The OECD QSAR Toolbox for Grouping Chemicals into Categories

OECD (Q)SAR Toolbox v.4.4.1

Tutorial on how to Import/Export a custom database and Import/Export a database via IUCLID

Outlook

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

Aim

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

Note: Please note that building of custom items (such as profilers, (Q)SAR models as well as importing of custom databases) is only enabled in single user mode. So, if your Toolbox is installed in multiuser mode, you will be not able to follow this tutorial.

Outlook

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- Import
- Export

Keywords

TARGET CHEMICAL - chemical of interest

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

WORKFLOW – the use, in combination, of the different modules (e.g. prediction workflow: from input to report)

IMPORT – Toolbox allows to import a custom databases with experimental data. Import should follows a specific import layout (Excel type of IU format)

EXPORT – Toolbox allows to export data and prediction for chemicals available on data matrix in a format appropriate for Excel

ENDPOINT TREE – Endpoints are structured in a branched scheme, from a broader level (Phys-Chem properties, Environmental Fate and transport, Ecotoxicology, Human health hazard) to a more detailed one (e.g. EC3 in LLNA test under Human health hazard-Skin sensitization)

DATA MATRIX – Table reporting the chemical(s) and data (experimental results, profilers outcomes, predictions). Each chemical is in a different column and each data in a different row

Outlook

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- Keywords

Definition of Database and Inventory

- Import
- Export

Definition of database and inventory

- <u>A database</u> is a collection of structures accompanied with experimental data.
- <u>An inventory</u> is a collection of structures without experimental data.

Outlook

- Aim
- Keywords
- 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
- Keywords
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- Import:
 - Import of database
 - Vertical import
 - Horizontal import
 - Import of inventory
 - Import via IUCLID
- Export Data matrix

Import of database: Vertical import layout

• 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 <u>xlsx</u> or <u>tsv</u> 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 layout

• 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 in the following installation folder: C:\Program Files (x86)\Common Files\(Q)SAR Toolbox 4\Config\Examples

	А	В	С	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	C1(=O)C(CCCC)C(=O)N(c2ccccc2)	0.09	Negative
6	148-82-3	MELPHALAN	C(=O)(O)C(N)Cc1ccc(N(CCCI)CCC	5	Positive
7	154-93-8	carmustine	C(=O)(N(CCCI)N=O)NCCCI	0.09	Positive
8	61785-57-7	Benzofurazan,_4-(1-aziridiny	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)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
19					
-					

QSAR TOOLE Data Import Gather Inform IUCLU6 2 Document 1 Document	Korrest Constraints of the second secon	Data D	ram Files (x86) > Common Files > QSAR Toolbox 4.4 > Co	nfig > Examples	×		×
1. Go to <u>Data</u> module(1);	<	 ✓ Quick access ✓ Desktop ✓ Downloads 	Name III HL_Mutagenicity_template.xlsx III Skin sens_template.xlsx III HL_Skin sens_template.xlsx III Horizontal import_Carcinogenicity&mutagenicity_exa	Date modified 11/6/2018 2:11 PM 11/6/2018 2:11 PM 3/13/2017 12:00 PM	Type Microsoft Excel W Microsoft Excel W Microsoft Excel W	Size 11 KB 12 KB 15 KB	^
2. Click on <i>Import button</i> (2);		Documents Pictures ACT About TP 44	Horizontal import_Ecotox.xlsx Horizontal import_Genotoxicity.xlsx Horizontal import_Multiple_endpoints.xlsx Horizontal import_Multiple_endpoints.xlsx	3/13/2017 12:00 PM 3/13/2017 11:59 AM 11/6/2018 2:11 PM	Microsoft Excel W Microsoft Excel W Microsoft Excel W	28 KB 16 KB 20 KB	
3. Click on <u>Open file (</u> 3);		bin	Horizontal import_Skin sens.xlsx JIGC50 training set.xlsx JIGC50 validation set.xlsx	3/13/2017 11:58 AM 11/8/2019 8:16 AM 11/8/2019 8:16 AM	Microsoft Excel W Microsoft Excel W Microsoft Excel W	15 KB 12 KB 11 KB	
4. Select the file (Verical	F	Times OneDrive	Import_Custom Inventory.xlsx Import_Custom Inventory_Custom ID.xlsx Import_Custom Inventory_Custom IDs.xlsx Import_Custom Inventory_Custom IDs.xlsx	3/13/2017 11:58 AM 2/4/2019 9:29 AM 9/13/2019 5:55 PM	Microsoft Excel W Microsoft Excel W Microsoft Excel W	18 KB 19 KB 10 KB	
import_ BOD and		This PC Network	Verical import_ Ames.xlsx Verical import_ BOD and Ames.xlsx Verical import_ ChemID_LC50 and Skin sens.xlsx	3/13/2017 11:58 AM 3/13/2017 11:56 AM 3/13/2017 6:22 PM	Microsoft Excel W Microsoft Excel W Microsoft Excel W	10 КВ 10 КВ 11 КВ]
5. Click on <i>Open</i> (5).		File nan	ne: Verical import_BOD and Ames.xlsx		[All Usable Formats (*.tsv;*.xlsv Open 💽 Cance	ix) ∨ el

Import of database: Vertical import procedure

Open file	ventory Import to None Import title	Verical import_BOD and Ames_1		
review 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(CCCI)CCCI)cc1	5	Positive
154-93-8	carmustine	C(=O)(N(CCCI)N=O)NCCCI	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
		C(4.5	Magazius

- 2. The title of the imported file is also included;
- 3. Click on <u>Next</u> (3);

Importin	g to 1 import_BOD and Ames_1			_	×
 Vertica 	I O Horizontal 🗹 I have a header row	3	3		
Preview of fi	e				
CAS	NAME	Smiles	BOD	Ames	
CAS ~	Chemical Names ~	SMILES	No endpoint selected	No endpoint selected	
			Undefined 🗠	Uncefined ~	
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	Negativ 4	
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(CCCI)CCCI)cc1	5	Positive	
154-93-8	carmustine	C(=O)(N(CCCI)N=O)NCCCI	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(=0)C(l)=CN(C2CC(0)C(C0)02)C(=0)N1	0.09	Negative	

1. Select Vertical radio button (1).

2. Checkbox indicating the file for import includes Header row (2)

3. First three columns includes chemical ID information. These columns are automatically recognized by the system that they includes chemical ID. Recognition is displayed via assigning the correct ID identifiers on the second row (first column is recognized that it includes CAS#, second includes names and third includes SMILES). In this situation no action is needed from the user here.

4. However the columns with endpoint data are not recognized by system. In other words in the second row it is written "No endpoint selected". In this respect in order to assign the endpoints to the respective column you need to click individually on each No endpoint selected button under the endpoints names (4)(see on next slide). The OECD (Q)SAR Toolbox for Grouping Chemicals into Categories

Import of database: Vertical import procedure

For **BOD**:

Once click on "Endpoint not selected" a new window appears. First you need to select the hard path of the tree to which the data should be assigned. Open "Biodegradation node" (1)select "Ready Biodegradability" (2) from the endpoint tree and then to press Next (3).

Importing to Verical impo	rt_BOD and Ames	— C	I X
Dat	a defining Designation must be mapped to a field in order to continue		
Import mode	💽 Select endpoint 🛛 🕹 🗶		
Vertical	Filter: Close		
Preview of file CAS C CAS C 60-34-4 METHYLHYDR/ 50-29-3 C 50-29-3 DICHLORO_DIF 50-32-8 BENZOPYRENE 50-33-9 PHENYLBUTAZ 148-82-3 MELPHALAN 154-93-8 carmustine 61785-57-7 Benzofurazan, 62-75-9 N-NITROSODII 91-59-8 2-NAPHTHYLA 96-09-3 STYRENE_OXIL 107-13-1 2-propenenitri 51-79-6 URETHANE 53-96-3 2-ACETYLAMIN 54-11-5 Pyridine,_3-(1- 54-42-2 idoxuridine 55-38-9 FENTHION 55-48-1 atropine_sulph	Physical Chemical Properties Environmental Fate Transport Bioaccumulation 1 tic Bioaccumulation 1 tic Biodegradation in Sewage Treatment Plant Biodegradation in water and sediment: simulation tests Biodegradation in Water: Screening T Biodegradation Probability Photodegradation Stability in Water Transport and Distribution Between Environmental Compartments Ectotoxicological Information Human Health Hazards	Ames ndpoint su Judefined ive ative ative ive ive ive ive ive ive ative	

	Family/Scale	Biodegradability (%)	Unit	%(Biodegra	dability (%)) 🛛 🗸
 Environment Biodegra Biode R 	al Fate and Transpor dation :gradation in Water: eady Biodegradabilit	t Screening Tests Y			
Test guideline Duration Endpoint	+	↓ ↓	~	Selection o	fadditional
				A	dd
			Г	Up	Down

For **BOD**:

Additionally select the Family/Scale from the drop-down menu (Biodegradability (%)(4)) and after that select the unit (% Biodegradability(%))(5). Press <u>Next</u> (6).

Select endpoint		×
Family/Scale	Biodegradability (%) 🛛 Y	Unit %(Biodegradability (%)) *
 Environmental Fate and Transpo Biodegradation Biodegradation in Water: Ready Biodegradabili 	rt Screening Tests ty 8	3
Test guideline	OECD 301C	v
Duration	+	
Endpoint	BOD 7	 Selection of additional metadata fields:
		~ ~
		Add
		Up Down
		Clear Remove
Undefine		Back Finish

<u>For **BOD**</u>: In order to define the endpoint more specifically please select *BOD endpoint* (7) from the drop-down menu. Then from the drop-down menu associated with test guideline select *OECD301C* (8).

Select endpoint					\times
Family/Sca	le	Biodegradability (%) 🔻	Un	it %(Biodegradability (%)) ~
 Environmental Fate and Trans Biodegradation Biodegradation in Wa Ready Biodegrada 	sport ter: S bility	creening Tests			
Test guideline	ļ	OECD 301C	Ŷ		
Duration	+ +				
indpoint	Ħ	BOD	~	Selection of additior metadata fields:	nal
					Y
				Add	
				Up Dowr	n
				Clear Remov	/e
					Ļ
Undefine				Back Einisk	

For BOD: Once all the data fields are filled , press *Finish* (9).

Importing to	verical import_BOD and Ames			- 0	×
Import mode -					
Vertical	◯ Horizontal 🔽 I have a header row				
			10		
Preview of file			Y		
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)(O)C(N)Cc1ccc(N(CCCI)CCCI)cc1	5	Positive	
154-93-8	carmustine	C(=O)(N(CCCI)N=O)NCCCI	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	
			Back	Next Imp	ort

For BOD: The edited fields are displayed in the main table (10).

Import of database: Vertical import procedure

For Ames:

1. Click on <u>No endpoint</u>

<u>selected (</u>1);

2. Expand the Human Health

hazard tree and select

"Genetic toxicity" (2).

3. Click on <u>Next</u> (3)

🦲 Importing	to Verical import_ BOD and Ames			-	\Box ×
Import mode	2				
Vertical	○ Horizontal 🔽 I have a header row				
0.000					
Preview of file					1
CAS	NAME	Smiles	BOD	Am	es
CAS ~	Chemical Names	SMILES ~	Test guideline=OE	No endpoir	nt selected
				Undefin	ned ~
60-34-4	METHYLHYDRAZINE	CNN	0.2	Positive	
148-82-3	MELPHALAN		-		
154-93-8	carmustine	Select endpoint			
61785-57-7	Benzofurazan, 4-(1-aziridinyl)-7-nitro-, 3-	ter:			Close
62-75-9	N-NITROSODIMETHYLAMINE	Physical Chemical Properties			
91-59-8	2-NAPHTHYLAMINE	Environmental Fate and Transport			
96-09-3	STYRENE OXIDE	Ecotoxicological Information Human Health Hazards			
107-13-1	2-propenenitrile	Acute Toxicity			
50-29-3	DICHLORO DIPHENYL TRICHLOROETHAN	▷ ADME			
50-32-8	BENZOPYRENE;3,4-";_BENZOPYRENE;3,4	Bioaccumulation			
50-33-9	PHENYLBUTAZONE	Developmental Toxicity / Teratogenicity			
51-79-6	URETHANE	Genetic Toxicity			
53-96-3	2-ACETYLAMINOFLUORENE	Immunotoxicity			
54-11-5	Pyridine,_3-(1-methyl-2-pyrrolidinyl)-,_(S)-	Irritation / Corrosion			
54-42-2	idoxuridine	Photoinduced toxicity			
55-38-9	FENTHION	Repeated Dose Toxicity			
55-48-1	atropine_sulphate	Sensitisation			
		loxCast Toxicity to Reproduction			
		 Toxicokinetics, Metabolism and Distributio 	n		
		·			
					3
					<u> </u>
		Jndefine			Next

	Family/S	cale Gene m	utation I × Unit
 Human Health Hazards Genetic Toxicity 			
Type of method	R	~	
lest organisms (species)			
Metabolic activation		~	Selection of additional
Strain	R .	~	metadata fields:
Endpoint	R .	~	
5	Filter:		
	Chromosom	e aberration	
	DNA and pr	otein damage	n
	DNA and pro DNA damag	otein damage e and repair	n ve

For Ames:

Select scale Gene mutation I (4). From the drop-down menu of the *Endpoint* field (5) select Gene mutation(6).

Import of database: Vertical import procedure

	Family/Scale Greenwetting LX Unit
	Family/Scale Gene mutation + Offic
 Human Health Hazards Genetic Toxicity 	
Tune of method	7
Test type	Bacterial Reverse Mu
Test organisms (species)	
Metabolic activation	
Strain	Bacillus Subtilis Recombination Assay Bacterial Reverse Mutation Assay (e.g. Ames Test)
Endpoint	in Vitro Gene Mut in Vitro Mammalian Cell Micronucleus Test Mammalian Cell Gene Mutation Assay
	Mouse Spot Test n Other
	Transgenic Rodent Mutation Yeast Cytogenetic Assay

For Ames:

From the drop-down menu of <u>Type of method</u>, select In vitro (7) and from <u>Test type</u> field select: Bacterial reverse Mutation assays (e.g. Ames test) (8).

Elect endpoint	×
	Family/Scale Gene mutation I Y Unit
 Human Health Hazards Genetic Toxicity 	
Type of method	in Vitro v
Test type	Bacterial Reverse Mu 9
Test organisms (species)	Salmonella typhimuri
Metabolic activation	 Selection of additional
Strain 📕	Filter:
Endpoint 📕	
	×
	No Data
	No S9 Into
	Not Specified
	With
	With and Without
	With S9 10
Undefine	Without
	Without S9

For Ames:

Select <u>*Test organism (species)*</u>: Salmonella typhimurium (9) and for <u>*Metabolic activation*</u> select Without S9 (10).

Import of database: Vertical import procedure

Select endpoint		×	
	Family/Scale Gene m	nutation I Y Unit V	
 Human Health Hazards Genetic Toxicity 			
Type of method	in Vitro ~		
Test type	Bacterial F J ~		
Test organisms (species)	🛚 Salmonell		
Metabolic activation	Without S	Selection of additional	
Strain	TA 100 ~	metadata fields:	
Endpoint	Gene mutation ~		
		~	
		Add	
		Up Down	
		Clear Remove	12
Undefine		Back Finish	

For Ames: Select Strain: TA 100 (11) for instance and then click Finish (12).

🦲 Import	ing to Verical import_BOD and Ames_1			- ð ×
Import n	node			
Vert	tical 🔿 Horizontal 🗹 I have a header row			
Preview o	f file			
CAS	NAME	Smiles	BOD	Ames
CAS ~	Chemical Names Y	SMILES	Test guideline=OECD 301C#E	Type of method=in Vitro#Test type=Bacterial Reverse Mutation Assav (e.g. Ames Test)#Test organisms (species)=Salmonella typhimurum#Metabolic activation=Without S9#Strain=TA 100#Endpoint=Gene mutation
-09-3	STYRENE OXIDE	c1(C2CO2)ccccc1	0.01	Positive
-59-8	2-NAPHTHYLAMINE	c12c(cc(N)cc1)cccc2	25	Positive
-75-9	N-NITROSODIMETHYLAMINE	CN(C)N=O	10	Positive
785-57-7	Benzofurazan,_4-(1-aziridinyl)-7-nitro-,_3-oxide	C1(N(=O)=O)C2C(C(N3CC3)=CC		Positive
-34-4	METHYLHYDRAZINE	CNN	0.2	Positive
-48-1	atropine_sulphate	C(=0)(C(c1ccccc1)C0)0C1CC2C0	4.5	Negative
-38-9	FENTHION	c1(SC)c(C)cc(OP(=S)(OC)OC)cc1	1.8	Negative
-42-2	Idoxuridine	C1(=0)C(I)=CN(C2CC(0)C(C0)O2	20.09	Negative
-11-5	2. ACETVLAMINOELLIOPENIE	c1(c2(c(N2()cccnc1	62	Negative Nanation
-79-6	URETHANE	C(N)(=0)QCC	1.8	negative Negative
-33-9	PHENYLBUTAZONE	C1(=0)C(CCCC)C(=0)N(c2ccccc2	0.09	Negative
-32-8	BENZOPYRENE;3,4-";_BENZOPYRENE;3,4-	c12c3c4c(c5c(cc4ccc3ccc1)cccc5)	60.7	Negative
-29-3	DICHLORO_DIPHENYL_TRICHLOROETHANE	C(CI)(CI)(CI)C(c1ccc(CI)cc1)c1ccc(7.1	Negative
4-93-8	carmustine	C(=O)(N(CCCI)N=O)NCCCI	0.09	Positive
8-82-3	MELPHALAN	C(=O)(O)C(N)Cc1ccc(N(CCCI)CCC	5	Positive
7-13-1	2-propenenitrile	C(#N)C=C	2	Positive
<				13
				Back Next Import

For Ames: The edited fields are displayed in the main table (12). Finally, click on *Import* (13).

Import of database: Vertical import procedure



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

View of imported database

• The new database is displayed in the Databases panel (1) in two sections: <u>Environmental fate and transport group</u> and <u>Human health hazard group (2);</u>

• Right-click menu (3) is implemented where you can see the database statistics or delete the database.



Outlook

- Aim
- Keywords
- 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 layout

• 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 in the following installation folder: C:\Program Files (x86)\Common Files\(Q)SAR Toolbox 4\Config\Examples

	F1	$ f_x$	Data Mean value/Scale v	value									
	F	G	н	1	J	к	L	М	N	0	Р	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 typhimuriun	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 typhimuriun	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 typhimuriun	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 typhimuriun	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 typhimuriun	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 typhimuriun	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 typhimuriun	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 typhimuriun	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 typhimuriun	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 typhimuriun	TA 1535		U.S. Environ	The Salmonella typhimuri	1996	US_GTox
12	Positive	Gene mutation	Gene mutation	in vitro	alian cell gene mutation	n 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	n 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 chr	omosome aberra	Chinese Hamster	chinese ham		Japan Minist	Japan Ministry of Health L		
15	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chr	omosome aberra	Chinese Hamster	chinese ham		Japan Minist	Japan Ministry of Health L		
16	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chr	omosome aberra	Chinese Hamster	chinese ham		Japan Minist	Japan Ministry of Health L		
17	Negative	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian chr	omosome aberra	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 Invento	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 Invento	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 Invento	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 Invento	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 cel	l micronucleus te	est			Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
27	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cel	l micronucleus te	est			Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
28	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cel	l micronucleus te	est			Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
29	Positive	Chromosome aberr	Chromosome aberration	in vitro	in vitro mammalian cel	l micronucleus te	est			Kirkland et a	Mutation Research 587	2005	CPDB, NTP, IARC
30													

- 1. Go to *Data* module (1);
- 2. Click on *Import* (2);
- 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.xls x)(5);
- 6. Click on <u>Open (</u>6).



🜔 Import	ing to Horizontal import_Ge	notoxicity_1						_	
Op	en file Decimal	ators							
Impor	t as inventory	None - Import tit	e Horizontal import_Genotoxicity_1						
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)ccccc1	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)ccccc1	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)ccccc1	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)ccccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial rev
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	bacterial rev
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	bacterial rev
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCCI)CCCI)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)NNCCC(=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-methylbenzenesulfonam	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+}3C{P+}(C{P-}4C{P	Human health hazards#Genetic Toxicity	Chromosome aberratic	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mam \ >
							Back	Next	2

- 1. A preview of the imported file is shown (1);
- 2. Click on <u>Next</u> (2);

📋 Importing to Horizont	al import_Genotoxicity_1							– 🗆 X
		Data.M	leanValue must be map	ed to a field in order	to continue			
		Endp	ointPath must be mappe	ed to a field in order to	o continue			
Import mode			7					
					<u>\</u> 2			
U vertical U Horizor	ntal 🔽 i nave a neader row				2			
Draview of file		V						
Freview of file		Endpoint path	Scale	Data Mean value Scale value	Endpoint	Type of genotovicity	Tune of method	Test two
	Chall FC A	Lindefined y	Data Saala V	Undefined V	Endpoint V	Turn of anotherisity	Ture of mothed	Test typ
	3WILES	Underined	Data.scale	Underined .	Crateria	Type of genotoxicity	Type of method	lest type
		Human health hazards#Genetic Toxicity		Negative		Gene mutation	in vitro	bacterial reverse mutation a
	=1(N(=2====2)N=-0)====1	Human health hazards#Genetic Toxicity		Negative	3	Gene mutation	in vitro	bacterial reverse mutation a
	c1(N(c2cccc2)N=O)ccccc1	Human health hazards#Genetic Toxicity	Gana mutation I	Negative	Gen on In	Gene mutation	in vitro	bacterial reverse mutation a
	c1(w(c2cccc2)w=0)ccccc1	Human health hazards#Genetic Toxicity	Gene mutation I	Positivo	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation a
	c1(-c2cc(C)c(N=Nc3c(O)c4c(I)	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation a
	C1CCNIP(=0)(N/CCCI)CCCI)O	Human health hazards#Genetic Toxicity	Gene mutation I	Positivo	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation a
	C1(-S)C2-C(N-CN2)N-CN1	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation a
	c12c3c4c(c(N)ccc4ccc3ccc1)c	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation a
		Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation a
		Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	mammalian cell gene mutat
	C1(-0)C(E)-CNC(-0)N1	Human health hazards#Genetic Toxicity	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	mammalian cell gene mutat
henol (dnn):nhenol 24-c	c1(0)c(N(-0)-0)cc(N(-0)-(Human health hazards#Genetic Toxicity	Chromosome aberration L (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
namide/henzenesulfonar	c1(S(N)(-O)-O)ccc(C)cc1	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
er2 3-yulidiner2 3-dimethy	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
e:2.3-xylidine:2.3-dimethy	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
	C(=0)(0)c1c(NCC2=CC=CO2	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
	c12c(C{P+}3C{P+}(C{P-}4C{P-	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
	C(CI)(CI)(CI)CI	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
-	C12c3c(cc(OC)cc3)NC=1C1C0	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
-	C12(CI)C(CI)(CI)C(CI)(C(CI)=C	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
	c1(SC)c(C)cc(OP(=S)(OC)OC)c	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
-	c1(Cl)c(O)c(Cl)cc(Cl)c1	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
	c1(C)cc(C)nc(NS(=O)(=O)c2co	Human health hazards#Genetic Toxicity	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromo
)-3-methylbutyrate;_Fenv	C(#N)C(c1cc(Oc2cccc2)ccc1)	Human health hazards#Genetic Toxicity	Micronucleus I	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cell mic
1	C12C(=0)C(C)=C(N)C(=0)C=	Human health hazards#Genetic Toxicity	Micronucleus I	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cell mic 🗡

- Select *Horizontal* radio button (1) ٠
- Column with chemical ID is automatically recognized by the system (for more details sees slide 15)
- 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). In order to map correctly the fields see next slide.

Import of database: Horizontal import procedure

			Data.Mean'	Value must be ma	pped t	o a field in order to c	ontinue			
		ſ	Endpoint	Path must be map	ped to	a field in order to con	ntinue			
Import mode -			4							
O Vertical	🖲 Horizontal 🗹 I have a	a header row	-							
Preview of file										
CAS	Chemical name	Smiles	Endpo 2	1		Data Mean value Scale value	Endpoint	Type of genotoxicity	Type of method	Te
CAS Y	Chemical Names Y	SMILES Y			~	Undefined Y	Endpoint Y	Type of genotoxicity ×	Type of method ~	Tes
86260	1,1'-biphenyl,_2-methox	c1(-c2c(OC)cccc2)ccccc1	Filter end			Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse muti ^
86260	1,1'-biphenyl,_2-methox	c1(-c2c(OC)cccc2)ccccc1	Files end	[Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
86306	N-NITROSODIPHENYLA	c1(N(c2ccccc2)N=O)ccccc1	Endpoint			Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
86306	N-NITROSODIPHENYLA	c1(N(c2ccccc2)N=O)ccccc1	Endpoint	2		Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c()	Endpoint	gned	_	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c()	Endpoint com	ments	γ	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCCI)CCCI)O'	Endpoint e. pla	nation	3	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
50442	Purine-6-thiol	C1(=S)C2=C(N=CN2)N=CN1	EndpointPa	ath		Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
1606673	1-PYRENAMINE	c12c3c4c(c(N)ccc4ccc3ccc1)c	Gender			Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
51127	nialamide	C(=O)(c1ccncc1)NNCCC(=O)	Organism ge	nder		Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mut
50760	Actinomycin_D	C(=O)(C1C2C(=C(C)C(=O)C=	Trend	[Positive	Gene mutation	Gene mutation	in vitro	mammalian cell gene
51218	FLUOROURACIL	C1(=O)C(F)=CNC(=O)N1	Human health hazards#Genetic	Gene mutation I		Positive	Gene mutation	Gene mutation	in vitro	mammalian cell gene
51285	2,4-dinitrophenol;2,4-di	c1(0)c(N(=0)=0)cc(N(=0)=0	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
70553	4-methylbenzenesulfon	c1(S(N)(=O)=O)ccc(C)cc1	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
87592	2,3-dimethylaniline;2,3-	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
87592	2,3-dimethylaniline;2,3-	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
54319	FUROSEMIDE	C(=O)(O)c1c(NCC2=CC=CO2	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
50282	Estradiol_[USAN:INN]	c12c(C{P+}3C{P+}(C{P-}4C{P-	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
56235	CARBON-TETRACHLORI	C(CI)(CI)(CI)CI	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
50555	reserpine	C12c3c(cc(OC)cc3)NC=1C1C(Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
76448	HEPTACHLOR	C12(CI)C(CI)(CI)C(CI)(C(CI)=C	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
55389	FENTHION	c1(SC)c(C)cc(OP(=S)(OC)OC)c	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
88062	2,4,6-TRICHLOROPHEN	c1(Cl)c(O)c(Cl)cc(Cl)c1	Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian c
57681	SULFAMETHAZINE	c1(C)cc(C)nc(NS(=O)(=O)c2c(Human health hazards#Genetic	Chromosome aberration	I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
51630581	cyano_(3-phenoxybenzy	C(#N)C(c1cc(Oc2ccccc2)ccc1)	Human health hazards#Genetic	Micronucleus I		Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian c
50077 <	Mitomycin IUSAN:BAN:	C12C(=O)C(C)=C(N)C(=O)C=	Human health hazards#Genetic	Micronucleus I		Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian ci 🗡

- 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 is also written in the top message (4).

Back Next Import

🦲 Importing to	o Horizontal import_Geno	toxicity_1							– 🗆 X
			Data.Mean	Value must be mapped t	o a field in order t	o continue			
Import mode	● Horizontal ✔ I have	a header row	4	1					
Preview of file									
CAS	Chemical name	Smiles	Endpoint path	Scale	Data Menn value Sc 🥏	e Endpoint	Type of genotoxicity	Type of method	Te
CAS ~	Chemical Names Y	SMILES Y	EndpointPath 🗸	Data.Scale v		 Endpoint 	Type of genotoxicity 🔻	Type of method ~	Tes
86260	1,1'-biphenyl,_2-metho	c1(-c2c(OC)cccc2)ccccc1	Human health hazards#Genetic	Gene mutation I	Filter date		Gene mutation	in vitro	bacterial reverse mut
86260	1,1'-biphenyl,_2-methox	c1(-c2c(OC)cccc2)ccccc1	Human health hazards#Genetic	Gene mutation I			Gene mutation	in vitro	bacterial reverse mut
86306	N-NITROSODIPHENYLA	c1(N(c2cccc2)N=O)ccccc1	Human health hazards#Genetic	Gene mutation I	Add as	metadata ^	Gene mutation	in vitro	bacterial reverse mut
86306	N-NITROSODIPHENYLA	c1(N(c2ccccc2)N=O)ccccc1	Human health hazards#Genetic	Gene mutation I	Agendy Responsib	le Sediment for Data	Gene mutation	in vitro	bacterial reverse mut
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c(N	Human health hazards#Genetic	Gene mutation I	BCF Data opera	ator.MeanQualifier	Gene mutation	in vitro	bacterial reverse mut
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c()	Human health hazards#Genetic	Gene mutation I	Consulte	d Databases	Gene mutation	in vitro	bacterial reverse mut
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCCI)CCCI)O'	Human health hazards#Genetic	Gene mutation I	Lata confid	ence category	Gene mutation	in vitro	bacterial reverse mut
50442	Purine-6-thiol	C1(=S)C2=C(N=CN2)N=CN1	Human health hazards#Genetic	Gene mutation I	Data	quality 3	Gene mutation	in vitro	bacterial reverse mut
1606673	1-PYRENAMINE	c12c3c4c(c(N)ccc4ccc3ccc1)c	Human health hazards#Genetic	Gene mutation I	Data.M	axQualifier	Gene mutation	in vitro	bacterial reverse mut
51127	nialamide	C(=O)(c1ccncc1)NNCCC(=O)	Human health hazards#Genetic	Gene mutation I	Data.	MaxValue	Gene mutation	in vitro	bacterial reverse mut
50760	Actinomycin_D	C(=O)(C1C2C(=C(C)C(=O)C=	Human health hazards#Genetic	Gene mutation I	ta.Me	anQualifier	Gene mutation	in vitro	mammalian cell gene
51218	FLUOROURACIL	C1(=O)C(F)=CNC(=O)N1	Human health hazards#Genetic	Gene mutation I	Data.N	1eanValue	Gene mutation	in vitro	mammalian cell gene
51285	2,4-dinitrophenol;2,4-di	c1(O)c(N(=O)=O)cc(N(=O)=C	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Data.M	inQualifier	Chromosome aberration	in vitro	in vitro mammalian cl
70553	4-methylbenzenesulfon	c1(S(N)(=O)=O)ccc(C)cc1	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Data.	MinValue	Chromosome aberration	in vitro	in vitro mammalian cl
87592	2,3-dimethylaniline;2,3-	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Dat	a.Scale	Chromosome aberration	in vitro	in vitro mammalian cl
87592	2,3-dimethylaniline;2,3-	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Dat	ta.Unit	Chromosome aberration	in vitro	in vitro mammalian cl
54319	FUROSEMIDE	C(=O)(O)c1c(NCC2=CC=CO2	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Dat	tabase	Chromosome aberration	in vitro	in vitro mammalian cl
50282	Estradiol_[USAN:INN]	c12c(C{P+}3C{P+}(C{P-}4C{P-}	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Databas	e affiliations	Chromosome aberration	in vitro	in vitro mammalian cl
56235	CARBON-TETRACHLORI	C(CI)(CI)(CI)CI	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Dotails on Me	vehological data	Chromosome aberration	in vitro	in vitro mammalian cl
50555	reserpine	C12c3c(cc(OC)cc3)NC=1C1C(Human health hazards#Genetic	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
76448	HEPTACHLOR	C12(CI)C(CI)(CI)C(CI)(C(CI)=C1	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
55389	FENTHION	c1(SC)c(C)cc(OP(=S)(OC)OC)c	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
88062	2,4,6-TRICHLOROPHEN	c1(Cl)c(O)c(Cl)cc(Cl)c1	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
57681	SULFAMETHAZINE	c1(C)cc(C)nc(NS(=O)(=O)c2cc	Human health hazards#Genetic	Chromosome aberration I (Oasis)	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cl
51630581	cyano_(3-phenoxybenzy	C(#N)C(c1cc(Oc2cccc2)ccc1)	Human health hazards#Genetic	Micronucleus I	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian c
50077	Mitomycin_[USAN:BAN:	C12C(=O)C(C)=C(N)C(=O)C=	Human health hazards#Genetic	Micronucleus I	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian c
50293	DICHLORO_DIPHENYL_1	C(CI)(CI)(CI)C(c1ccc(CI)cc1)c1(Human health hazards#Genetic	Micronucleus I	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian ci 🗸
								Back	ext 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 is also written in the top message (4).

Import of database: Horizontal import procedure

🦲 Importing to	Horizontal import_Geno	toxicity_1							- 🗆 ×
Import mode -									
· Vertical (Horizontal 🖌 I have	a header row							
Vertical	g nonzontar 💽 nave								
Preview of file -									
CAS	Chemical name	Smiles	Endpoint path	Scale	Data Mean value So	Endpoint	Type of genotoxicity	Type of method	Test type
CAS ~	Chemical Names ~	SMILES ~	EndpointPath ~	Data.Scale ~	Data.MeanVal ~	Endpoint ~	Type of genotoxicity 👋	Type of method 🗠	Test type 🗸 🗸 🗸
86260	1,1'-biphenyl,_2-metho>	c1(-c2c(OC)cccc2)ccccc1	Human health hazards#Genetic	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
86260	1,1'-biphenyl,_2-metho>	c1(-c2c(OC)cccc2)ccccc1	Human health hazards#Genetic	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
86306	N-NITROSODIPHENYLA	c1(N(c2ccccc2)N=O)ccccc1	Human health hazards#Genetic	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
86306	N-NITROSODIPHENYLA	c1(N(c2ccccc2)N=O)ccccc1	Human health hazards#Genetic	Gene mutation I	Negative	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c()	Human health hazards#Genetic	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
72571	Trypan_Blue	c1(-c2cc(C)c(N=Nc3c(O)c4c()	Human health hazards#Genetic	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
50180	CYCLOPHOSPHAMIDE	C1CCNP(=O)(N(CCCI)CCCI)O	Human health hazards#Genetic	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
50442	Purine-6-thiol	C1(=S)C2=C(N=CN2)N=CN1	Human health hazards#Genetic	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
1606673	1-PYRENAMINE	c12c3c4c(c(N)ccc4ccc3ccc1)c	Human health hazards#Genetic	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
51127	nialamide	C(=O)(c1ccncc1)NNCCC(=O)	Human health hazards#Genetic	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	bacterial reverse mutation assay (e.g. Ames test)
50760	Actinomycin_D	C(=O)(C1C2C(=C(C)C(=O)C=	Human health hazards#Genetic	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	mammalian cell gene mutation assay
51218	FLUOROURACIL	C1(=O)C(F)=CNC(=O)N1	Human health hazards#Genetic	Gene mutation I	Positive	Gene mutation	Gene mutation	in vitro	mammalian cell gene mutation assay
51285	2,4-dinitrophenol;2,4-di	c1(O)c(N(=O)=O)cc(N(=O)=C	Human health hazards#Genetic	Chromosome aber	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
70553	4-methylbenzenesulfon	c1(S(N)(=O)=O)ccc(C)cc1	Human health hazards#Genetic	Chromosome aber	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
87592	2,3-dimethylaniline;2,3-	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic	Chromosome aber	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
87592	2,3-dimethylaniline;2,3-	c1(N)c(C)c(C)ccc1	Human health hazards#Genetic	Chromosome aber	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
54319	FUROSEMIDE	C(=O)(O)c1c(NCC2=CC=CO2	Human health hazards#Genetic	Chromosome aber	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
50282	Estradiol_[USAN:INN]	c12c(C{P+}3C{P+}(C{P-}4C{P-	Human health hazards#Genetic	Chromosome aber	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
56235	CARBON-TETRACHLORI	C(CI)(CI)(CI)CI	Human health hazards#Genetic	Chromosome aber	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
50555	reserpine	C12c3c(cc(OC)cc3)NC=1C1C(Human health hazards#Genetic	Chromosome aber	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
76448	HEPTACHLOR	C12(CI)C(CI)(CI)C(CI)(C(CI)=C	Human health hazards#Genetic	Chromosome aber	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
55389	FENTHION	c1(SC)c(C)cc(OP(=S)(OC)OC)c	Human health hazards#Genetic	Chromosome aber	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
88062	2,4,6-TRICHLOROPHEN(c1(Cl)c(O)c(Cl)cc(Cl)c1	Human health hazards#Genetic	Chromosome aber	Positive	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
57681	SULFAMETHAZINE	c1(C)cc(C)nc(NS(=O)(=O)c2c(Human health hazards#Genetic	Chromosome aber	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian chromosome aberration test
51630581	cyano_(3-phenoxybenz)	C(#N)C(c1cc(Oc2ccccc2)ccc1)	Human health hazards#Genetic	Micronucleus I	Negative	Chromosome aberration	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test
50077	Mitomycin_[USAN:BAN:	C12C(=O)C(C)=C(N)C(=O)C=	Human health hazards#Genetic	Micronucleus I	Positive	mosome aberration	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test
50293	DICHLORO_DIPHENYL_1	C(CI)(CI)(CI)C(c1ccc(CI)cc1)c1(Human health hazards#Genetic	Micronucleus I	Positive	mosome aberration	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test
50328	BENZOPYRENE;3,4-";_BE	c12c3c4c(c5c(cc4ccc3ccc1)cc	Human health hazards#Genetic	Micronucleus I	Positive	mosome aberration	Chromosome aberration	in vitro	in vitro mammalian cell micronucleus test
<									

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

The OECD (Q)SAR Toolbox for Grouping Chemicals into Categories

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

View of imported database

- The new database is displayed in the Databases panel (1) in the <u>Human health hazard group</u> (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
- Keywords
- 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
- Keywords
- 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 Layout

- As already presented an inventory is a collection of chemicals without any data.
- In the current example import of chemicals along with their external identifiers (custom ID) will be illustrated.

Import of inventory Layout

• Import layout contains two main sections: substance information (1) and column with external ID information (custom ID number)(2);

• The external ID number could be different types: strings only, integer (numbers) only or combination of integer and strings (3)

The imported file can be in <u>xlsx</u> or <u>tsv</u> format

• An example file could be found in the following installation folder: C:\Program Files (x86)\Common Files\(Q)SAR Toolbox 4\Config\Examples

X	, ⊻) • (≌ - ,	Import_Custom	Inventory_Custom IDs.xlsx - Microsoft Excel		- 0	×
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	A21 • (/		*
	А	В	<u> </u>	D	E	
1	CAS #	NAME	SMILES	External ID		
2	000051-28-5	2,4-dinitrophenol; Phenol, 2,4	c1(O)c(N(=O)=O)cc(N(=O)=O)cc	1		
3	000059-50-7	4-Chloro-m-cresol; 3-methyl-	c1(Cl)c(C)cc(O)cc1	2		2
4	000065-45-2	2-hydroxybenzamide; Benza	C(N)(=O)c1c(O)cccc1	3		5
5	000069-72-7	2-hydroxybenzoic_acid; Benz	C(=O)(O)c1c(O)cccc1	EID1		
6	000079-94-7	4,4'-(1-methylethylidene)bis[c1(C(C)(C)c2cc(Br)c(O)c(Br)c2)c	ED2		
7	000080-05-7	4,4'-(1-methylethylidene)bisp	c1(C(C)(C)c2ccc(O)cc2)ccc(O)cc	VOT		
8	000080-09-1	Phenol, 4,4'-sulfonylbis-; Phe	c1(S(=O)(=O)c2ccc(O)cc2)ccc(O	NEC		
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12	Sheet1 Sheet2	Sheet3 / PI	[] 4 [•
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Import of inventory Procedure

	→ + Profiling 1 → Data	Category definition Category definition Category definition Category definition	► Report
Data Import Export Delete Import Import			
Documents Documents	Open file Decimal Thousan	nds 4	
	Preview of file Preview of file	« Common Files » QSAR Toolbox 4.4 » Config » Examples « folder	earch Examples
Databases Options F Select All Unselect All Invert Physical Chemical Properties Chemical Reactivity COLIPA ECHA CHEM Experimental pKa CAL Experimental pKa	PROFILERS 18.4 OneDrive OneDrive 10.5 PC	Name Import_Custom Inventory_Custom IDsxlsx Import_Custom Inventory_Custom IDxlsx Import_Custom Inventory_Custom IDxlsx Import_Castom IDxlsx Import_Castom Inventory_Custom IDxlsx Import_Castom Inventory_Custom IDxlsx Import_Castom Inventory_Custom IDxlsx Import_Castom Inventory_Castom IDxlsx Import_Castom IDxlsx Impor	Date multified Type Size 9/13/2019 11:58 AM Microsoft Excel W 2/4/2019 9:29 AM Microsoft Excel W 1/1/2019 9:29 AM Microsoft Excel W 1/1/2019 9:25 AM Microsoft Excel W 1/1/2019 2:11 PM Microsoft Excel W 1/16/2018 2:11 PM Microsoft Excel W 1/16/2018 2:11 PM Microsoft Excel W
Go to Data module (1); Click on <u>Import</u> (2);	⇒ 30 Ubjects ■ Deskop ■ Documents ↓ Downloads → Music ■ Pictures	The store of	11/6/2018 2:11 PM Microsoft Excel W 11/6/2018 2:11 PM Microsoft Excel W 11/6/2018 2:11 PM Microsoft Excel W 11/6/2018 2:11 PM Microsoft Excel W 3/13/2017 6:22 PM Microsoft Excel W
ïck "Import as inventory" (3)		File <u>Barne</u> Import_Custom Inventory_Custom IDs.xlsx	All Usable Formats ('.tsrg':sdst) ~

4. Type in the name of the inventory as you would want it to be displayed in roolbox (4). Otherwise the name of the file will be used as the name of the inventory.

5. Click on Open file

1.

- 6. Select the file (Import_Custom Inventory_Custom IDs.xlsx)(6),
- 7. Click Open (7) then a message appears informing that only the first worksheet will be used for import, click OK

Import of inventory Procedure

- 1. A preview of the imported file is shown (1);
- 2. Click on <u>Next</u> (2);

() Importing	to My custom inventory_1			-		×				
Open file Used separators Decimal , Thousands										
✓ Import as	nventory Import to None Import title My custor									
Preview of file										
CAS	NAME	SMILES	External ID							
000051-28-5	2,4-dinitrophenol; Phenol, 2,4-dinitro-	c1(0)c(N(=0)=0)cc(N(=0)=0)cc1	1							
000059-50-7	4-Chloro-m-cresol; 3-methyl-4-chlorophenol; Phenol, 4-chloro-3-methyl-; m-Cresol, 4-chl	c1(Cl)c(C)cc(O)cc1	2							
000065-45-2	2-hydroxybenzamide; Benzamide, 2-hydroxy-; Salicylamide	C(N)(=O)c1c(O)cccc1	3							
000069-72-7	2-hydroxybenzoic_acid; Benzoic acid, 2-hydroxy-; Salicylic acid	C(=O)(O)c1c(O)cccc1	EID1							
000079-94-7	4,4'-(1-methylethylidene)bis[2,6-dibromophenol]; Phenol, 4,4'-(1-methylethylidene)bis 2,6	c c1(C(C)(C)c2cc(Br)c(O)c(Br)c2)cc(Br)c(O)c(Br)c1	ED2							
000080-05-7	4,4'-(1-methylethylidene)bisphenol; Phenol, 4,4'-(1-methylethylidene)bis-; Phenol, 4,4'-iso	r c1(C(C)(C)c2ccc(O)cc2)ccc(O)cc1	VOT							
000080-09-1	Phenol, 4,4'-sulfonylbis-; Phenol, 4,4'-sulfonyldi-	c1(S(=O)(=O)c2ccc(O)cc2)ccc(O)cc1	NEC							
		Baci	< Ne	xt	2	Port				

Import of inventory Procedure

🦲 Importing to	My custom inventory_1			-		×		
Import mode								
Vertical	🖲 Horizontal 🛛 I have a header row							
Provinu of file				2				
CAS	NAME	SMILES	External ID	7				
CAS ~	Chemical Names v	SMILES	Undefined	1				
000051-28-5	2,4-dinitrophenol; Phenol, 2,4-dinitro-	c1(0)c(N(=0)=0)cc(N(=0)=0)cc1	1	Filter:	custo			
000059-50-7	4-Chloro-m-cresol; 3-methyl-4-chlorophenol; Phenol, 4-chloro-3-methyl-; m-Cresol, 4-chlo	c1(Cl)c(C)cc(O)cc1	2			Add as o	rustom id(integer)	- 7/
000065-45-2	2-hydroxybenzamide; Benzamide, 2-hydroxy-; Salicylamide	C(N)(=O)c1c(O)cccc1	3			Add ac	custom id/string)	
000069-72-7	2-hydroxybenzoic_acid; Benzoic acid, 2-hydroxy-; Salicylic acid	C(=O)(O)c1c(O)cccc1	EID1			Aug as	custom iu(string)	
000079-94-7	4,4'-(1-methylethylidene)bis[2,6-dibromophenol]; Phenol, 4,4'-(1-methylethylidene)bis 2,6-c	c1(C(C)(C)c2cc(Br)c(O)c(Br)c2)cc(Br)c(O)c(Br)c1	ED2					
000080-05-7	4,4'-(1-methylethylidene)bisphenol; Phenol, 4,4'-(1-methylethylidene)bis-; Phenol, 4,4'-isopr	c1(C(C)(C)c2ccc(O)cc2)ccc(O)cc1	VOT					
000080-09-1	Phenol, 4,4'-sulfonylbis-; Phenol, 4,4'-sulfonyldi-	c1(S(=O)(=O)c2ccc(O)cc2)ccc(O)cc1	NEC					

- 1. On the second top row are displayed the chemical identifiers as they will be shown in Toolbox (1);
- 2. The last column includes external ID and it is not recognized by the system (the second row is named "Undefined"). Open the drop-down menu and type "custo" (2). Two options appeared:
 - Add as custom id(integer)
 - Add as custom id(string)
- 3. If your external IDs are only numbers (integer) you should select the first option. If your custom IDs are letters only you should select the second option. In case your IDs are combination of letters and numbers, you should select again the second option. In our case external IDs are combination of letters and strings, so second option is selected here (3).
- 4. Click *Import* (4);

4

Import

Import of inventory Procedure



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

View of imported inventory

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



Outlook

- Aim
- Keywords
- Definition of Database and Inventory
- Import:
 - Import of database
 - Vertical import
 - Horizontal import
 - Import of inventory
 - Import of data from IUCLID to TB
 - Export Data matrix

IUCLID - background

- IUCLID (International Uniform ChemicaL Information Database) is a software application to record, store, maintain and exchange data on intrinsic and hazard properties of chemical substances. It is a key software application for both regulatory bodies and the chemical industry where it is used in the implementation of various regulatory programmes
- QSAR Toolbox is connected to IUCLID (IU) through WebServices. Experimental data is allowed to be imported from IU to Toolbox only.
- Prediction obtained in the Toolbox could also be exported to IU. An example is shown in tutorial:

Predicting aquatic toxicity to daphnia by trend analysis.pdf

Import of data from IUCLID to Toolbox

Simplified UI

Delete

Export

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IUCLID6

- 1. Go to **Data** module (1);
- 2. Click on *IUCLID6* button (2);
- 3. Select New database (3);
- 4. Write the database name (4);
- 5. Click on *Next* (5).

Note: Importing data from IUCLID requires:

- 1) To have access to IU 6.3 (or 6.4)
- 2) IU web services to be running
- 3) To have a substance in the running IU server



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Import

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Data

Gather

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IUCLID6

Documents



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Report

Import of data from IUCLID to Toolbox

- 1. Write *IUCLID Server name* (1);
- 2. Next Port(2);
- 3. Next Username (3);
- 4. Password: root(4);
- 5. Click on <u>*Next*</u>(5).

Note:

In case you don't know your IUCLID account, please ask your administrator.

Connect to an IUCLID6 server
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
IUCLID Server: localhost v 8080
Username: Password: 4
Test connection options
5
Cancel < Back Next > Finish

Import of data from IUCLID to Toolbox

- Click Get All Substances (1).
- Select the substance which you would like to import in the Toolbox (2)
- 3. Finish (3)

0		_		×
CAS# Name	Owner	_	See	arch
	Get All Substances			
Show substances from dos	iers 🗌 Import all "Type of inforr	nation" as measu	ired data.	
	Cancel < Back	Next >	Finis	sh

D			-		×
CAS#	Name	Owner			
51-55-8	Test substance	Laboratory of	Mathematic		
		2			
		2			
CAS					Search
Name					Search
	Ge	t All Substances			
Show subst	ances from dossiers 📃 li	mport all "Type of ir	nformation" as meas	ured dat	a. 3
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Import of data from IUCLID to Toolbox

QSAR Toolbox 4.4 [Document 2]	
	H Data Gap Filling > Report
Data Import Export Delete Import Import Import Import Gather Import IUCLID6 Database Inventory	
Occuments ✓ Document 1 # [C: 1;Md: 0;P: 0] CAS: 120832 ➢ Document 2	
	CAS# Name Owner 51-55-8 Test substance Laboratory of Mathematic
Databases Options a 0 Selected f Select All Invert a Physical Chemical Properties • Chemical Reactivity COLIPA ECHA REACH • E CHA REACH • • E SH Experimental pKa • • GSH Experimental pKa • • B GSH Experimental RCS0 • • Phys-chem EPISUITE • • B bioaccumulation Canada • • B bioaccumulation filsh CEFIC LRI • • B bioaccumulation NITE • • B bioaccumulation Filsh CEFIC LRI • •	CAS Import completed! Name CAS Name CAS Show substances from dossiers Import all "Type of information" as measured data. Cancel < Back Next > Finish Cancel import
Options ∠ 0 Selected f Select All Canada DSL Invert COSING ECOSING DSSTOX ECHA PR EINECS HPVC OECD	port completed(1).

Import of data from IUCLID to Toolbox



- 1. Click on *Input* module, then click on *Database* button (1)
- 2. Select the imported IUCLID database (in our case named Test import database) in order to load it in the data matrix (2) and click <u>OK</u> (3).

Outlook

- Aim
- Keywords
- Definition of Database and Inventory
- Import data:
 - Import of database
 - Vertical import
 - Horizontal import
 - Import of inventory
 - Import IUCLID
- Export data

Export Types of export

- Data could be exported via:
 - Data matrix export
 - IUCLID Export*

*IUCLID Export is allowed for predictions only. An example of export is shown in the tutorial "Predicting aquatic toxicity to daphnia by trend analysis"

Data matrix export:

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

Two options to export:

- Export data from a row
- 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.

Data matrix Export: Collecting data



- 3. Select from Database (3);
- 4. Select <u>Aquatic OASIS(4);</u>
- 5. Click on <u>OK(5)</u>.

Data matrix Export: Collecting data



Data matrix Export: Collecting data

- The following steps need to be executed to collect the experimental data for the chemicals available on data matrix
- 1. Go to **<u>Data</u>** module (1);
- Select <u>Aquatic OASIS</u>
 (2);
- 3. Click on *Gather* (3);
- 4. Click on <u>OK</u> in the Read Data window (4).
- Click on <u>OK</u> in the information window (5).





The OECD (Q)SAR Toolbox for Grouping Chemicals into Categories

- Keep the Aquatic toxicity level selected (1); Unselect Sediment and Terrestrial toxicity (not shown)
- Expand the Profiling level

 (2) and then select Acute
 aquatic toxicity MOA by
 OASIS;
- 3. Click on *Export* (3).

Matrix export	—		\times
Select All Unselect All			
Filter			
 Structure info Parameters Physical Chemical Properties Environmental Fate and Transport Cotoxicological Information Aquatic Toxicity Sediment Toxicity Terrestrial Toxicity Human Health Hazards Profiling Endpoint Specific Acute aquatic toxicity MOA by OASIS 			
Export detailed metadata Distribute profiling results Remove empty columns Do not multiply chemical ID	[Expo	3 ort

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File <u>n</u> ame: Export data		~
Save as type: CSV Files (*.csv)		~
Hide Folders		ave Cancel



- 1. Specify the name of the file (e.g. Export data) (1). The file is saved in *csv* format.
- 2. Click on <u>Save (</u>2).
- 3. Click <u>OK</u> in the information message (3).

Horizontal export

		1			2			3			4					[5	
1	A B		D	E	F F	G	Н		J	K		Μ	Ν	0	Р	Q	R	
#	CAS Nu	mb Chemical	r SMILES	EndpointPath	Endpoint	Value.Mean	/Value.	Jni Value.Scale	Fest organ Class	s F	Phylum	Kingdom	Effect	Duration.M	Duration.l	Acute aquatic toxicity N	OA by OASI	s
	98-01-1	2-furaldel	nO=Cc1ccco1	Ecotoxicologica	IGC50	145.42563	mg/L	Mass concentrati	Fetrahyme Ciliat	tea (Ciliophora	Protozoa	Growth	48	h	Aldehydes		
	98-01-1	2-furaldel	O=Cc1ccco1	Ecotoxicologica	LC50	10.535155	mg/L	Mass concentrati	Poecilia re Actir	nopter (Chordata (Animalia (Mortality	96	h			
	98-01-1	2-furaldel	n O=Cc1ccco1	Ecotoxicologica	LC50	20.541916	mg/L	Mass concentrati	Pimephale Actir	nopter (Chordata <mark>(</mark>	Animalia (Mortality	96	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	LC50	17.138008	mg/L	Mass concentrati	Daphnia m Bran	nchiop A	Arthropod	Animalia (Mortality	48	h	Phenols and Anilines		
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	EC50	411.11218	mg/L	Mass concentrati	Escherichi Gam	nmapr F	Proteobac	Bacteria (b	Growth	12	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	LC50	94.180359	mg/L	Mass concentrati	Rana japoi Amp	ohibia (Chordata <mark>(</mark>	Animalia (Mortality	12	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	EC50	12.415389	mg/L	Mass concentrati	Daphnia <mark>m</mark> Bran	nchiop A	Arthropod	Animalia (Intoxicatio	48	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	IGC50	163.66671	mg/L	Mass concentrati	Fetrahyme Ciliat	tea (Ciliophora	Protozoa	Growth	48	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	рТ	2.7161912	mg/L	Mass concentrati	/ibrio fiscl Und	efined l	Jndefined	Undefined	Physiology	0.5	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	рТ	2.3657037	mg/L	Mass concentrati	/ibrio fiscl Und	efined l	Jndefined	Undefined	Physiology	0.5	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	LC50	19.677066	mg/L	Mass concentrati	Poecilia re Actir	nopter (Chordata (Animalia (Mortality	96	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	LC50	16.366671	mg/L	Mass concentrati	Pimephale Actir	nopter (Chordata (Animalia (Mortality	96	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	EC50	8.2027663	mg/L	Mass concentrati	Daphnia <mark>m</mark> Bran	nchiop A	Arthropod	Animalia (Intoxicatio	24	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	EC50	0.3191246	mg/L	Mass concentrati	Daphnia <mark>m</mark> Bran	nchiop A	Arthropod	Animalia (Intoxicatio	24	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	рТ	2.3118537	mg/L	Mass concentrati	/ibrio fiscl Und	efined l	Jndefined	Undefined	Physiology	0.25	h			
	2 106-44	5 p-cresol;4	Cc1ccc(O)cc	Ecotoxicologica	рТ	2.0604417	mg/L	Mass concentrati	/ibrio fiscl Und	efined l	Jndefined	Undefined	Physiology	0.0834	h			
	3 589-34	4 3-Methylk	n CCCC(C)CC	Ecotoxicologica	MRC50	24.035596	mg/L	Mass concentrati	Hydractini Hydi	rozoa (Cnidaria (c	Animalia (Mortality	3	h	Basesurface narcotics		
	4 28575-	17 diethylbip	CCc1ccc(cc1	Ecotoxicologica	LC50	8.181733	mg/L	Mass concentrati	Dryzias lat Actir	nopter (Chordata (Animalia (Mortality	48	h	Basesurface narcotics		
	586-98	1 2-hydroxy	OCc1ccccn1	Ecotoxicologica	IGC50	3531.2345	mg/L	Mass concentrati	Tetrahyme Ciliat	tea (Ciliophora	Protozoa	Growth	48	h	Basesurface narcotics		

The file can be opened in excel. It contains the following main sections: <u>chemical identity of each chemical</u> (red, 1), <u>endpoint</u> (pink, 2) <u>experimental</u> <u>data and unit</u> (purple, 3), metadata (blue, 4), profiler results (green, 5). Here, if the chemical has several experimental data each one is listed on a separate row (e.g. CAS 98-01-1).

Additional option to export profiling results in a format approved by EFSA

- Keep the Aquatic toxicity level selected (1); Unselect Sediment and Terrestrial toxicity (not shown)
- Expand the Profiling level (2) and then select Acute aquatic toxicity MOA by OASIS;
- 3. Check Distribute profiling results
- 4. Click on *Export* (3).

For more details, see next slide.

Matrix export	_		×
Select All Unselect All			
Filter			
 Structure info Parameters Physical Chemical Properties Environmental Fate and Transport Ecotoxicological Information Aquatic Toxicity Sediment Toxicity Terrestrial Toxicity Human Health Hazards Profiling Endpoint Specific Acute aquatic toxicity MOA by OASIS 			
Export detailed metadata Distribute profiling results Remove empty columns Do not multiply chemical ID	[Exp	ort



This is a new template where each chemical is listed in a separate row, while the different profiling results identified for the list of analyzed chemicals appear as captions in separate columns. Indication for the chemicals that have specific profiling results according to the applied profiler is labeled with "X" sign.

Congratulations!

- You have now been introduced to the functionality of import and export of data;
- You have now been introduced to the import of data from IUCLID to the Toolbox;
- Note, proficiency comes with practice!