

Export functionality in Toolbox

There are two type of export **Horizontal** and **Vertical**.

1. Horizontal export:

- The layout of the horizontal export is:
 - **Data records (experimental data) are exported in rows**
 - **Multiple data records for a single chemicals are presented in separate rows**

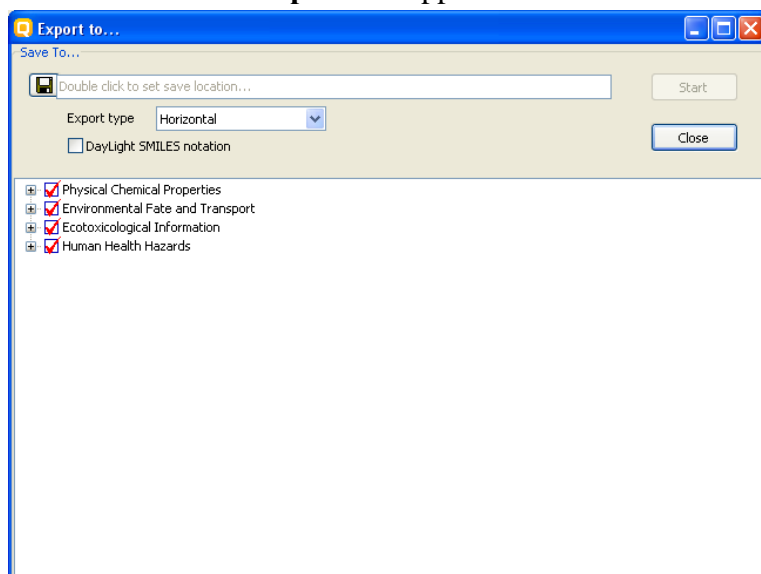
Once you are in the Endpoint section and experimental data are extracted and assigned to the chemicals on the data matrix, click the active **Export** button:

The screenshot shows the QSAR Toolbox 2.1.2.939 interface. The 'Endpoint' section is active, displaying a tree structure with various categories like Substance Identity, Physical Chemical Properties, Environmental Fate and Transport, Ecotoxicological Information, and Human Health Hazards. The 'Export' button is highlighted in red. A text box states: "Experimental data for chemicals from data matrix are extracted and assigned to the leaves of the endpoint tree."

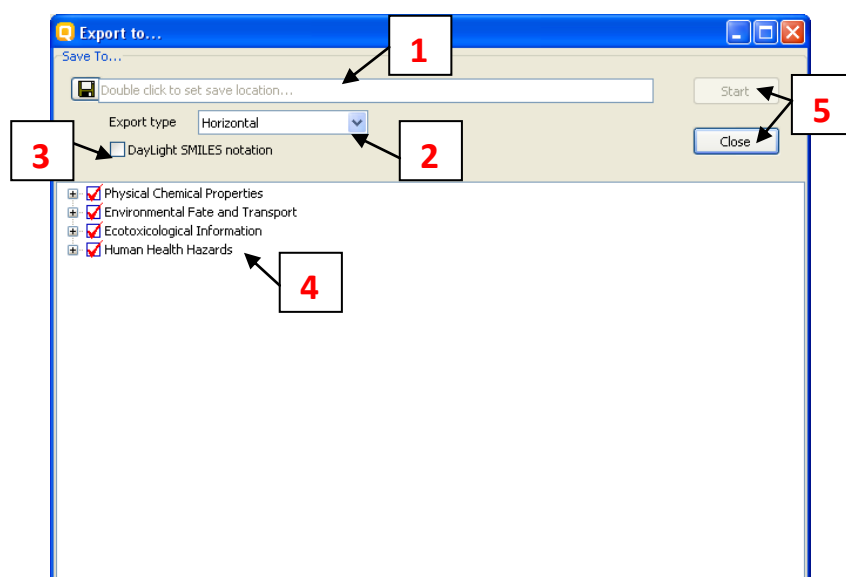
Click the **Export** button:

This is a close-up screenshot of the QSAR Toolbox software interface, focusing on the 'Export' button which is highlighted with a red box. The interface shows the 'Data' and 'Import' sections, with the 'Export' button clearly visible and highlighted.

Then the window “**Export to**” appears:



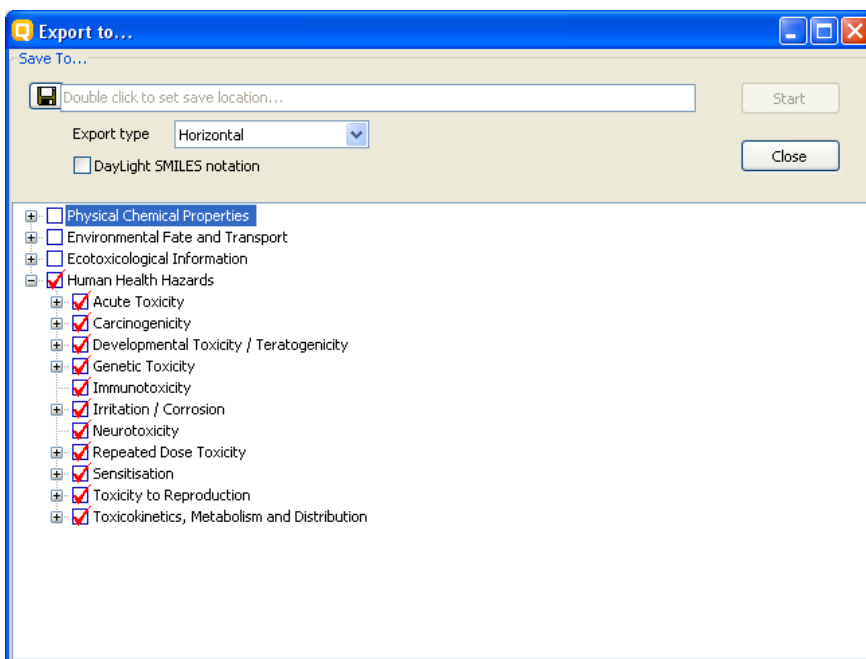
Description of fields of **Export to** window:



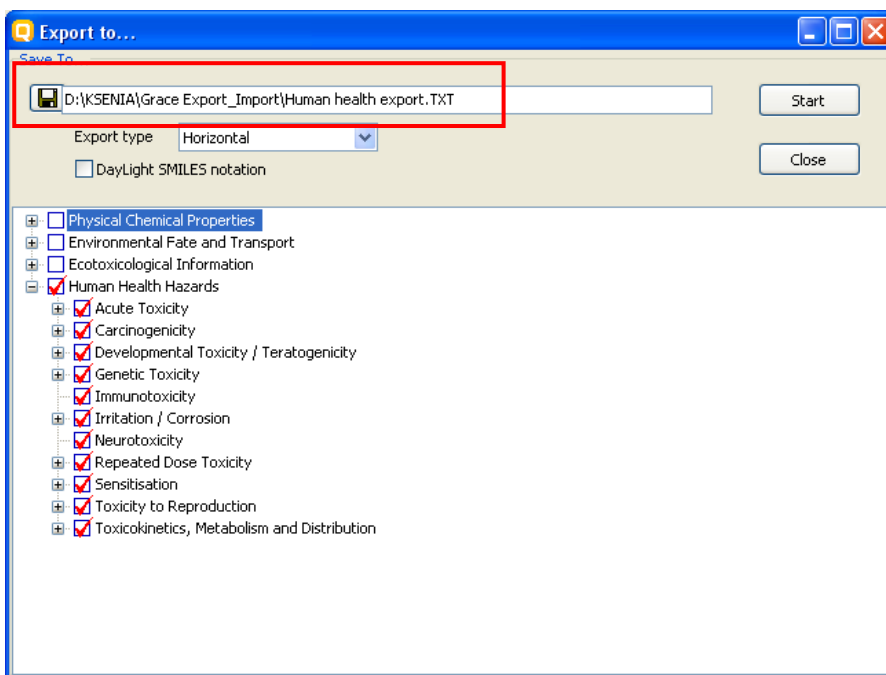
1. Fields where the user should specify the name of the file and file location
2. Pop-up menu to select horizontal or vertical type export
3. Box where the user could specify if the exported SMILES is in Daylight format
4. Endpoint tree – the experimental data are assigned to the leaves of the endpoint tree
5. Start and Close buttons

Example with Horizontal export:

Select nodes with data for export that you are interest in (e.g human health hazard):

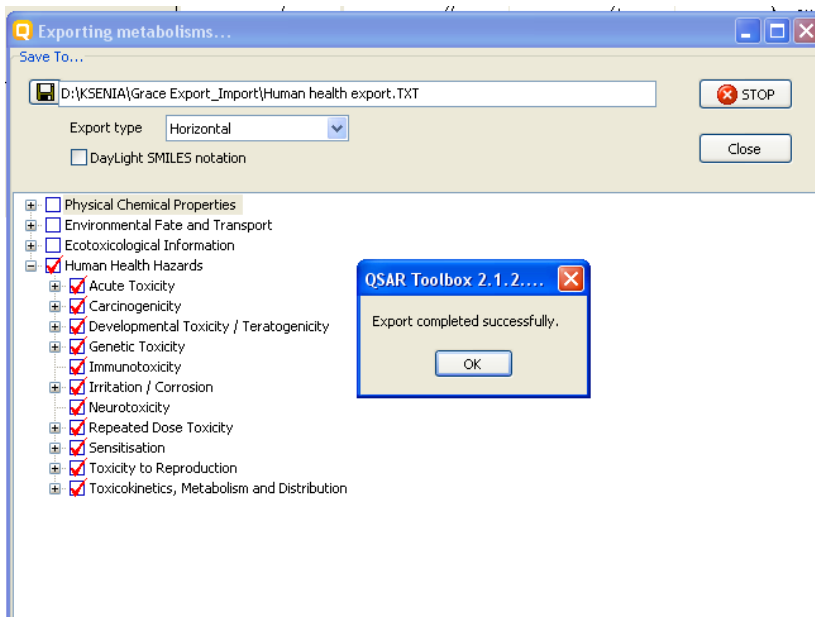


Specify the file and folder for export:

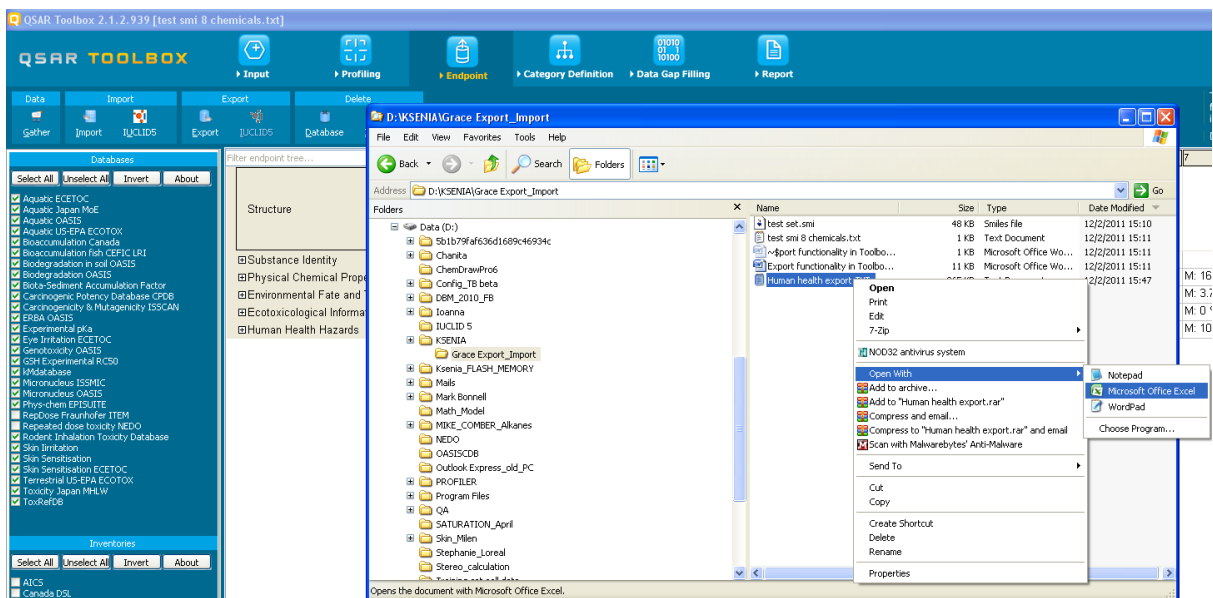


Specify the type of export. In this case horizontal type is selected

Click **Start** button, when the export is ready close the appeared message:



Open the saved file via excel:



Overview of excerpt from the saved excel file:

CAS	NAME	SMILES	Data	Duration	Endpoint End	Unit	Endpoint	Database	QA (CAS-2 Assigned)	Age	Assign	Author	Control Ty	Creation Date	Date Publish	Document	Dose	Nur	Effect	Exposure	Measured	Meas
66-25-1	hexaldehyd	C(O)CCCCC																				
107-02-8	2-propenyl C(=O)C=C		2 mg/kg/d	22 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		7/24/2006	11/12/2008	95	4	Reproduct	gavage	NC	Prog	
107-02-8	2-propenyl C(=O)C=C		2 mg/kg/d	3 day(s)	LOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	X	Parent, R. Concurrer		7/24/2006	11/12/2008	95	4	Growth	gavage	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		0.75 mg/kg/d	3 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	X	Parent, R. Concurrer		7/24/2006	11/12/2008	95	4	Growth	gavage	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		0.75 mg/kg/d	12 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		7/24/2006	11/12/2008	95	4	Developm	gavage	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		2 mg/kg/d	22 day(s)	LOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		7/24/2006	11/12/2008	95	4	Developm	gavage	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		0.75 mg/kg/d	22 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		7/24/2006	11/12/2008	95	4	Developm	gavage	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		0.5 mg/kg/d	12 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	X	Parent, R. Concurrer		7/24/2006	11/12/2008	95	6	Reproduct	gavage	NC	Reso	
107-02-8	2-propenyl C(=O)C=C		0.5 mg/kg/d	22 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		7/24/2006	11/12/2008	95	6	Developm	gavage	NC	Deve	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	70 day(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES	58 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Reproduct	intraperic	NC	Gest.	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	130 day(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES	58 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Populatio	intraperic	NC	Viabi	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	70 day(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES	58 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Growth	intraperic	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	130 day(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES	58 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Reproduct	intraperic	NC	Ferti	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	22 day(s)	LOEL	mg/kg	Human He Terrestria	High Qual	YES	58 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Growth	intraperic	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	1 day(s)	LOEL	mg/kg	Human He Terrestria	High Qual	YES	22 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Growth	intraperic	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	125 day(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES	22 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Populatio	intraperic	NC	Viabi	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	125 day(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES	22 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Reproduct	intraperic	NC	Ferti	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	125 day(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES	22 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Reproduct	intraperic	NC	Gest.	
107-02-8	2-propenyl C(=O)C=C		6 mg/kg	85 day(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES	22 d	X	Parent, R. Concurrer		7/24/2006	9/21/2006	100	4	Growth	intraperic	NC	Weig	
107-02-8	2-propenyl C(=O)C=C		0.5 mg/kg	2 hour(s)	NOEL	mg/kg	Human He Terrestria	High Qual	YES		X	Green, M. Multiple t		7/24/2006	9/21/2006	92	7	Physiolog	intraperic	NC	Blood	

Each data is presented on a separate row, so for a single chemical there could be more than one row with experimental data (e.g CAS 107-02-8 have more than one experimental data (see red colored shape)):

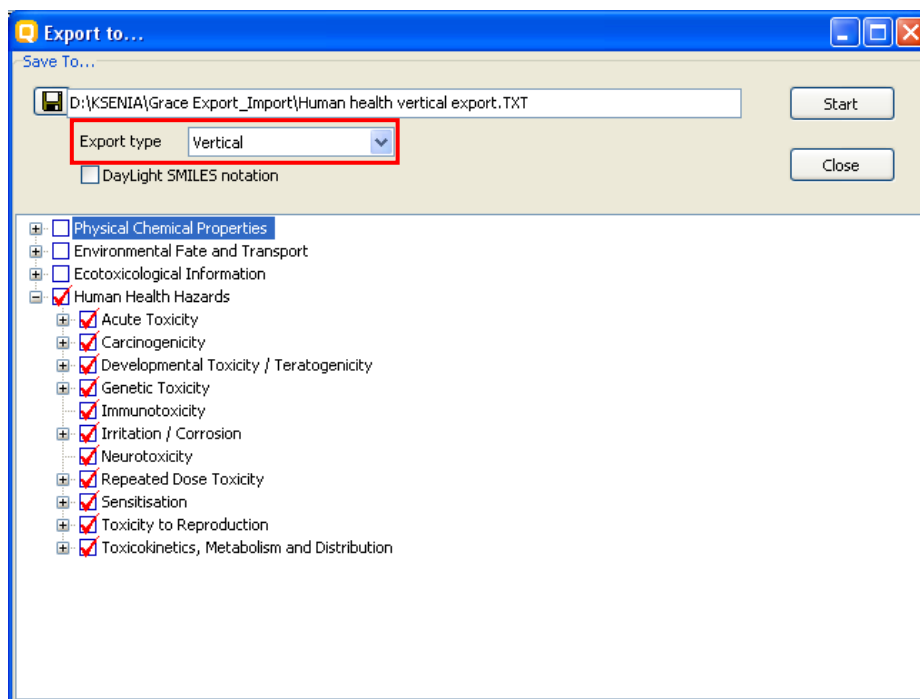
CAS	NAME	SMILES	Data	Duration	Endpoint End	Unit	Endpoint	Database	QA (CAS-2 Assigned)	Age	Assign	Author	Control Ty	Cr
66-25-1	hexaldehyd	C(O)CCCCC												
107-02-8	2-propenyl C(=O)C=C		2 mg/kg/d	22 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		
107-02-8	2-propenyl C(=O)C=C		2 mg/kg/d	3 day(s)	LOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	X	Parent, R. Concurrer		
107-02-8	2-propenyl C(=O)C=C		0.75 mg/kg/d	3 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	X	Parent, R. Concurrer		
107-02-8	2-propenyl C(=O)C=C		0.75 mg/kg/d	12 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		
107-02-8	2-propenyl C(=O)C=C		2 mg/kg/d	22 day(s)	LOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		
107-02-8	2-propenyl C(=O)C=C		0.75 mg/kg/d	22 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		
107-02-8	2-propenyl C(=O)C=C		0.75 mg/kg/d	22 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	X	Parent, R. Concurrer		
107-02-8	2-propenyl C(=O)C=C		0.5 mg/kg/d	22 day(s)	NOEL	mg/kg/d	Human He Terrestria	High Qual	YES	>5 mo	R	Parent, R. Concurrer		

2. Vertical export

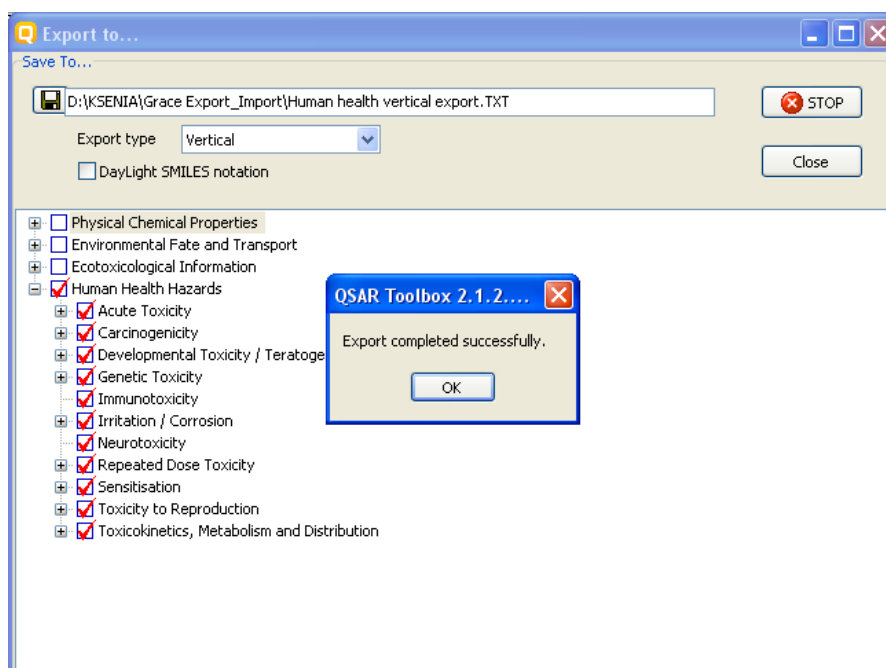
- The layout of the vertical export is:
 - Data records (experimental data) are exported in columns. Column heading contain metadata labels
 - Multiple records for a single chemical are presented in a single row

Example with Vertical export:

The only difference with horizontal export is the type of selected export:



Click **Start** button, when the export is ready close the appeared message:



Overview of excerpt from the saved vertical file:

91	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	
92					Test guideline, qualifier																				
93					Type of inhalation exposure																				
94					Vehicle																				
95					ISSN																				
96					Results Remarks																				
97					Organ/Tissue																				
98					Overall																				
99					Institution and country																				
100					Organ																				
101					Test method / Data source																				
102					StudyType																				
103					OECD SIDS Dossier label																				
104					Type of coverage																				
105					NT Technical Report																				
106					Database affiliation																				
107					Tissue analyzed																				
108	#	CAS	NAME	SMILES																					
109	1	66-25-1	hexaldehyd C(=O)CCCCC																						
110	2	107-02-8	2-propeni C(=O)C=C		2 mg/kg/c2 mg/kg/c0.75 mg/k	0.75 mg/k	2 mg/kg/c0.75 mg/k	0.5 mg/k	0.5 mg/k	0.5 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	6 mg/kg	0.5 mg/kg	0.5
111	3	107-22-2	glyoxal et C(=O)C=O																						
112	4	107-86-8	3-methyl C(C)(C)C=O																						
113	5	111-30-8	pentaned C(=O)CCCC=O																						
114	6	50-00-0	formalin f C=O																						
114	7	98-01-1	furfural 2, C(C=O)-CC=CO1																						

In this type of export the first columns contains metadata information, while the chemicals with their substance information and experimental data are presented after the columns with metadata.

Note: If the experimental data prepared for export contains diversity of metadata, the horizontal type of export is recommended.

3. Export of experimental data from a row from data matrix:

There is an option where the software could export data from a row (e.g export skin sensitization exp.data):

The screenshot shows the QSAR Toolbox interface. On the left is a 'Databases' list. The main area displays an 'Endpoint tree' on the left and a data matrix on the right. The 'Skin' endpoint is highlighted in red in the tree. The data matrix shows results for various chemicals across different endpoints.

Endpoint	Chemical 1	Chemical 2	Chemical 3	Chemical 4	Chemical 5	Chemical 6	Chemical 7
Substance Identity	(744) M: 131 °C, 4.41, 1...	M: 52.6 °C, -0.01, ...	M: 50.4 °C, 15 °C, ...	M: 134 °C, 925 mg/l...	M: 188 °C, 0.6 mm Hg...	M: -19.1 °C, 0.36, ...	M: 162 °C, 0.41, -3...
Physical Chemical Properties	(6/21) M: 2.13E-4 atm-m3...	M: 344, 1.22E-4 at...	M: 3.33E-9 atm-m3...	M: 2.38E-11 cm3/l...	M: 3.37E-7 atm-m3...	M: 3.77E-6 atm-m3...	M: 3.77E-6 atm-m3...
Environmental Fate and Transport	(7/1347) M: 22(21-23) mg/L, ...	M: -100 %, 10 %, 2...	M: 550 mg/L, 230 ...	M: 68.4 mg/L	M: 200-1.6E3 mg/L...	M: 224(180-321) m...	M: 0 %, 0.01 ml/or...
Ecotoxicological Information							
Human Health Hazards							
Acute Toxicity	(3/18)	M: 13.9 mg/kg, =0...				M: 340(270-440) m...	M: 1.04E3 mg/L
Carcinogenicity	(4/37)	M: Negative, Negati...			M: Negative, Negative	M: Positive, Positiv...	M: Positive, Positiv...
Developmental Toxicity / Teratogenicity					M: Positive, Positiv...	M: Positive, Positiv...	M: Positive, Positiv...
Genetic Toxicity	(5/49)	M: Negative, Negati...	M: Positive		M: Positive, Positiv...	M: Positive, Positiv...	M: Positive, Positiv...
Immunotoxicity							
Irritation / Corrosion	(1/1)				M: <2		
Neurotoxicity							
Repeated Dose Toxicity	(3/75)	M: 2 mg/kg/d, 2 mg...				M: 5 %, 1 %, 1 %	M: 100 mg/kg, 200 ...
Sensitisation							
Skin							
In Vivo	(3/13)		M: Strongly positive		M: Positive, Strongl...	M: Positive, Strongl...	M: Positive, Strongl...
Skin Sensitisation	(4/4)						M: 0
Toxicity to Reproduction							
Toxicokinetics, Metabolism and Distribution							

Once you are open the endpoint tree to the leaf with data which you want to export, right click over the endpoint tree. Then select export:

QSAR Toolbox 2.1.2.939 [test smi 8 chemicals.txt]

QSAR TOOLBOX

Input Profiling Endpoint Category Definition Data Gap Filling Report

Data Import Export Delete

Gather Import IUCLID5 Export IUCLID5 Database Inventory

The OECD QSAR Tool for Grouping Chemicals into Categories
Developed by ILMC

Select All Unselect All Invert About

Filter endpoint tree...

Structure

1	2	3	4	5	6	7
<ul style="list-style-type: none"> Substance Identity Physical Chemical Properties Environmental Fate and Transport Ecotoxicological Information Human Health Hazards <ul style="list-style-type: none"> Acute Toxicity (3/16) Carcinogenicity (4/37) Developmental Toxicity / Teratogenicity Genetic Toxicity (5/49) Immunotoxicity Irritation / Corrosion (1/1) Neurotoxicity Repeated Dose Toxicity (3/75) Sensitisation <ul style="list-style-type: none"> Skin In Vivo <ul style="list-style-type: none"> Skin Sensitisation Toxicity to Reproduction Toxicokinetics, Metabolism and Distribution 						
(7/44) M: 131 °C, 4.41, 1...	M: 52.6 °C, -0.01, ...	M: 50.4 °C, 15 °C, ...	M: 134 °C, 925 mg/...	M: 188 °C, 0.6 mm Hg	M: -19.1 °C, 0.35, ...	M: 162 °C, 0.41, -3...
(6/21) M: 2.13E-4 atm-m3...	M: 344, 1.22E-4 at...	M: 3.33E-9 atm-m3...	M: 2.38E-11 cm3/...	M: 3.37E-7 atm-m3...	M: 3.77E-6 atm-m3...	M: 0 %, 0.01 ml/or...
(7/1347) M: 22(21-23) mg/L, ...	M: -100 %, 10 %, 2...	M: 550 mg/L, 230 ...	M: 68.4 mg/L	M: 200-1.6E3 mg/L...	M: 224(180-321) m...	M: 0 %, 0.01 ml/or...
					M: 340(270-440) m...	M: 1.04E3 mg/L
				M: Negative, Negati...	M: Positive, Positiv...	M: Positive, Positiv...
	M: Negative, Negati...	M: Positive		M: Positive, Positiv...	M: Positive, Positiv...	M: Positive, Positiv...
				M: <2		
					M: 5 %, 1 %, 1 %	M: 100 mg/kg, 200 ...
			M: Strongly positive	M: Positive, Strongl...	M: Positive, Strongl...	M: 0

Hide Show hidden Collapse all Sort (targets priority) Sort Function... Filter effects Set tree hierarchy...

Export CAS list Export

7 test smi 8 chemicals.txt 1/10

The Export to window appears:

Export to...

Save To...

Double click to set save location...

Start

Export type Horizontal

DayLight SMILES notation

Close

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

In this case the skin data will be exported only.

Note: The red thick mark should be bold like , not . In second case the data will not be exported.