

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

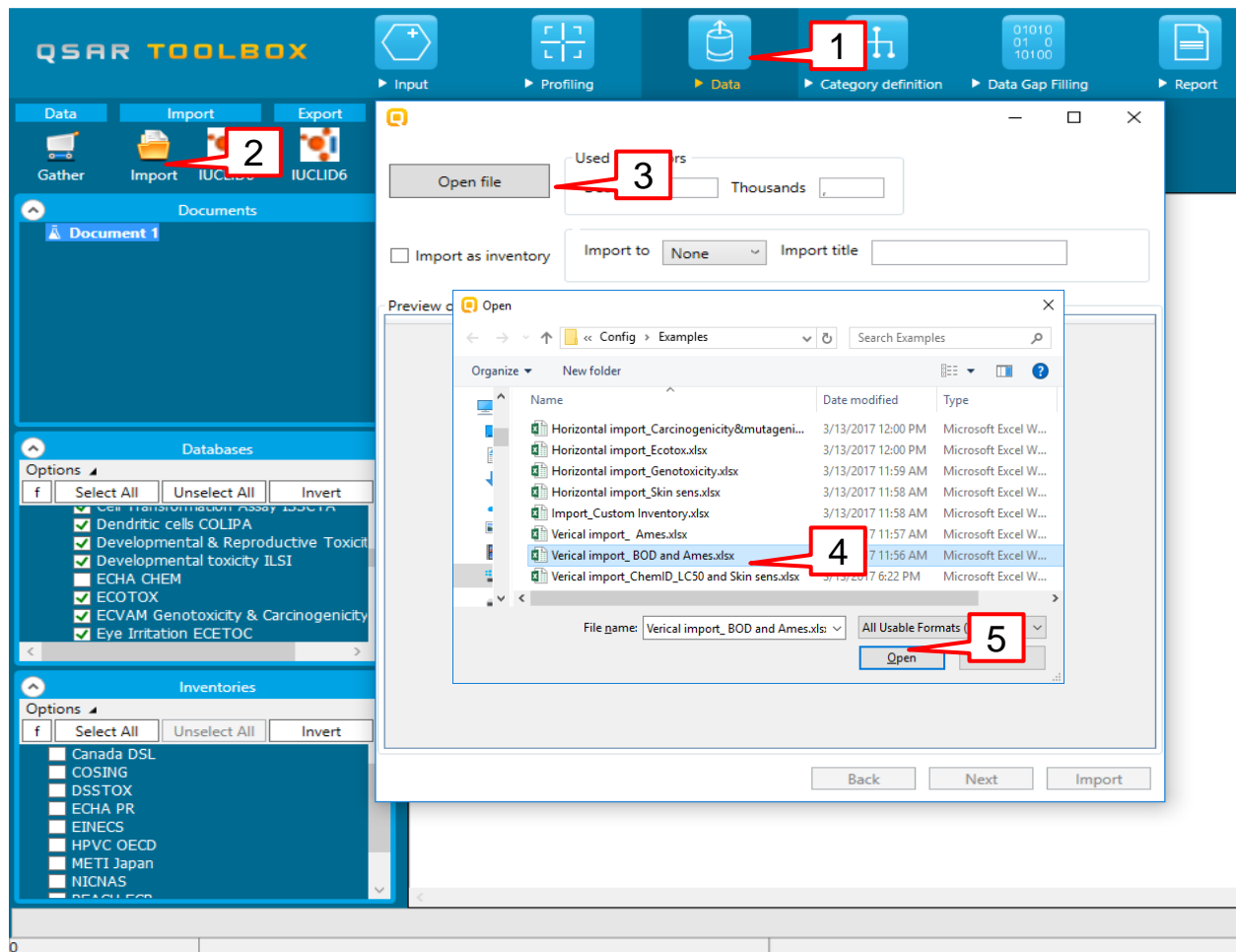
Import of database: Vertical import

- 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-";_BENZO	c12c3c4c(c5c(cc4ccc3ccc1)cccc5)c	60.7	Negative
5	50-33-9	PHENYLBUTAZONE	C(=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-aziridin	C1(N(=O)=O)C2C(C(N3CC3)=CC=	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)cccc1	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(C2CCCN2)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(c1cccc1)CO)OC1CC2CC	4.5	Negative
19					
20					

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

Importing to Verical import_ BOD and Ames_1

Open file

Used separators
 Decimal Thousands

Import as inventory

Import to Import title 2

Preview of file

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	Negative
148-82-3	MELPHALAN	C(=O)(O)C(N)Cc1ccc(N(CCC)CC)cc1	5	Positive
154-93-8	carmustine	C(=O)(N(CCC)N=O)NCCC1	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)cccc1	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-ACETYLAMINOFUORENE	c12-c3c(cc(NC(C)=O)cc3)Cc1cccc2	6.2	Negative
54-11-5	Pyridine_3-(1-methyl-2-pyrrolidinyl)-_(S)-	c1(C2CCCN2C)cccc1	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(c1cccc1)CO)OC1CC2CCC(C1)N(+)(+2(C).O(-)S(=O)(=O)O	4.5	Negative

Back 3 Next Import

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

Importing to Verical import_BOD Ames_1

Import mode

Vertical Horizontal I have a header row

Preview of file

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)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(CCC)CC)cc1	5	Positive
154-93-8	carmustine	C(=O)(N(CCC)N=O)NCCC1	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)cccc1	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(c1cccc1)CO)OC1CC2CCC(C1)N(+)(C2)O{-}S(=O)(=O)O	4.5	Negative

Back Next Import

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:

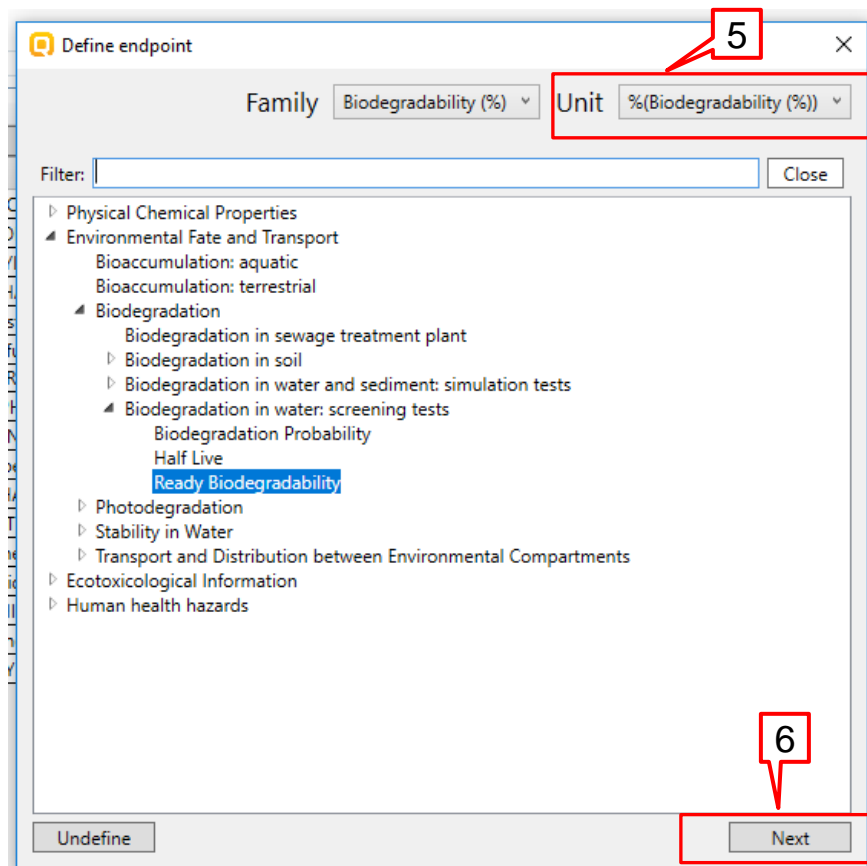
Define endpoint window is displayed (1).
Select Ready Biodegradability (2) from the endpoint tree, then select the family (Biodegradability %) (3) by using the filter options (4).

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).

Filter: BIC	Family	Unit	Value	Category
	Bioaccumulation			Negative
	Biodegradability (%)			Negative
	Biodegradability (categories)			Negative
	Biodegradation probability (EPI)			Positive
	Carcinogenicity V (ISSBIOC)			Positive
			0.09	Positive
			1.63	Positive
			80	Positive
			25	Positive
			0.01	Positive
			2	Positive
			1.8	Negative
			6.2	Negative
			75	Negative
			0.09	Negative
			1.8	Negative
			4.5	Negative
			0.2	Positive

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

Select endpoint

Family/Scale: Biodegradability (%) Unit: %(Biodegradability (%))

- Environmental Fate and Transport
 - Biodegradation
 - Biodegradation in Water: Screening Tests
 - Ready Biodegradability

Test organisms (species): Microorganisms

Test guideline: OECD 301C

Duration: []

Endpoint: BOD

Selection of additional metadata fields:

[]

Add

Up Down

Clear Remove

Undefined Back Finish

10

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

Import of database: Vertical import

Importing to Verical import_BOD and Ames_1

Import mode
 Vertical Horizontal I have a header row

Preview of file

CAS	NAME	Smiles	BOD	Ames
CAS	Chemical Names	SMILES	Test guideline=OECD 301C Endpoint=BOD	No endpoint selected 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)C(N)C(C)C1ccc(N(CCC)CCC)cc1	5	Positive
154-93-8	carmustine	C(=O)N(CCC)N=O)NCCC1	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)cccc1	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)C1cccc2	6.2	Negative
54-11-5	Pyridine_3-(1-methyl-2-pyrrolidinyl)-_(S)-	c1(C2CCCN2C)cccc1	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(c1cccc1)CO)OC1CC2CCC(C1N(+)2(C)O(-)S(=O)(=O)O	4.5	Negative

Back Next 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
<chem>)C(C)C(c1ccc(C)cc1)c1ccc(C)cc1</chem>	7.1	Negative
<chem>4c(c5c(cc4ccc3ccc1)cccc5)cc2</chem>	60.7	Negative
<chem>C(CCCC)C(=O)N(c2ccccc2)N1c1ccccc1</chem>	0.09	Negative
<chem>2)C(N)Cc1ccc(N(CCC)CCC)cc1</chem>	5	Positive
<chem>V(CCC)N=O)NCCC</chem>	0.09	Positive
<chem>O)=O)C2C(C(N3CC3)=CC=1)=N(=O)ON=2</chem>	1.63	Positive
<chem>I=O</chem>	80	Positive

Define endpoint

Family/Scale: Gene mutation I Unit: []

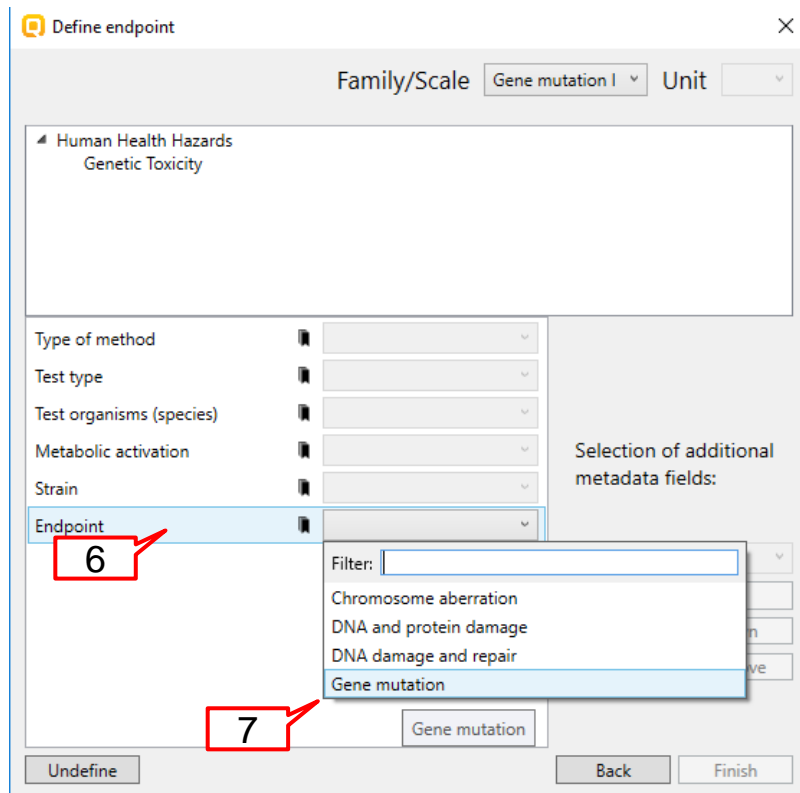
Filter: [] Close

- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazards
 - Acute Toxicity
 - Bioaccumulation
 - Carcinogenicity
 - Developmental Toxicity / Teratogenicity
 - Genetic Toxicity
 - Immunotoxicity
 - Irritation / Corrosion
 - Neurotoxicity
 - Photoinduced toxicity
 - Repeated Dose Toxicity
 - Sensitisation
 - ToxCast
 - Toxicity to Reproduction
 - Toxicokinetics, Metabolism and Distribution

Undefined

Next

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

Importing to Verical import_BOD and Ames_1

Import mode

Vertical Horizontal I have a header row

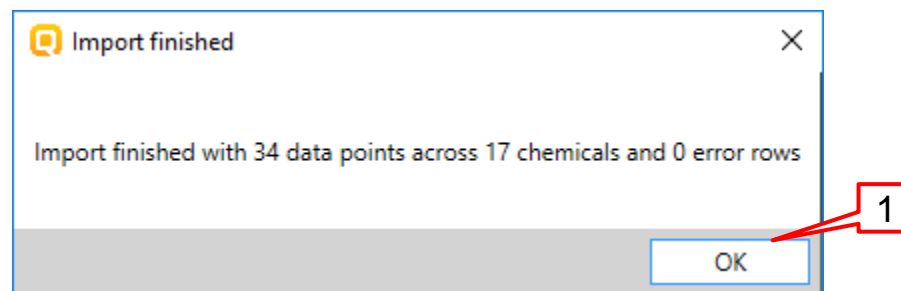
Preview of file

CAS	NAME	Smiles	BOD	Ames
CAS	Chemical Names	SMILES	Test guideline=OECD 301 Endpoint=BOD	Type of method=in Vivo Test type=Bacterial Reverse Mutation Assay (e.g. Ames Test) Test organisms (species)=Salmonella typhimurium Metabolic activation=Without S9 Strain=TA 100 Endpoint=Gene mutation
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(c2cccc2)N1c1cccc1	0.09	Negative
148-82-3	MELPHALAN	C(=O)(O)C(N)Cc1ccc(N(CCC)CCC)cc1	5	Positive
154-93-8	carmustine	C(=O)(N(CCC)N=O)NCCC1	0.09	Positive
61785-57-7	Benzofurazan,_4-(1-aziridiny)-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)cccc1	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(=O)cc3)C)1cccc2	6.2	Negative
54-11-5	Pyridine,_3-(1-methyl-2-pyrrolidiny)-,(S)-	c1(C2CCCN2C)cccc1	75	Negative
54-42-2	idoxuridine	C1(=O)C(l)=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

Back Next Import

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

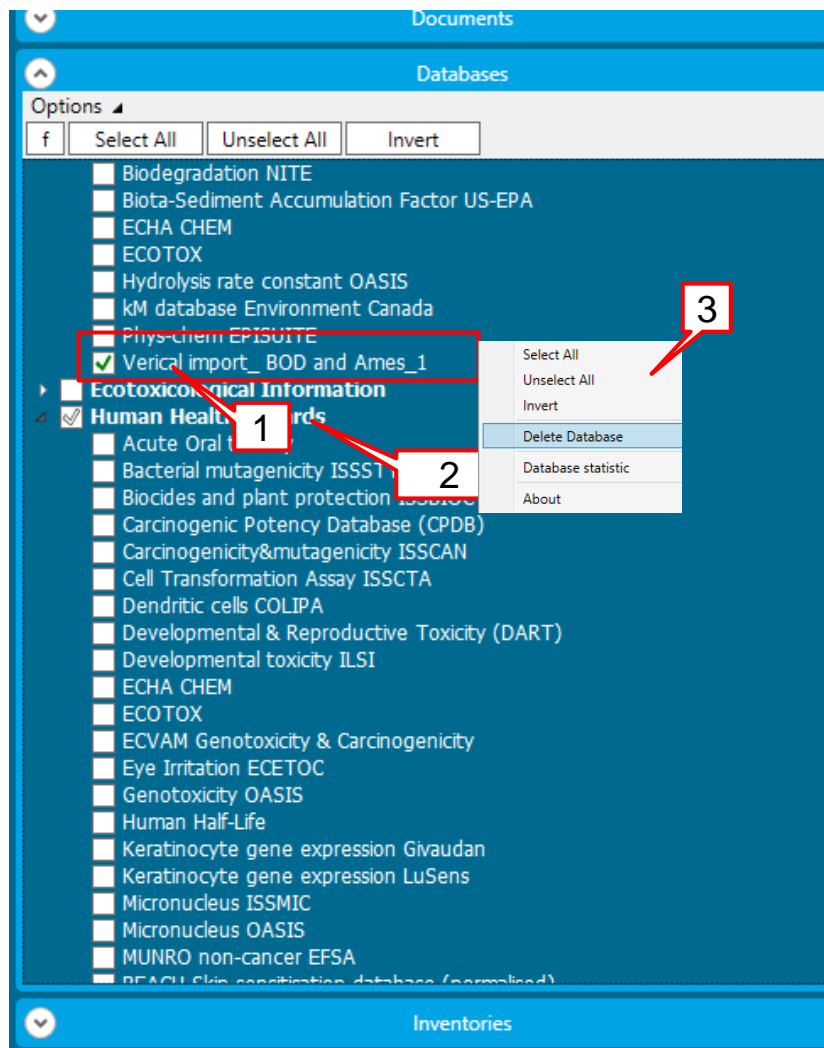
Import of database: Vertical import



- 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

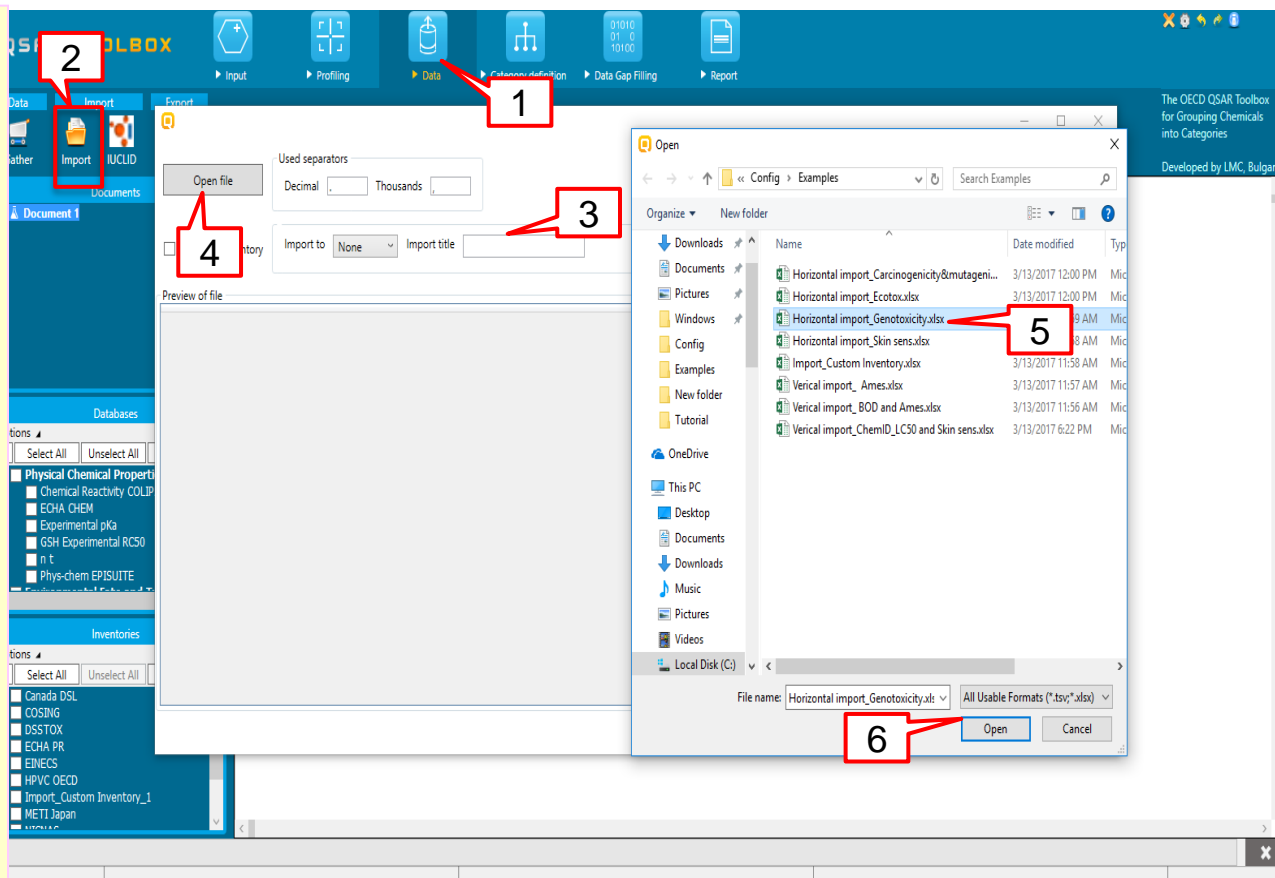
Import of database: Horizontal import

- 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

F	G	H	I	J	K	L	M	N	O	P	Q	R	
Data Mean value/Scale value	Endpoint	Type of genotoxicity	Type of method	Test type	Metabolic activation	Test organisms (species)	Strain	Source of metabolic 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 Progr		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 Progr		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 al	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 al	Mutation Research 587	2005	CPDB, NTP, IARC
14	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chromosome aberr		Chinese Hamster	chinese ham:		Japan Minist	Japan Ministry of Health L		
15	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chromosome aberr		Chinese Hamster	chinese ham:		Japan Minist	Japan Ministry of Health L		
16	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chromosome aberr		Chinese Hamster	chinese ham:		Japan Minist	Japan Ministry of Health L		
17	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chromosome aberr		Chinese Hamster	chinese ham:		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 al	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 al	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 al	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 al	Mutation Research 587	2005	CPDB, NTP, IARC
26	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test					Kirkland et al	Mutation Research 587	2005	CPDB, NTP, IARC
27	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test					Kirkland et al	Mutation Research 587	2005	CPDB, NTP, IARC
28	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test					Kirkland et al	Mutation Research 587	2005	CPDB, NTP, IARC
29	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test					Kirkland et al	Mutation Research 587	2005	CPDB, NTP, IARC
30													

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

Importing to Horizontal import_Genotoxicity_1

Open file

Used separators
Decimal . Thousands ,

Import as inventory

Import to None Import title Horizontal import_Genotoxicity_1

Preview of file

CAS	Chemical name	Smiles	Endpoint path	Scale	Data Mean value	Endpoint	Type of genotoxicity	Type of method	
86260	1,1'-biphenyl_2-methoxy-	c1(-c2c(OC)cccc2)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial rev
86260	1,1'-biphenyl_2-methoxy-	c1(-c2c(OC)cccc2)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial rev
86306	N-NITROSODIPHENYLAMI	c1(N(c2cccc2)N=O)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial rev
86306	N-NITROSODIPHENYLAMI	c1(N(c2cccc2)N=O)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial rev
72571	Trypan_Blue	c1(-c2cc(C)(N=Nc3c(O)c4c	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial rev
72571	Trypan_Blue	c1(-c2cc(C)(N=Nc3c(O)c4c	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial rev
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCC)CCC)C	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial rev
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	bacterial rev
1606673	1-PYRENAMINE	c12c3c4c(c(N)ccc4ccc3ccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial rev
51127	nialamide	C(=O)(c1ccncc1)NNCCCC(=O	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial rev
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	mammalian
51218	FLUOROURACIL	C1(=O)C(F)=CNC(=O)N1	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	mammalian
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	in vitro mam
70553	4-methylbenzenesulfonamr	c1(S(N)(=O)=O)ccc(C)cc1	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mam
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	in vitro mam
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	in vitro mam
54319	FUROSEMIDE	C(=O)(O)c1c(NCC2=CC=CO	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mam
50282	Estradiol_[USAN:INN]	c12c(C(P+3)C(P+3)C(P-4)C(P	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mam

Back Next

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

Import of database: Horizontal import

Importing to Horizontal import_Genotoxicity_1

Data.MeanValue must be mapped to a field in order to continue
EndpointPath must be mapped to a field in order to continue

Import mode
 Vertical Horizontal I have a header row

Preview of file

CAS	Chemical Name	Smiles	Endpoint path	Scale	Data Mean value Scale value	Endpoint	Type of genotoxicity	Type
CAS	Chemical Names	SMILES	Undefined	Data.Scale	Undefined	Endpoint	Type of genotoxicity	Type
86260	1,1'-biphenyl_2-meth	c1(-c2c(OC)cccc2)cccc1	Human health hazards#Gene	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86260	1,1'-biphenyl_2-meth	c1(-c2c(OC)cccc2)cccc1	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
86306	N-NITROSODIPHENYL	c1(N(c2cccc2)N=O)cccc	Human health hazards#Gene	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86306	N-NITROSODIPHENYL	c1(N(c2cccc2)N=O)cccc	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCC)CC	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
50442	Purine-6-thiol	C1(=S)C2=C(N=CN2)N=	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
1606673	1-PYRENAMINE	c12c3c4c(c(N)ccc4ccc3cc	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
51127	nialamide	C(=O)(c1ccncc1)NNCCC	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
50760	Actinomycin_D	C(=O)(C1C2C(=C(C)C(=C	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
51218	FLUOROURACIL	C1(=O)C(F)=CNC(=O)N1	Human health hazards#Gene	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro
51285	2,4-dinitrophenol;2,4-c	c1(O)c(N(=O)=O)cc(N(=	Human health hazards#Gene	Chromosome aberra	Positive	Chromosome aberration	Chromosome aberration	in vitro
70553	4-methylbenzenesulfo	c1(S(N)(=O)=O)ccc(C)cc	Human health hazards#Gene	Chromosome aberra	Negative	Chromosome aberration	Chromosome aberration	in vitro
87592	2,3-dimethylaniline;2,3	c1(N)c(C)c(C)ccc1	Human health hazards#Gene	Chromosome aberra	Positive	Chromosome aberration	Chromosome aberration	in vitro
87592	2,3-dimethylaniline;2,3	c1(N)c(C)c(C)ccc1	Human health hazards#Gene	Chromosome aberra	Negative	Chromosome aberration	Chromosome aberration	in vitro
54319	FUROSEMIDE	C(=O)(O)c1c(NCC2=CC=	Human health hazards#Gene	Chromosome aberra	Negative	Chromosome aberration	Chromosome aberration	in vitro
50282	Estradiol_[USAN:INN]	c12c(C(P+)+3C(P+))C(P-)	Human health hazards#Gene	Chromosome aberra	Negative	Chromosome aberration	Chromosome aberration	in vitro

Back Next 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

Importing to Horizontal import_Genotoxicity_1

Data.MeanValue must be mapped to a field in order to continue
EndpointPath must be mapped to a field in order to continue **1**

Import mode
 Vertical Horizontal I have a header row

Preview of file

CAS	Chemical name	Smiles	Endpoint path	Scale	Data Mean value	Endpoint	Type of genotoxicity	Type of method
CAS	Chemical Names	SMILES	Endpoint path	Data.Scale	Undefined	Endpoint	Type of genotoxicity	Type of method
86260	1,1'-biphenyl_2-methoxy-	c1(-c2c(OC)cccc2)cccc1	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)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86306	N-NITROSODIPHENYLAMINE	c1(N(c2ccccc2)N=O)cccc1		I	Negative	Gene mutation	Gene mutation	in vitro
86306	N-NITROSODIPHENYLAMINE	c1(N(c2ccccc2)N=O)cccc1		I	Negative	Gene mutation	Gene mutation	in vitro
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3ccccc3)cc2)cc1		I	Positive	Gene mutation	Gene mutation	in vitro
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3ccccc3)cc2)cc1		I	Positive	Gene mutation	Gene mutation	in vitro
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCC)CC)C1		I	Positive	Gene mutation	Gene mutation	in vitro
50442	Purine-6-thiol	C1(=S)C2=C(N=CN2)N=CN1		I	Positive	Gene mutation	Gene mutation	in vitro
1606673	1-PYRENAMINE	c12c3c4c(c(N)ccc4ccc3ccc1)		I	Positive	Gene mutation	Gene mutation	in vitro
51127	nialamide	C(=O)(c1ccncc1)NNCCC(=O)N		I	Positive	Gene mutation	Gene mutation	in vitro
50760	Actinomycin_D	C(=O)(C1C2C(=C(C)C(=O)C2)N1)C		I	Positive	Gene mutation	Gene mutation	in vitro
51218	FLUOROURACIL	C1(=O)C(F)=CNC(=O)N1		I	Positive	Gene mutation	Gene mutation	in vitro
51285	2,4-dinitrophenol;2,4-dinitrophenol	c1(O)c(N(=O)=O)cc(N(=O)=O)c1		aberratic	Positive	Chromosome aberration	Chromosome aberration	in vitro
70553	4-methylbenzenesulfonamide	c1(S(N)(=O)=O)ccc(C)cc1	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
87592	2,2-dimethylalanine;2,2-dimethylalanine	c1(N)(C)C(C)C1	Human health hazards#Genetic Toxicity	Chromosome aberratic	Positive	Chromosome aberration	Chromosome aberration	in vitro
87592	2,2-dimethylalanine;2,2-dimethylalanine	c1(N)(C)C(C)C1		I	Positive	Chromosome aberration	Chromosome aberration	in vitro
54319				I	Positive	Chromosome aberration	Chromosome aberration	in vitro
50282				I	Positive	Chromosome aberration	Chromosome aberration	in vitro

Filter: end

Endpoint
Endpoint 2
Endpoint assigned
Endpoint comment
Endpoint explanation
EndpointPath
Gender
Organism gender
Trend

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

Import

Import of database: Horizontal import

Importing to Horizontal import_Genotoxicity_1

Import mode
 Vertical Horizontal I have a header row

Preview of file

CAS	Chemical name	Smiles	Endpoint path	Scale	Data Mean	Endpoint	Type of genotoxicity	Type of method
CAS	Chemical Names	SMILES	EndpointPath	Data.Scale		Endpoint	Type of genotoxicity	Type of method
86260	1,1'-biphenyl,_2-methoxy-	c1(-c2c(OC)cccc2)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I				
86260	1,1'-biphenyl,_2-methoxy-	c1(-c2c(OC)cccc2)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I				
86306	N-NITROSODIPHENYLAMI	c1(N(c2cccc2)N=O)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I				
86306	N-NITROSODIPHENYLAMI	c1(N(c2cccc2)N=O)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I				
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c	Human health hazards#Genetic Toxicity	Gene mutation I				
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c	Human health hazards#Genetic Toxicity	Gene mutation I				
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCC)CCC)C	Human health hazards#Genetic Toxicity	Gene mutation I				
50442	Purine-6-thiol	C1(=S)C2=C(N=CN2)N=CN	Human health hazards#Genetic Toxicity	Gene mutation I				
1606673	1-PYRENAMINE	c12c3c4c(c(N)ccc4ccc3ccc1	Human health hazards#Genetic Toxicity	Gene mutation I				
51127	nialamide	C(=O)(c1ccncc1)NNCCC(=O	Human health hazards#Genetic Toxicity	Gene mutation I				
50760	Actinomycin_D	C(=O)(C1C2C(=C(C)C(=O)C	Human health hazards#Genetic Toxicity	Gene mutation I				
51218	FLUOROURACIL	C1(=O)C(F)=CNC(=O)N1	Human health hazards#Genetic Toxicity	Gene mutation I				
51285	2,4-dinitrophenol;2,4-dinit	c1(O)c(N(=O)=O)cc(N(=O)=	Human health hazards#Genetic Toxicity	Chromosome aberratic				
70553	4-methylbenzenesulfonamr	c1(S(N)(=O)=O)ccc(C)cc1	Human health hazards#Genetic Toxicity	Chromosome aberratic				
87592	2,3-dimethylaniline;2,3-dir	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic Toxicity	Chromosome aberratic				
87592	2,3-dimethylaniline;2,3-dir	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic Toxicity	Chromosome aberratic				
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+)(C(P-)(C(P-	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
56235	CARBON-TETRACHLORIDE	C(Cl)(Cl)C(Cl)Cl	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro

Data.MeanValue must be mapped to a field in order to continue

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

Importing to Horizontal import_Genotoxicity_1

Import mode
 Vertical Horizontal I have a header row

Preview of file

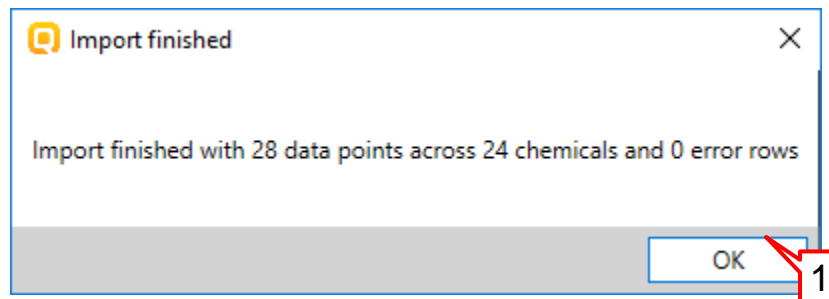
CAS	Chemical name	Smiles	Endpoint path	Scale	Data Mean value	Endpoint	Type of genotoxicity	Type of method
CAS	Chemical Names	SMILES	EndpointPath	Data.Scale	Data.MeanV...	Endpoint	Type of genotoxicity	Type of method
86260	1,1'-biphenyl_2-methoxy-	c1(-c2c(OC)cccc2)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86260	1,1'-biphenyl_2-methoxy-	c1(-c2c(OC)cccc2)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86306	N-NITROSODIPHENYLAMI	c1(N(c2ccccc2)N=O)cccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro
86306	N-NITROSODIPHENYLAMI	c1(N(c2ccccc2)N=O)cccc1	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(CCC)CCC)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)(c1ccccc1)NCCCC(=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-methylbenzenesulfonamr	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)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)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	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
50555	reserpine	C12c3c(cc(OC)cc3)NC=1C1C	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro
76448	HEPTACHLOR	C12(C)C(C)C(C)C(C)C1=O	Human health hazards#Genetic Toxicity	Chromosome aberratic	Positive	Chromosome aberration	Chromosome aberration	in vitro

Next Import

- 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)

4

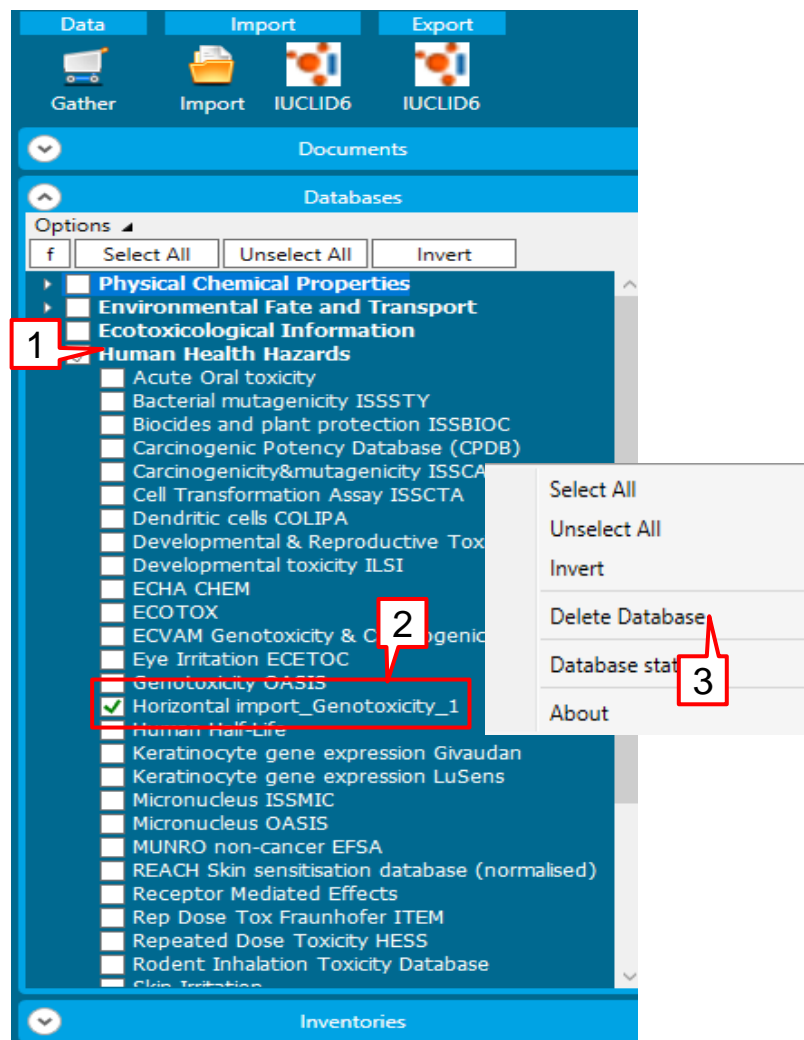
Import of database: Horizontal import



- 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

The screenshot shows the QSAR Toolbox interface with the 'Data' panel active. The 'Import' button is highlighted with a red box labeled '2'. The 'Import title' field is highlighted with a red box labeled '3'. The 'Import as inventory' checkbox is checked and highlighted with a red box labeled '4'. The 'Open file' button is highlighted with a red box labeled '5'. An 'Open' file dialog is open, showing a list of files. The file 'Import_Custom Inventory.xlsx' is selected and highlighted with a red box labeled '6'. The 'Open' button in the dialog is highlighted with a red box labeled '7'. The 'Data' panel is highlighted with a red box labeled '1'.

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);

Importing to Import_Custom Inventory_1

Open file

Used separators
 Decimal Thousands

Import as inventory

Import to Import title

1

Preview of file

CAS	Name	SMILES
000051-28-5	2,4-dinitrophenol; Phenol, 2,4-dinit	<chem>c1(O)c(N(=O)=O)cc(N(=O)=O)cc1</chem>
000059-50-7	4-Chloro-m-cresol; 3-methyl-4-chk	<chem>c1(C)c(C)cc(O)cc1</chem>
000065-45-2	2-hydroxybenzamide; Benzamide, 2	<chem>C(N)(=O)c1c(O)cccc1</chem>
000069-72-7	2-hydroxybenzoic_acid; Benzoic aci	<chem>C(=O)(O)c1c(O)cccc1</chem>
000079-94-7	4,4'-(1-methylethylidene)bis[2,6-dit	<chem>c1(C(C)(C)c2cc(Br)c(O)c(Br)c2)cc(Br)c(O)c(Br)c1</chem>
000080-05-7	4,4'-(1-methylethylidene)bisphenol	<chem>c1(C(C)(C)c2ccc(O)cc2)ccc(O)cc1</chem>
000080-09-1	Phenol, 4,4'-sulfonylbis-; Phenol, 4,	<chem>c1(S(=O)(=O)c2ccc(O)cc2)ccc(O)cc1</chem>
000080-46-6	4-(1,1-dimethylpropyl)phenol; Pher	<chem>C(C)(C)(c1ccc(O)cc1)CC</chem>
000081-64-1	1,4-dihydroxy-9,10-anthracenedior	<chem>c12C(=O)c3c(C(=O)c1c(O)ccc2O)cccc3</chem>
000088-06-2	2,4,6-trichlorophenol; Phenol, 2,4,6	<chem>c1(Cl)c(O)c(Cl)cc(Cl)c1</chem>
000088-18-6	2-(1,1-dimethylethyl)phenol; Phenc	<chem>C(C)(C)(C)c1c(O)cccc1</chem>
000088-60-8	Phenol, 2-(1,1-dimethylethyl)-5-me	<chem>C(C)(C)(C)c1c(O)cc(C)cc1</chem>
000088-75-5	2-nitrophenol; Phenol, 2-nitro-; Phē	<chem>c1(O)c(N(=O)=O)cccc1</chem>
000088-85-7	dinoseb; Phenol, 2-(1-methylpropy	<chem>c1(N(=O)=O)c(O)c(C(C)C)cc(N(=O)=O)c1</chem>

Back Next Import

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);

Importing to Import_Custom Inventory_1

Import mode

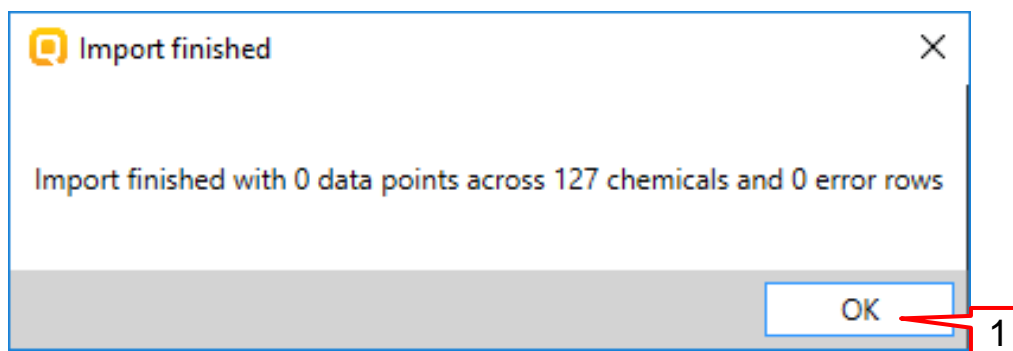
Vertical Horizontal I have a header row

Preview of file

CAS	Name	SMILES
CAS	Chemical Names	SMILES
000051-28-5	2,4-dinitrophenol; Phenol, 2,4-dinit	<chem>c1(O)c(N(=O)=O)cc(N(=O)=O)cc1</chem>
000059-50-7	4-Chloro-m-cresol; 3-methyl-4-chl	<chem>c1(Cl)c(C)cc(O)cc1</chem>
000065-45-2	2-hydroxybenzamide; Benzamide, 2	<chem>C(N)(=O)c1c(O)cccc1</chem>
000069-72-7	2-hydroxybenzoic_acid; Benzoic aci	<chem>C(=O)(O)c1c(O)cccc1</chem>
000079-94-7	4,4'-(1-methylethylidene)bis[2,6-dit	<chem>c1(C(C)(C)C2cc(Br)c(O)c(Br)c2)cc(Br)c(O)c(Br)c1</chem>
000080-05-7	4,4'-(1-methylethylidene)bisphenol	<chem>c1(C(C)(C)C2ccc(O)cc2)ccc(O)cc1</chem>
000080-09-1	Phenol, 4,4'-sulfonylbis-; Phenol, 4,	<chem>c1(S(=O)(=O)c2ccc(O)cc2)ccc(O)cc1</chem>
000080-46-6	4-(1,1-dimethylpropyl)phenol; Pher	<chem>C(C)(C)(c1ccc(O)cc1)CC</chem>
000081-64-1	1,4-dihydroxy-9,10-anthracenedior	<chem>c12C(=O)c3c(C(=O)c1c(O)ccc2O)cccc3</chem>
000088-06-2	2,4,6-trichlorophenol; Phenol, 2,4,6	<chem>c1(Cl)c(O)c(Cl)cc(Cl)c1</chem>
000088-18-6	2-(1,1-dimethylethyl)phenol; Phenc	<chem>C(C)(C)(C)c1c(O)cccc1</chem>
000088-60-8	Phenol, 2-(1,1-dimethylethyl)-5-me	<chem>C(C)(C)(C)c1c(O)cc(C)cc1</chem>
000088-75-5	2-nitrophenol; Phenol, 2-nitro-; Phe	<chem>c1(O)c(N(=O)=O)cccc1</chem>
000088-85-7	dinoseb; Phenol, 2-(1-methylpropy	<chem>c1(N(=O)=O)c(O)c(C(C)CC)cc(N(=O)=O)c1</chem>
000088-89-1	2,4,6-trinitrophenol; Phenol, 2,4,6-t	<chem>c1(N(=O)=O)c(O)c(N(=O)=O)cc(N(=O)=O)c1</chem>
000089-72-5	o-sec-butylphenol; Phenol, 2-(1-me	<chem>c1(O)c(C(C)CC)cccc1</chem>
000089-83-8	5-methyl-2-(1-methylethyl)phenol;	<chem>c1(O)c(C(C)C)ccc(C)c1</chem>

Back Next Import

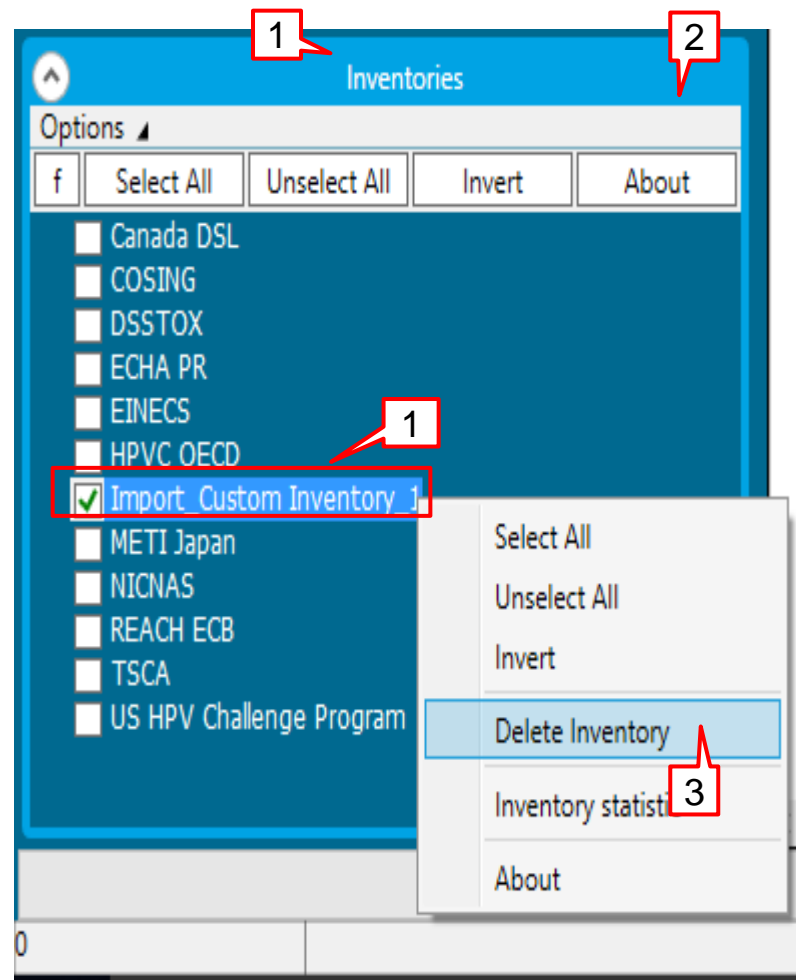
Import of inventory



- 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.

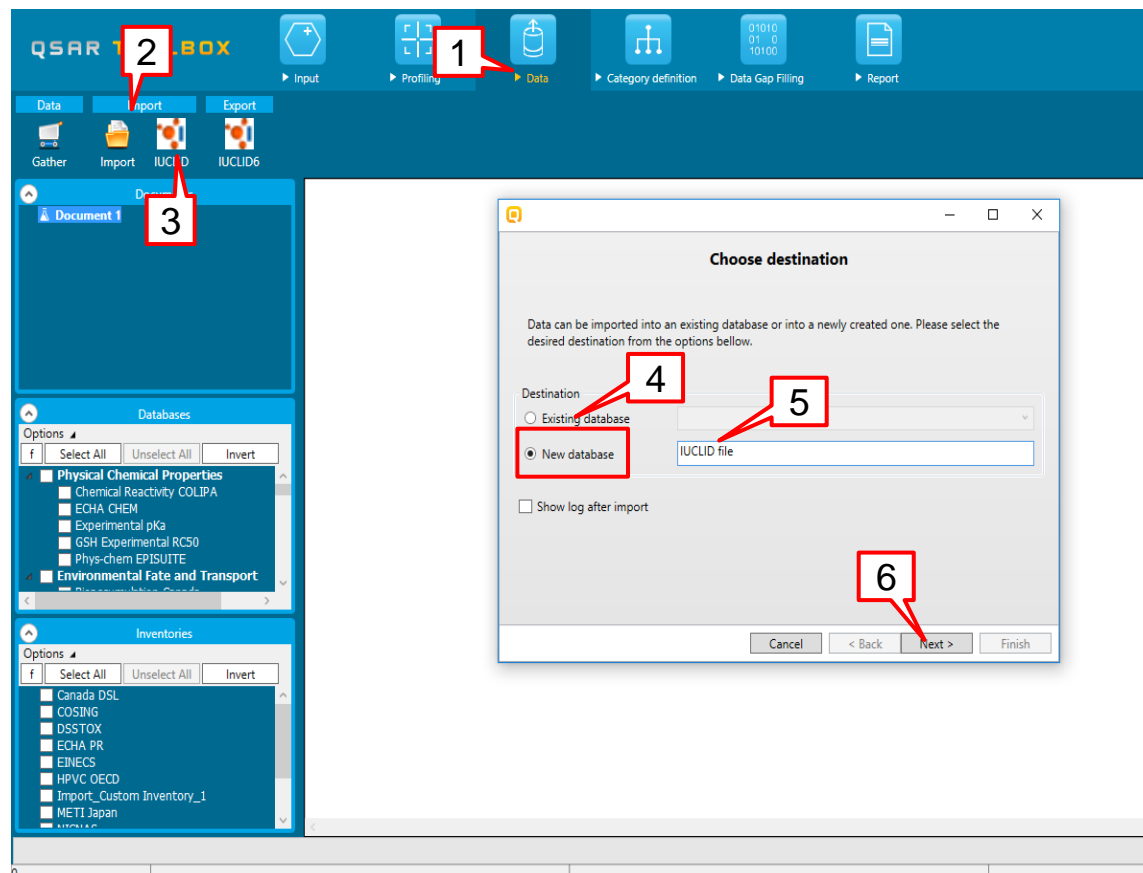


Outlook

- 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).

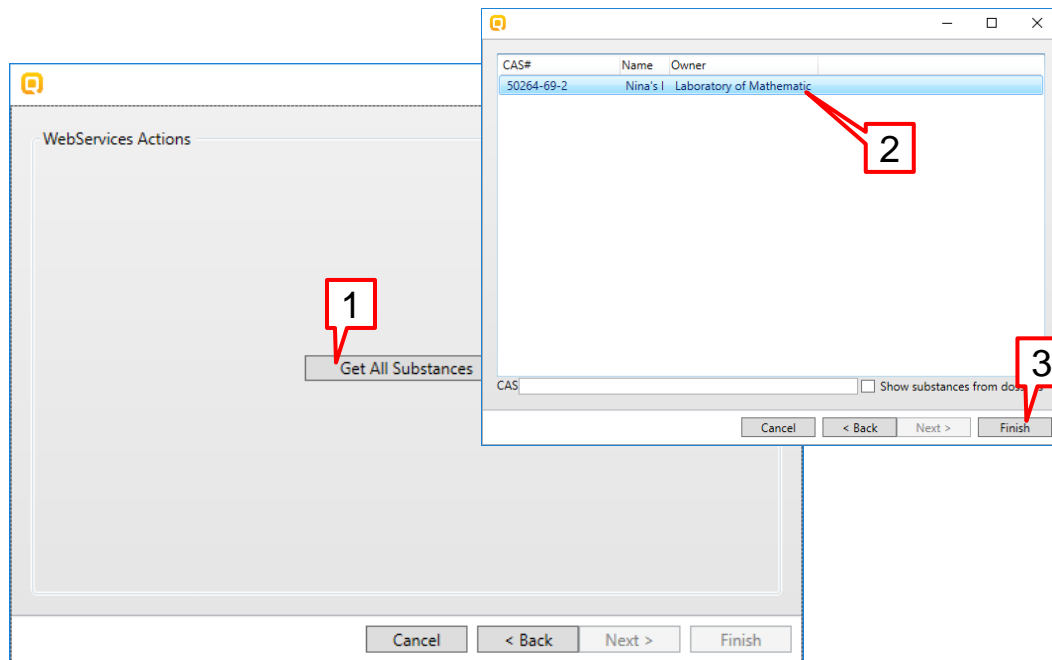
The screenshot shows a dialog box titled "Connect to an IUCLID6 server". The text inside reads: "In order to use a IUCLID server you should establish a network connection with it. Please provide the needed connection parameters below and then click Next".

The dialog contains the following fields and controls:

- IUCLID Server:** A dropdown menu with "localhost" selected. A red callout box with the number "1" points to this field.
- Port:** A text input field containing "8080". A red callout box with the number "2" points to this field.
- Username:** A text input field containing "SuperUser". A red callout box with the number "3" points to this field.
- Password:** A text input field with masked characters (dots). A red callout box with the number "4" points to this field.
- Test connection options:** A button located below the Username and Password fields.
- Navigation buttons:** At the bottom, there are four buttons: "Cancel", "< Back", "Next >", and "Finish". A red callout box with the number "5" points to the "Next >" button.

Import IUCLID

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



Import IUCLID

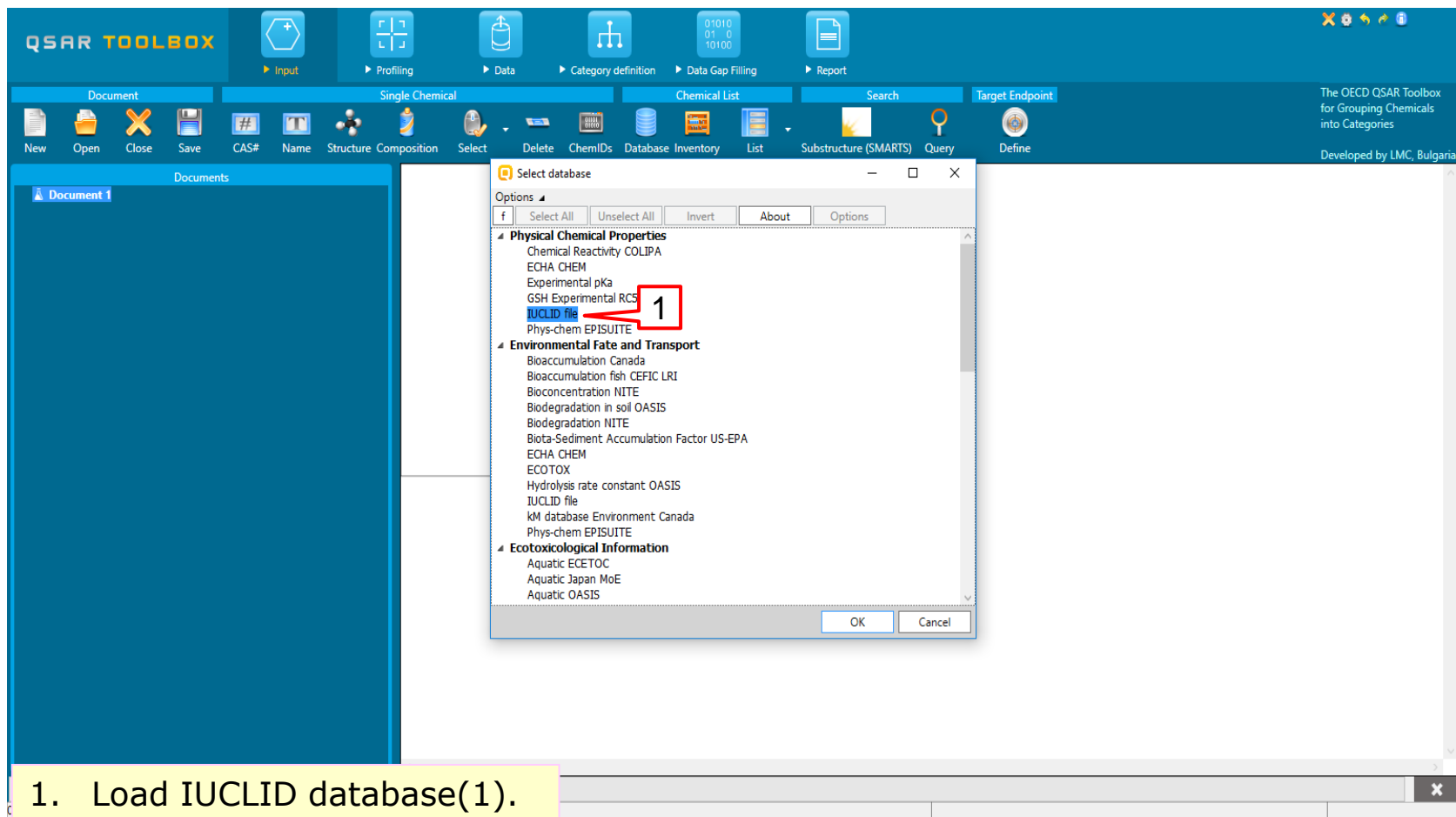
The screenshot shows the QSAR Toolbox software interface. The top menu bar includes 'Data', 'Import', and 'Export'. Under 'Import', there are icons for 'Gather', 'Import', 'IUCLID6', and 'IUCLID6'. The main workspace is divided into 'Documents', 'Databases', and 'Inventories' sections. A dialog box titled 'Import completed(1)' is overlaid on the workspace, with a red box around the number '1' and a red arrow pointing to it. The dialog box contains a table with the following data:

CAS#	Name	Owner
50264-69-2	Nina's I	Laboratory of Mathematic

Below the table, there is a checkbox labeled 'Show substances from dossiers' which is currently unchecked. At the bottom of the dialog box, there are buttons for 'Cancel', '< Back', 'Next >', and 'Finish'.

1. Import completed(1).

Import IUCLID



The screenshot displays the QSAR Toolbox software interface. A 'Select database' dialog box is open, showing a list of databases categorized into Physical Chemical Properties, Environmental Fate and Transport, and Ecotoxicological Information. The 'IUCLID file' option is highlighted with a red box and the number '1'. Below the screenshot, a yellow box contains the text '1. Load IUCLID database(1).'

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 Intput (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

The screenshot shows the Aquatic OASIS software window with a grid of 20 chemical structures. The first row, containing items 1 through 5, is highlighted with a red border and a red box labeled '1'. The 'OK' button at the bottom right of the window is also highlighted with a red box and a red box labeled '2'. The chemical structures are as follows:

Item	Chemical Structure
1	98-01-1: <chem>O=Cc1ccccc1</chem>
2	106-44-5: <chem>Oc1ccc(C)cc1</chem>
3	589-34-4: <chem>CC(C)CC(C)C</chem>
4	28575-17-9: <chem>O=Cc1ccc(O)cc1</chem>
5	586-98-1: <chem>Oc1ccc(O)cc1</chem>
6	768-94-5: <chem>O=C1C2CC3C1C2</chem>
7	1485-07-0: <chem>Oc1ccc(O)cc1</chem>
8	383-63-1: <chem>CC(C)C(C)C</chem>
9	100-46-9: <chem>Nc1ccccc1</chem>
10	1461-25-2: <chem>O=C(O)C(C)C</chem>
11	771-61-9: <chem>O=C(O)C(C)C</chem>
12	14660-52-7: <chem>O=C(O)C(C)C</chem>
13	96-50-4: <chem>Nc1ccncc1</chem>
14	109-00-2: <chem>O=C(O)C(C)C</chem>
15	5930-28-9: <chem>O=C(O)C(C)C</chem>
16	623-43-8: <chem>O=C(O)C(C)C</chem>
17	122-03-2: <chem>O=C(O)C(C)C</chem>
18	637-59-2: <chem>O=C(O)C(C)C</chem>
19	7251-61-8: <chem>O=C(O)C(C)C</chem>
20	75039-84-8: <chem>O=C(O)C(C)C</chem>

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).

The screenshot displays the QSAR Toolbox software interface. The top menu bar has 'Data' highlighted with a red box and the number 1. Below the menu bar, the 'Gather' button in the 'Documents' panel is highlighted with a red box and the number 3. In the 'Databases' panel, 'Aquatic OASIS' is selected with a red box and the number 2. A 'Read data?' dialog box is open, with the 'OK' button highlighted by a red box and the number 4. Below this, a confirmation dialog box displays the message '19 points added across 5 chemicals.' with the 'OK' button highlighted by a red box and the number 5. The main workspace shows a table with chemical structures and their corresponding data points.

Filter endpoint tree...	1	2	3	4
Structure	<chem>H2C=O</chem>	<chem>C1=CC=C(C=C1)C(=O)O</chem>	<chem>C1=CC=C(C=C1)C(=O)O</chem>	<chem>C1=CC=C(C=C1)C(=O)O</chem>
Structure info				
Parameters				
Physical Chemical Properties				
Environmental Fate and Transport				
Ecotoxicological Information (5/14)	M: 0.0498 mg/L	M: 485 mg/L	M: 0.00457 mg/L	M: 4.17E+04 r
Human Health Hazards				

Horizontal Export: Collecting data

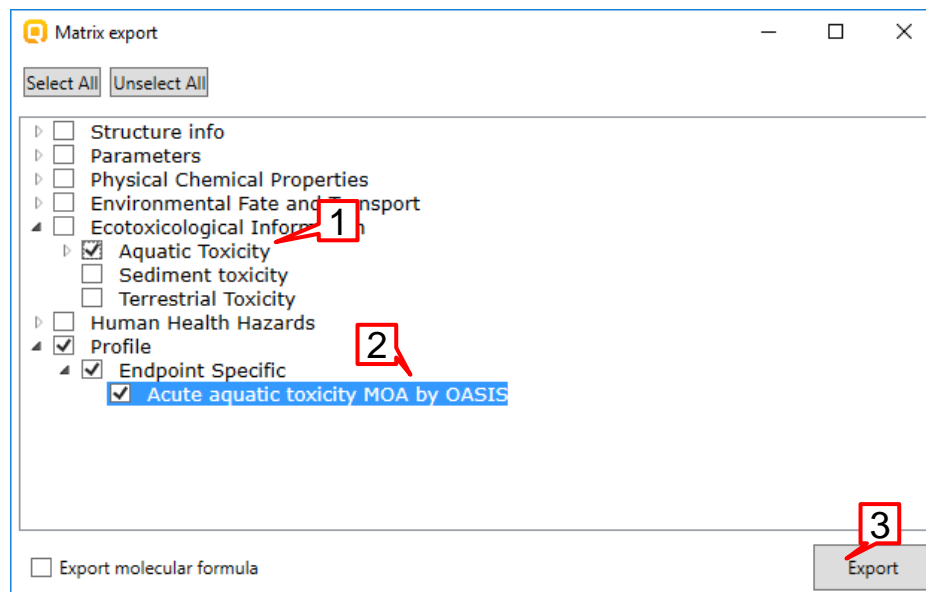
The screenshot displays the QSAR Toolbox interface. The top menu bar includes 'Input', 'Profiling', 'Data', 'Category definition', 'Data Gap Filling', and 'Report'. The 'Profiling' menu is open, showing options: 'Apply', 'View', 'New', and 'Delete'. The 'Apply' button is highlighted with a red box and labeled '1'. Below the menu, the 'Documents' panel shows 'Document 1' with a selection from the 'Aquatic OASIS' database. The 'Filter endpoint tree...' panel on the left shows a tree structure with 'Acute aquatic toxicity ...' selected. The 'Profiling methods' panel at the bottom left shows 'Acute aquatic toxicity MOA by OASIS' checked, also highlighted with a red box and labeled '1'. The main data matrix table has five columns, each with a chemical structure and a concentration value (M). A context menu is open over the table, with 'Export Data matrix' highlighted by a red box and labeled '2'. Other menu items include 'Expand branch', 'Collapse branch', 'Expand All', 'Collapse All', 'Target endpoint', 'Open path', 'Copy path', 'Function', 'Sort', 'Acute aquatic toxicity MOA by OASIS', 'Activate AOP', and 'Profile Statistic'.

Structure	1	2	3	4	5
<chem>O=Cc1ccoc1</chem>	<chem>Oc1ccc(C)cc1</chem>	<chem>CC(C)CC(C)C</chem>	<chem>OCC1=CC=C(C=C1)C=C2C=CC(=C2)C=C1</chem>	<chem>OCC1=CC=C(C=C1)C=C2C=CC(=C2)C=C1</chem>	<chem>OCC1=CC=C(C=C1)C=C2C=CC(=C2)C=C1</chem>
Structure info					
Parameters					
Physical Chemical Properties					
Environmental Fate and Transport					
Ecotoxicological Information (5/19)	M: 10.5 mg/L	M: 0.319 mg/L	M: 24 mg/L	M: 8.18 mg/L	M: 3.53E+03 mg/L
Human Health Hazards					
Profile					
Endpoint Specific					
Acute aquatic toxicity ...	Aldehydes	Phenols and Anilines	Basesurface narcotics	Basesurface narcotics	Basesurface narcotic

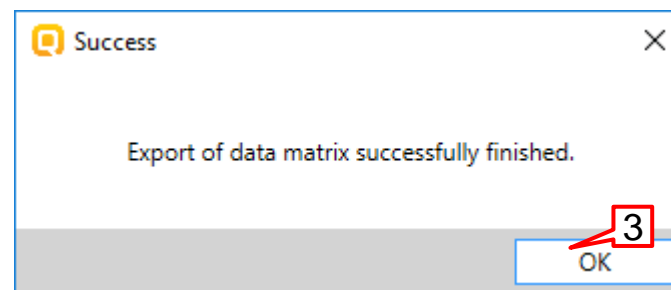
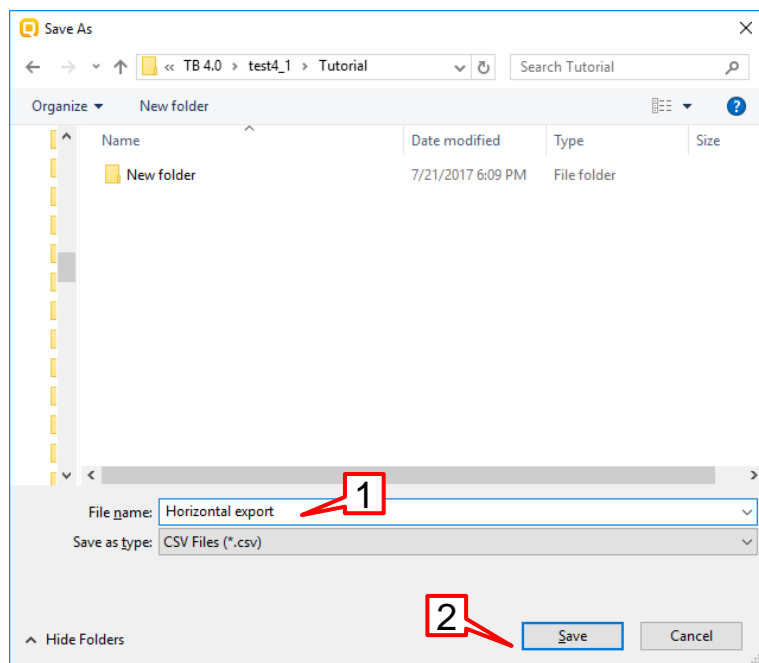
1. Select Acute aquatic toxicity MOA by OASIS and apply the profiler(1)
2. Perform right click over the data matrix and select Export data matrix (2)

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

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	CAS Num	Structural	Data.Meas	Data.Uni	Data.Min	Data.Max	Data.Scale	Data.Qual	Year	Title	Author	Effect	Comment	Endpoint	Referen
2	62-53-3	Nc1cccc1	84.93154	mg/L			Mass concentration		1997	Tetratox: Schultz, T.	Growth	Impairme	IGC50		
3	62-53-3	Nc1cccc1	45.61094	mg/L			Mass concentration		2003	Estimating	Furusjö, E	Intoxicati	Effective	EC50	
4	62-53-3	Nc1cccc1	24.49452	mg/L			Mass concentration		1998	QSAR stuc	Zhao, Y.H.	Intoxicati	Immobiliz	IC50	
5	62-53-3	Nc1cccc1	23.39209	mg/L			Mass concentration		1985	QSARs for	Vighi, M.,	Mortality	Lethal con	LC50	
6	62-53-3	Nc1cccc1	0.435581	mg/L			Mass concentration		2005	Structural	Peter C. v	Mortality	Lethal con	LC50	
7	62-53-3	Nc1cccc1	0.099786	mg/L			Mass concentration		2005	Structural	Ohe, P.C.	Mortality	Lethal con	LC50	
8	62-53-3	Nc1cccc1	61.52746	mg/L			Mass concentration		2003	Estimating	Furusjö, E	Mortality	Lethal con	LC50	
9	62-53-3	Nc1cccc1	106.9225	mg/L			Mass concentration		1997	PREDICTIN	Russom, C	Mortality	Lethal con	LC50	
10	62-53-3	Nc1cccc1	114.5695	mg/L			Mass concentration		2004	Creation c	raevsky, (Mortality	Lethal con	LC50	
11	62-53-3	Nc1cccc1	48.873	mg/L			Mass concentration		1998	QSAR of cl	Zhao, Y.H.	Physiolog	Millimolai	PT	
12	62-53-3	Nc1cccc1	70.64298	mg/L			Mass concentration		1994	Mechanis	Jaworska,	Physiolog	Millimolai	PT	
13	5428-54-6	Cc1ccc(cc1	33.50241	mg/L			Mass concentration		1997	Tetratox: Schultz, T.	Growth	Impairme	IGC50		
14	5428-54-6	Cc1ccc(cc1	16.40877	mg/L			Mass concentration		1992	Biodegradat	ion and	Mortality	Lethal con	LC50	
15	90-01-7	OCC1cccc	1106.341	mg/L			Mass concentration		1997	Tetratox: Schultz, T.	Growth	Impairme	IGC50		
16	110-40-7	CCOC(=O)	19.15149	mg/L			Mass concentration		1997	Tetratox: Schultz, T.	Growth	Impairme	IGC50		
17	110-40-7	CCOC(=O)	2.705219	mg/L			Mass concentration		1997	PREDICTIN	Russom, C	Mortality	Lethal con	LC50	
18	1122-91-4	Brc1ccc(C	47.55482	mg/L			Mass concentration		1997	Tetratox: Schultz, T.	Growth	Impairme	IGC50		

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).