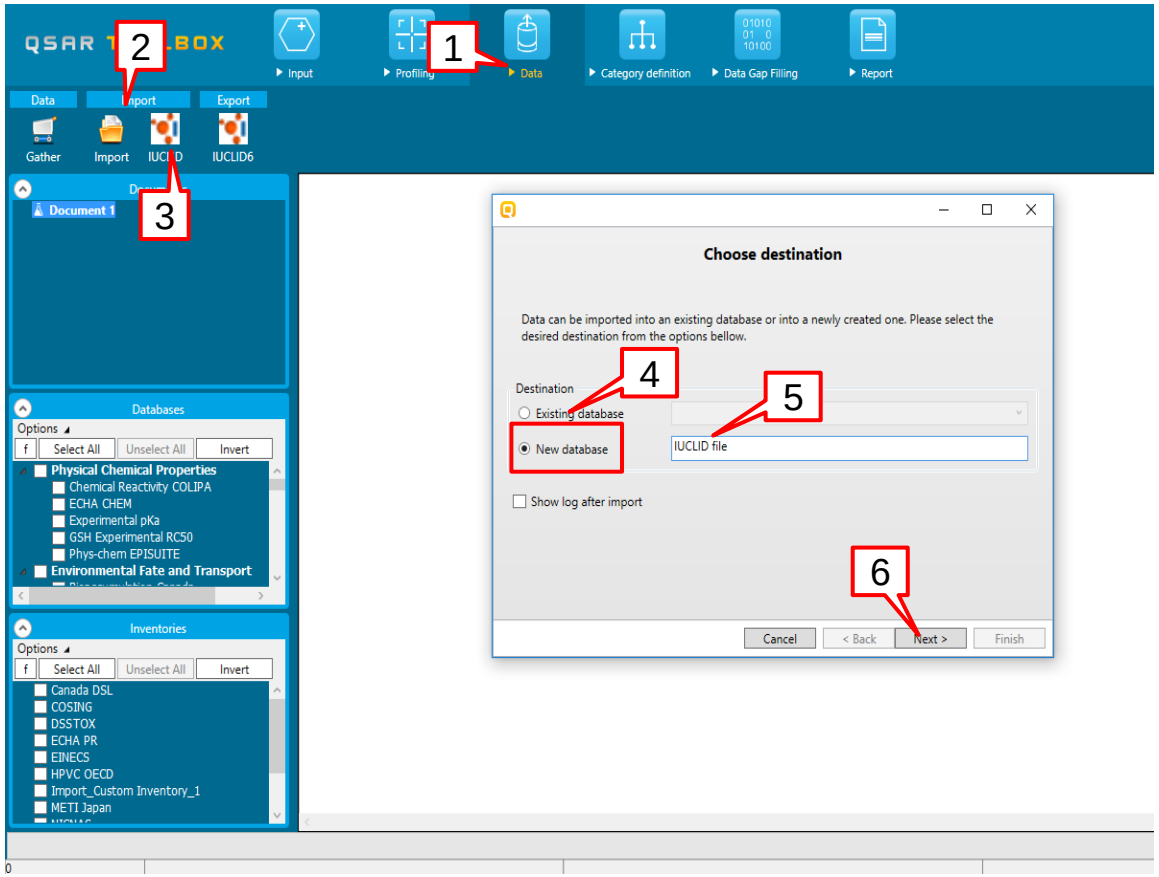


Outlook

- Aim
- Definition of Database and Inventory
- **Import:**
  - ❖ Import of database
    - ➢ Vertical import
    - ➢ Horizontal import
  - ❖ Import of inventory
  - ❖ **Import IUCLID**
- Export Data matrix

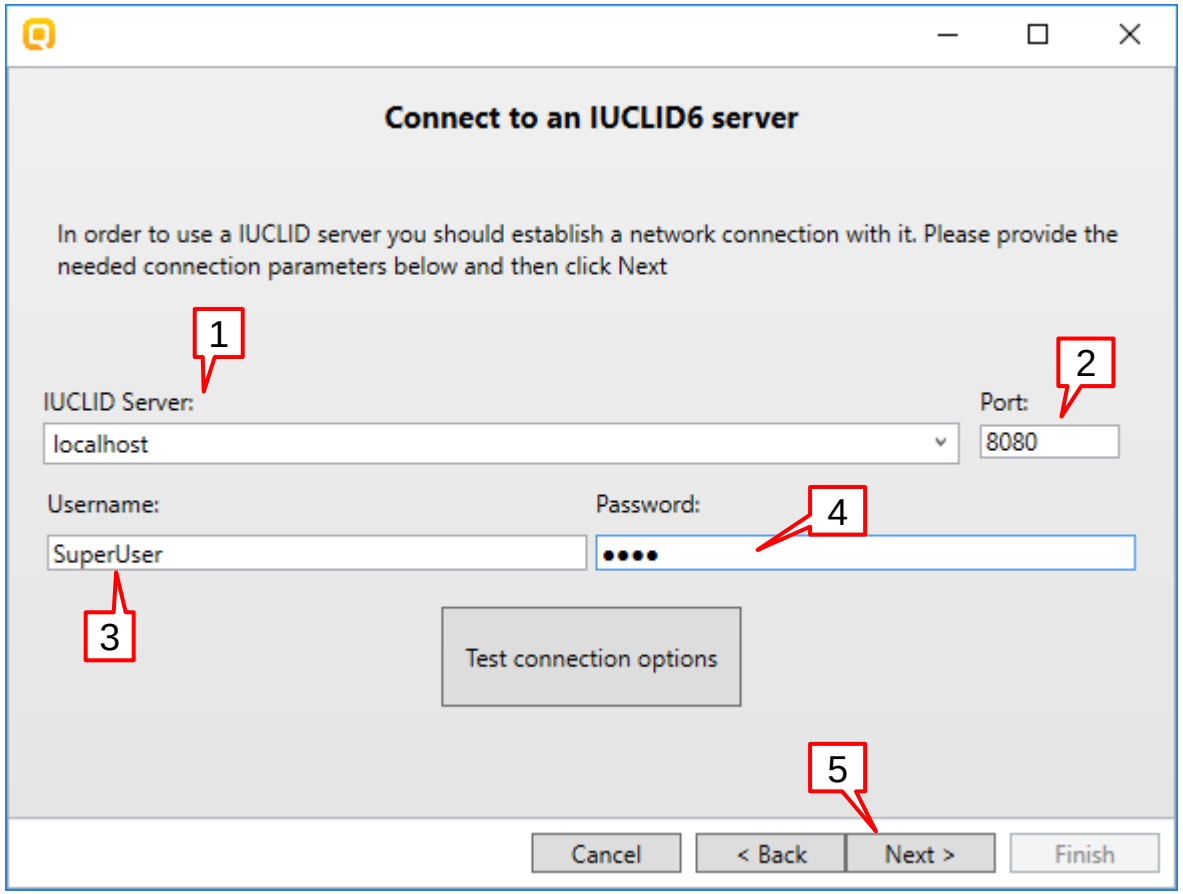
Import of IUCLID

1. Go to *Data* panel (1);
2. Click on *Import* (2);
3. Click on *IUCLID*(3);
4. Select New database(4);
5. Write the database name(5);
6. Click on *Next*(6).



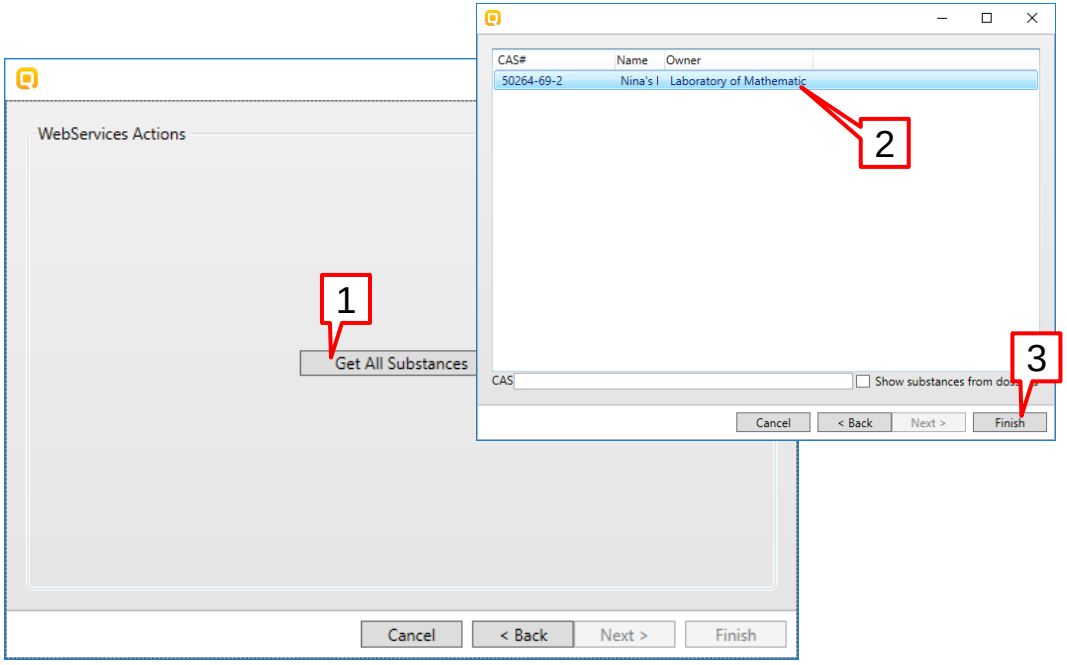
Import IUCLID

1. Write *IUCLID Server name* (1);
2. Next Port(2);
3. Next Username (3);
4. Password(4);
5. Click on *Next*(5).

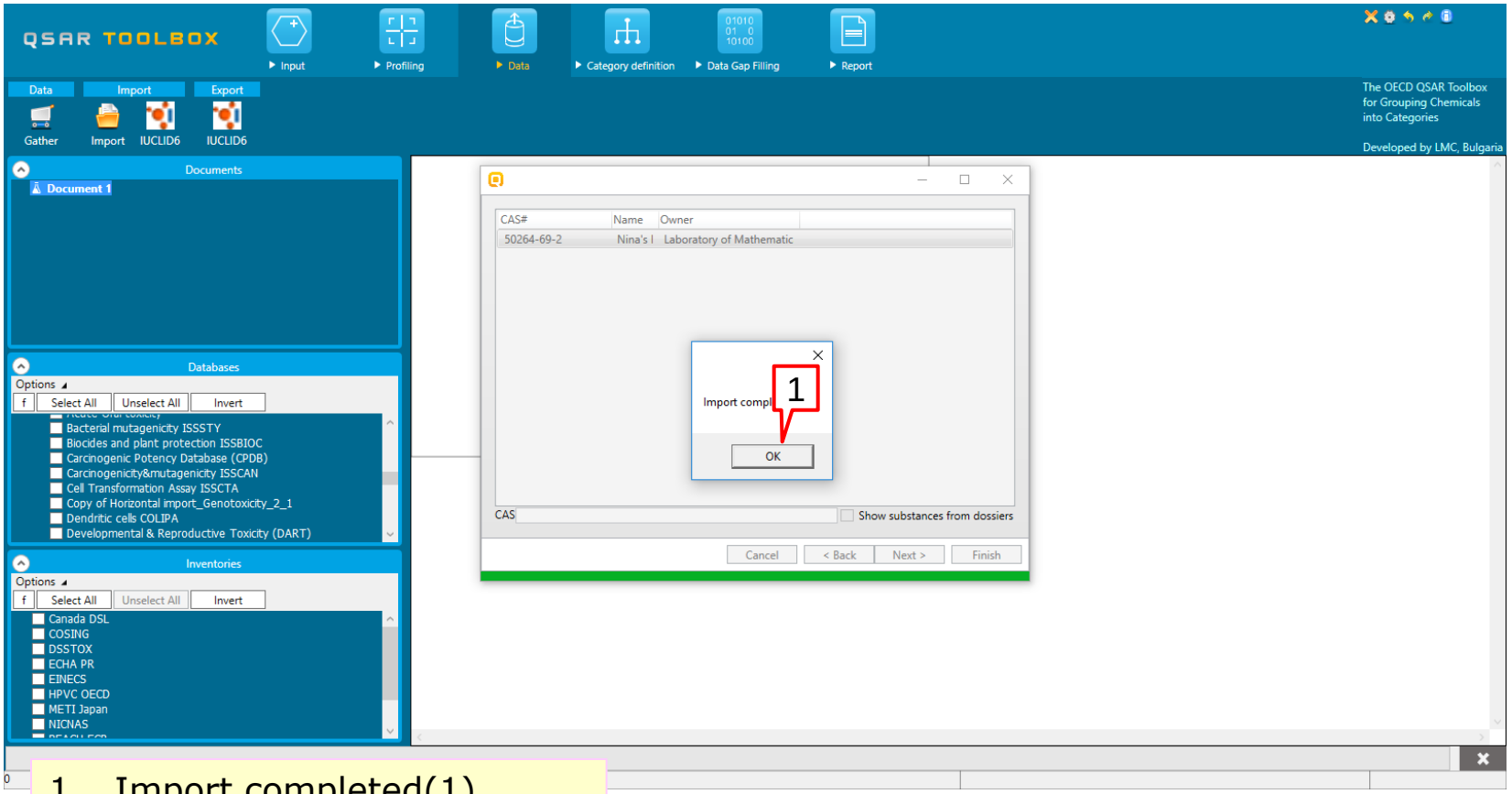


Import IUCLID

1. Get All Substances (1).
2. Select the substance (2)
3. Finish (3)

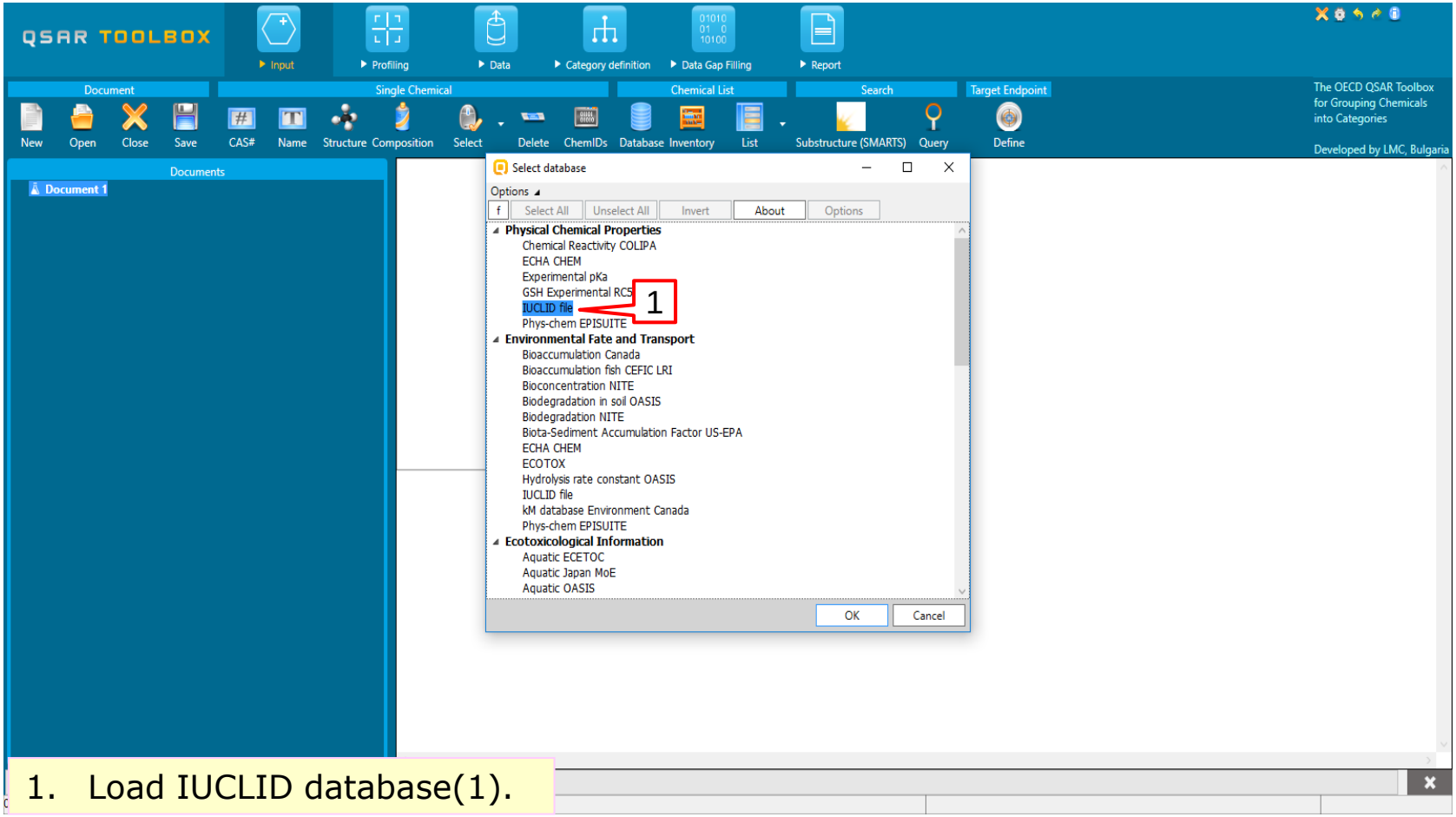


Import IUCLID



1. Import completed(1).

Import IUCLID



1. Load IUCLID database(1).

Outlook

- Aim
- Definition of Database and Inventory
- Import:
  - Import of database
    - Vertical import
    - Horizontal import
  - Import of inventory
  - Import IUCLID
- **Export Data matrix**

Export data matrix: Type of export

- One type of export are available in Toolbox:
  - **Horizontal**

- **Export IUCLID**

Horizontal Export

Horizontal Export:

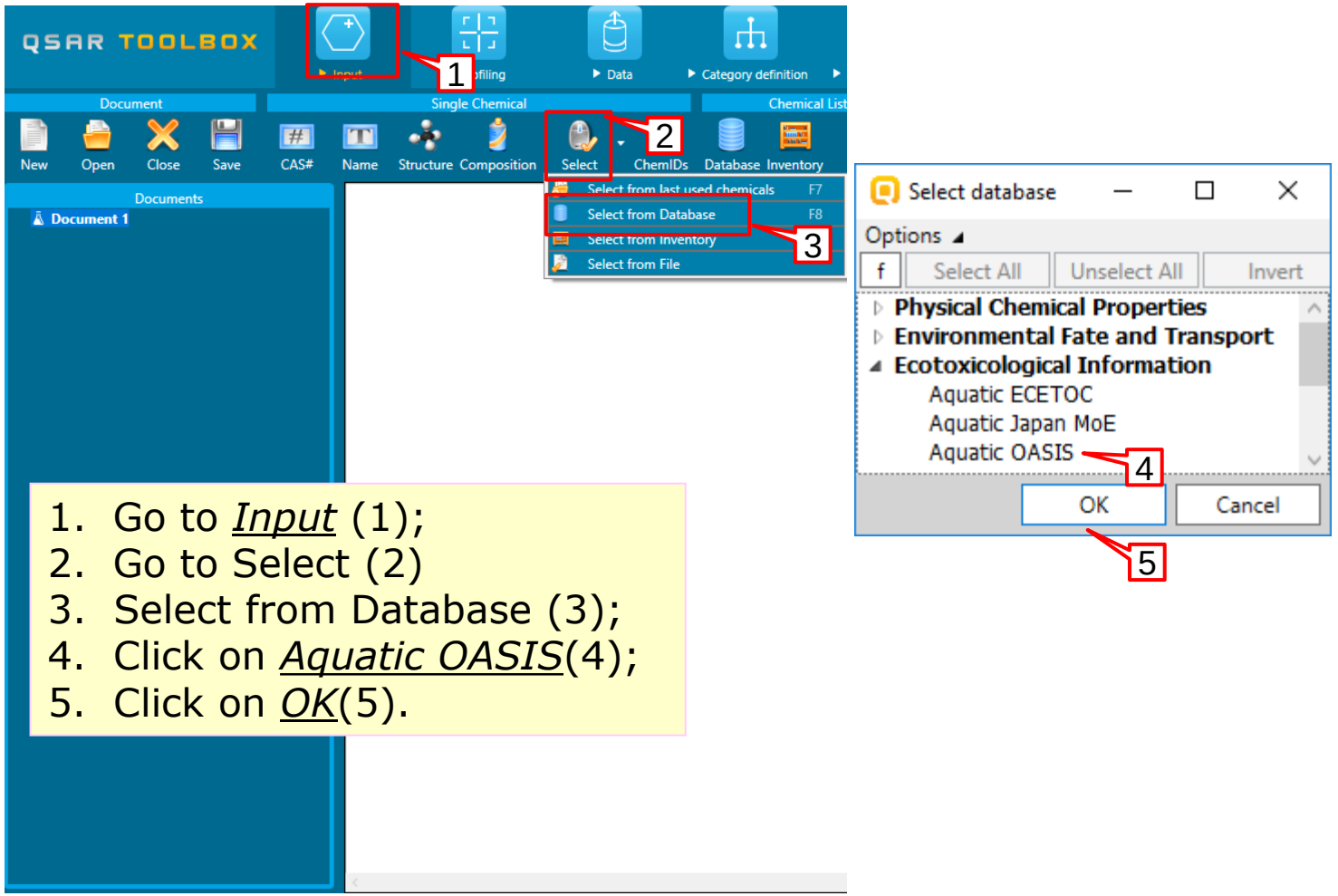
Possibility to export chemicals with data and supporting information (e.g. profiling results, 2D/3D parameters, molecular formula, etc.) available on Data matrix in text format organized in a horizontal layout.

Two options of export:

- Export row from data matrix
- Export whole data matrix

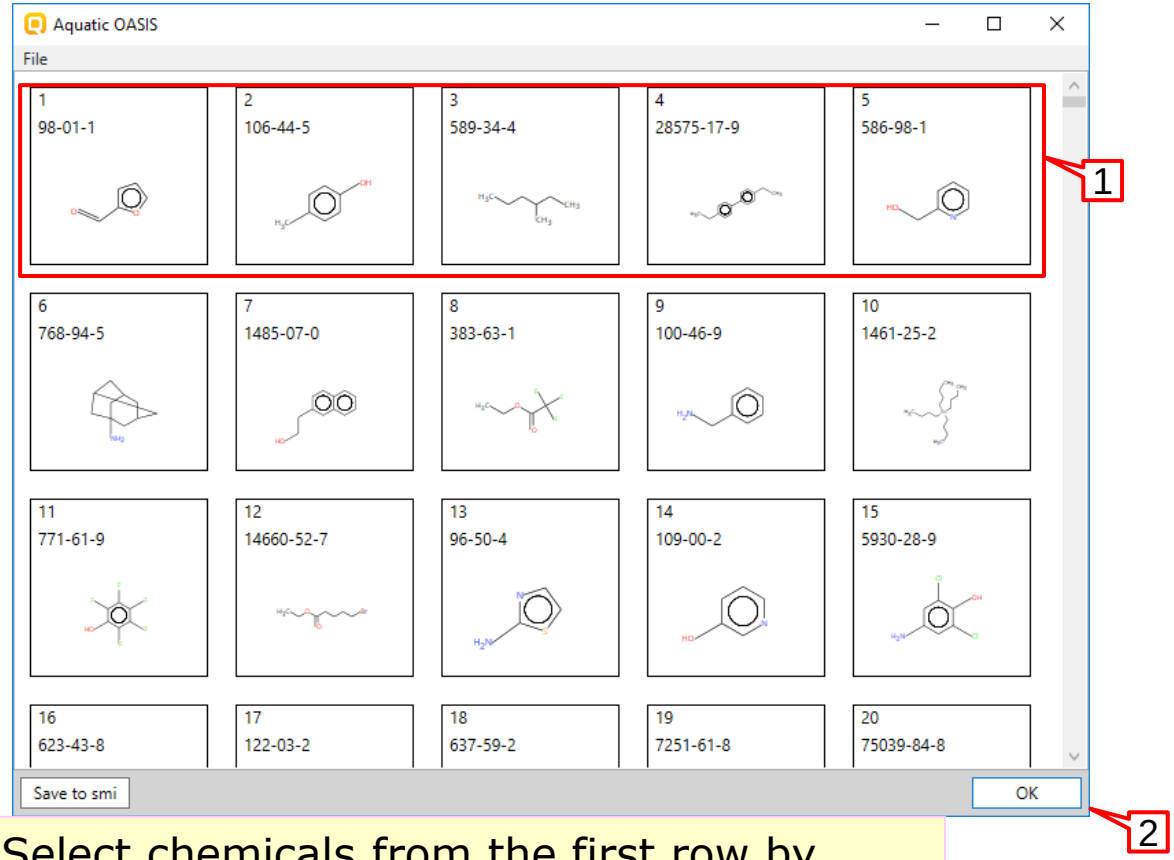
In this tutorial only the export of the whole data matrix is shown as it encompasses the first option as well.

Horizontal Export: Collecting data



1. Go to *Input* (1);
2. Go to Select (2)
3. Select from Database (3);
4. Click on *Aquatic OASIS*(4);
5. Click on *OK*(5).

Horizontal Export: Collecting data

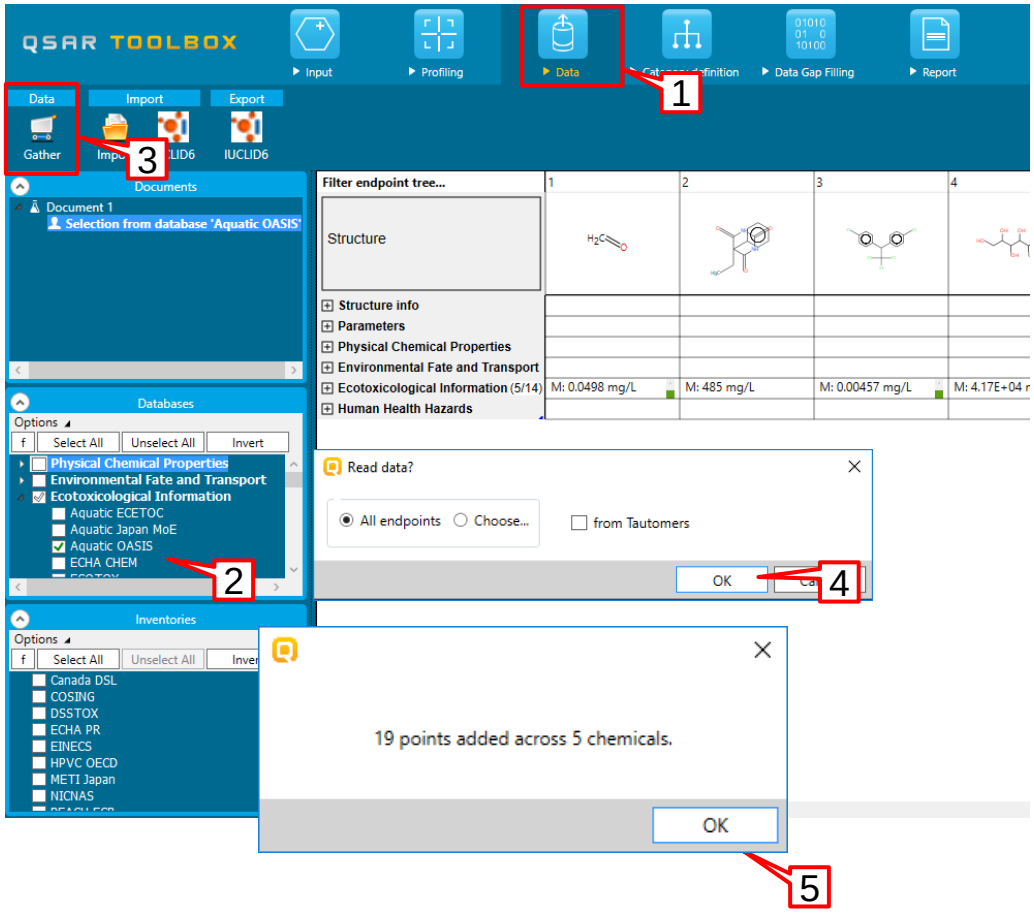


1. Select chemicals from the first row by holding Ctrl button and click over the chemicals (1);
2. Click on *OK*(2).

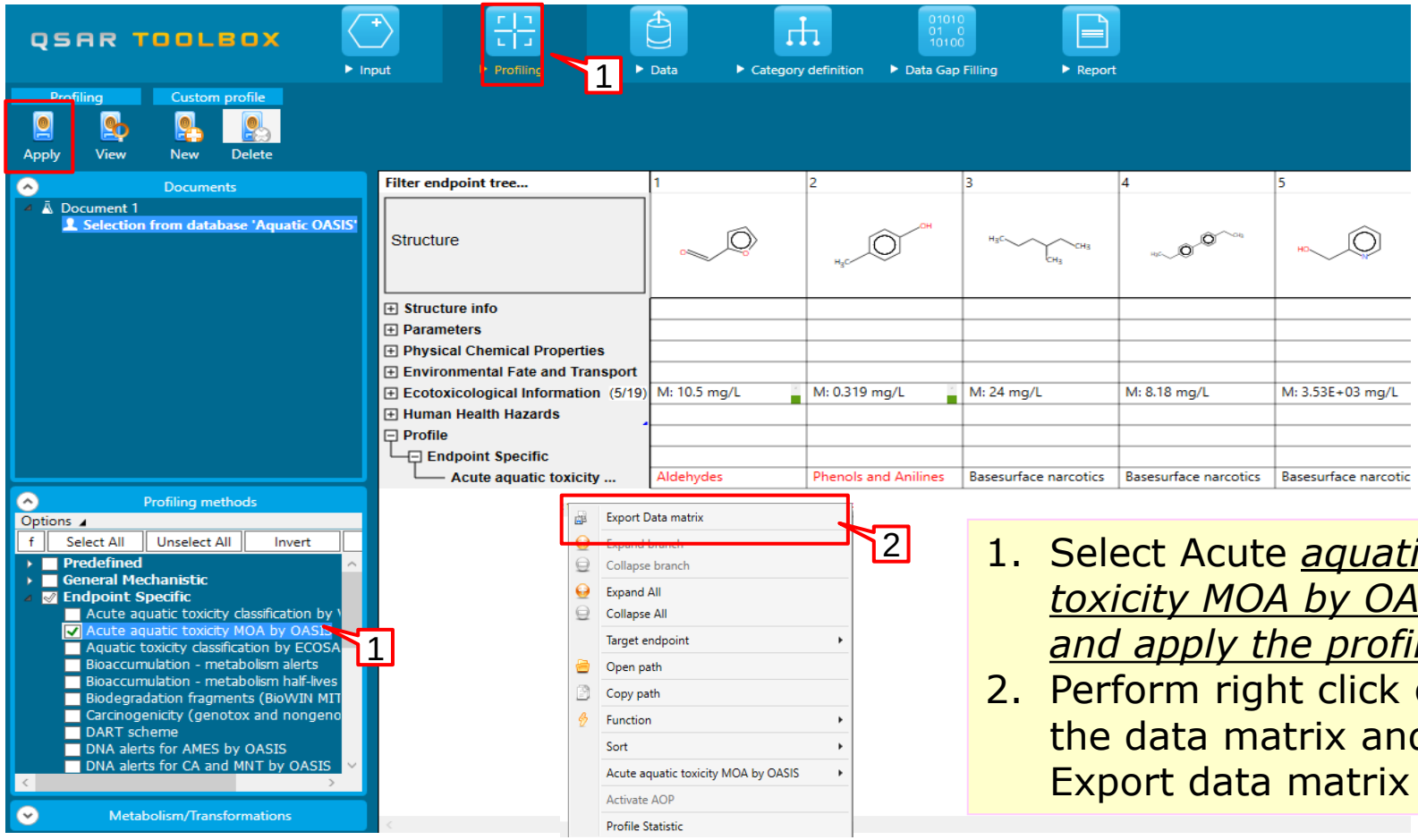
Horizontal Export: Collecting data

The following steps need to be executed to gather the experimental data for the chemicals loaded on data matrix

1. Go to *Data* (1);
2. Select *Aquatic OASIS* (2);
3. Click on *Gather* (3);
4. Click on *OK* in the Read Data window (4).
5. Click on *OK* in the information window (5).



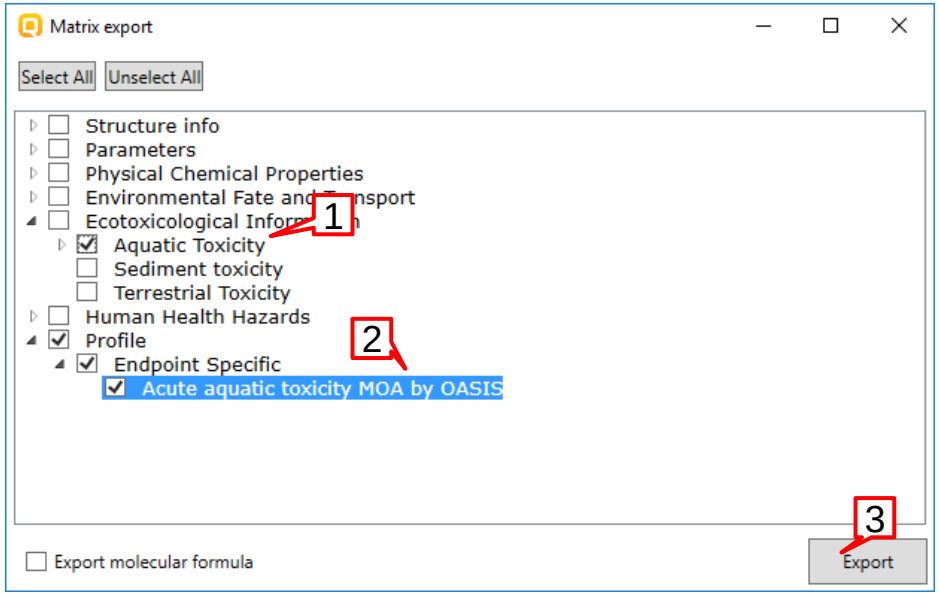
Horizontal Export: Collecting data



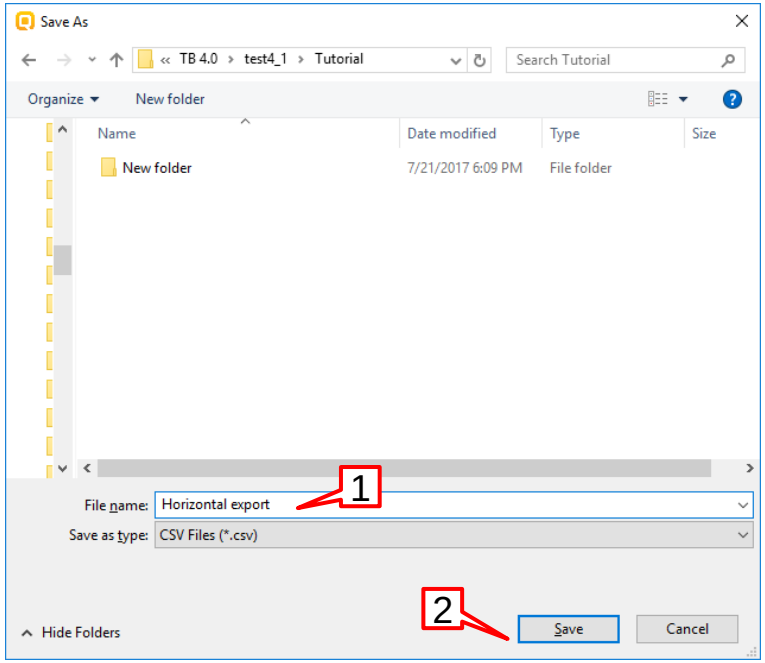
1. Select Acute *aquatic toxicity MOA by OASIS and apply the profiler*(1)
2. Perform right click over the data matrix and select Export data matrix (2)

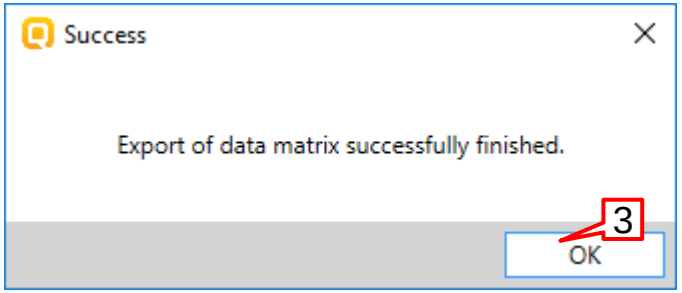
Horizontal Export

1. Aquatic toxicity (1) is selected as the right click was next to that branch;
2. Expand the Profile level (2) and then select Acute aquatic toxicity MOA by OASIS(3);
3. Click on *Export* (5).



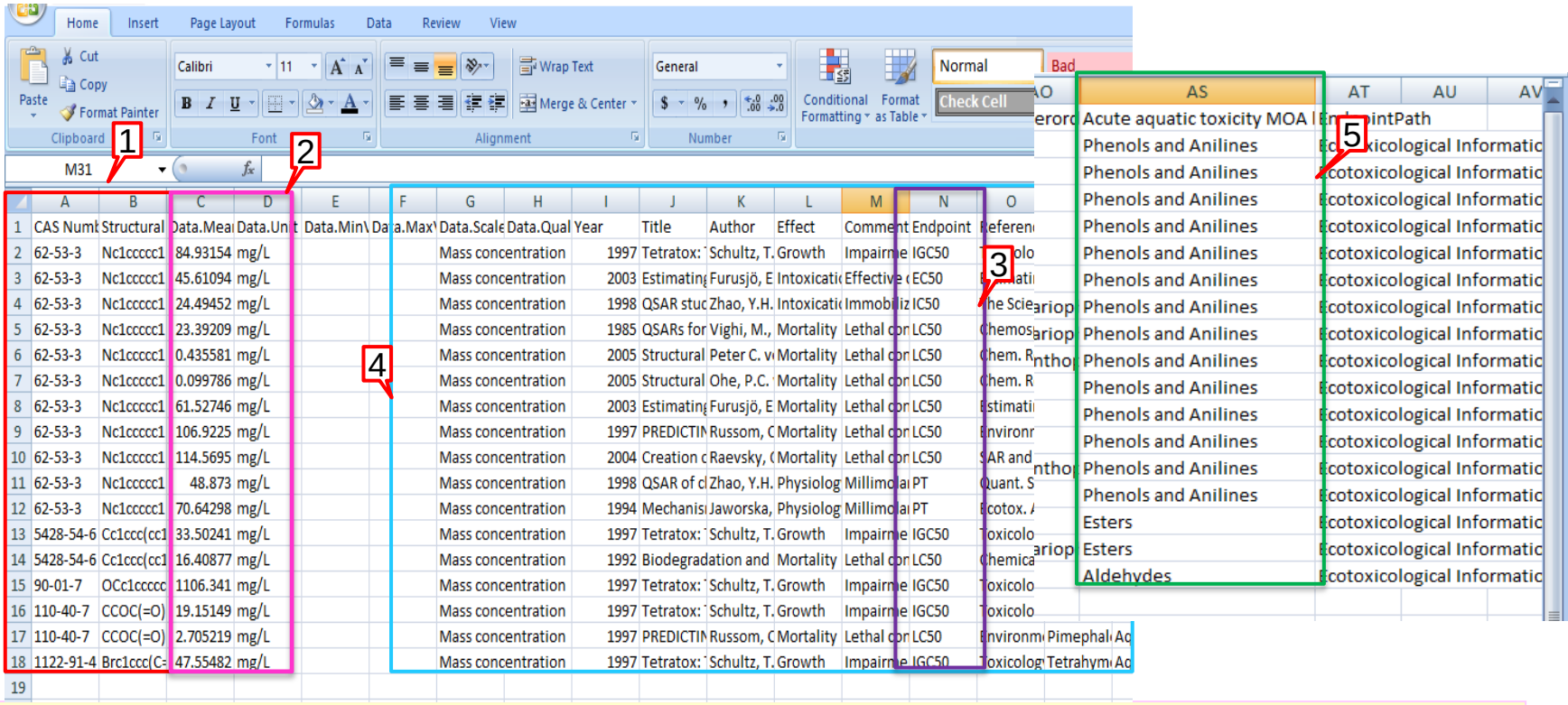
Horizontal export





1. Type in the name (e.g. Horizontal_export) (1). The file is saved in *csv* format.
2. Click on *Save* (2).
3. Click *OK* in the information message (3).

Horizontal export



The file can be opened in excel. It contains the following main sections: *chemical identity of each chemical* (red, 1), *experimental data* (pink, 2), endpoint (purple, 3), metadata (blue, 4), profiler results (green, 5). Here, if the chemical has several experimental data each one is listed on separate row (e.g. CAS 62-53-3).