

**WaterTOP COST Action (CA18225)
for Water Taste and Odor Problems**

Risk Assessment approaches for water T&O 16-18 October 2023

Istituto Superiore di Sanità (ISS), Rome, Italy

**Presenter:
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ISS, Department of Environment and Health**



Data Management in the OECD QSAR Toolbox:

- **Import of a database**
- **Import of an inventory**
- **Profiling of a database**
- **Data gathering from other database present in the TB**
- **Applying a QSAR to fill a data gap**
- **Trend analysis to retrieve an endpoint value**
- **Save result as a QSAR model**
- **Data matrix report and export in Excel**

WaterTop database <https://fsbi-db.de/waterTop/>

Export as a CSV file



Leibniz Institute for
Food Systems Biology
at the Technical University of Munich



Water
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Funded by the
European Union

WaterTOP COST
for Water Taste and Odor Problems

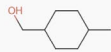
 Completato — 219 kB

 csv(6).csv
Completato — 219 kB

Visualizza tutti i download

Search:

CSV PDF Print Column visibility Show 10 entries

Compound	Structure	MW	Quality	OT	Links	Source
Search Compound	Structure Search Tool	Min Max	Search Quality	Min Max	Search Links	Search Source
(4-Methylcyclohexyl)methanol		128.21	licorice (details)	0.55 µg/L(details)	PubChem:118193 FSBI-DB	Industrial pollution (details)
(E)-2-Decenal		154.25	fishy (details)		PubChem:5283345 FSBI-DB	
(E)-2-Hexenal		98.14	(details)	17 µg/L(details)	PubChem:5281168 FSBI-DB	

WaterTop database <https://fsbi-db.de/waterTop/>

Importance of chemical identifiers: SMILES and CAS number

CSV

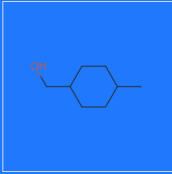
PDF

Print

Column visibility ▾

Show 10 ▾ entries

Search

Compound	Structure	MW	Quality	OT
Search Compound	Structure Search Tool	Min ▾ Max ▾	Search Quality	Min ▾ Max ▾
Search Synonyms	Search Links	Search		
(4-Methylcyclohexyl)methanol		128.21	licorice (details)	0.55 µg/L(details)
Synonyms (4-Methylcyclohexyl)methanol;34885-03-5;4-Methylcyclohexanemethanol;4-Methyl-1-cyclohexanemethanol;3937-49-3;3937-48-2;trans-4-Methyl-1-cyclohexanemethanol;[cis-4-methylcyclohexyl]methanol;cis-4-Methylcyclohexanemethanol;trans-4-Methylcyclohexanemethanol;(trans-4-methylcyclohexyl)methanol;MCHM;Cyclohexanemethanol, 4-methyl-, trans-;4-Methylcyclohexanemethanol, cis-;4-Methylcyclohexylcarbinol;p-Methylcyclohexanemethanol;4-MCHM;4-methylcyclohexane methanol;Cyclohexanemethanol, 4-methyl-, cis-;Cyclohexanemethanol, 4-methyl-;4-Methylcyclohexanemethanol, trans-;64PJK2GTXA;1-(Hydroxymethyl)-4-methylcyclohexane;((1R,4R)-4-Methylcyclohexyl)methanol;9TEH6BZ70K;DTXSID9041813;(1alpha,4alpha)-1-Hydroxymethyl-4-methylcyclohexane;(cis-4-Methylcyclohexyl)methanol;[(1R,4R)-4-METHYLCYCLOHEXYL]METHANOL;UNII-64PJK2GTXA;UNII-9TEH6BZ70K;UNII-1558K6RHM3;Hexahydro-p-methylbenzyl alcohol;HSDB 8182;A13-28423;4-methylcyclohexylmethanol;hexahydro-p-tolyl-carbinol;4-methylcyclohexyl-1-carbinol;SCHEMBL155951;4-methylcyclohexane-1-methanol;SCHEMBL3485266;SCHEMBL8216437;CHEMBL3184778;DTXCID7021813;SCHEMBL13164699;SCHEMBL13755133;DTXSID40274142;DTXSID80274141;CHEBI:157744;1558K6RHM3;trans-(4-methylcyclohexyl)methanol;ZINC2521583;Tox21_301528;(4-Methylcyclohexyl)methanol, (Z)-;AM9715;MFCD00152628;MFCD27997499;MFCD31705071;ZB1702;AKOS009158915;ZINC101975343;ZINC238483660;4alpha-Methylcyclohexane-1beta-methanol;SB84063;SB84581;NCGC00255649-01;AS-59463;AS-79175;BS-41685;(1beta,4beta)-4-Methylcyclohexanemethanol;cis-4-Methyl-1-(hydroxymethyl)cyclohexane;CAS-34885-03-5;DB-086888;CS-0035799;CS-0185316;CS-0205309;FT-0692545;M1412;(1a,4a)-1-Hydroxymethyl-4-methylcyclohexane;D91499;EN300-135109;P18076;EN300-6982689;A1-48509;Q15622250;Q27263773;Q27273174;				
Links PubChem:118193 FSBI-DB				
Source Industrial pollution (details)				



Curation process of CSV data in MS Excel

Compound,"Structure","MW","Quality","OT","Synonyms","Links","Source"										
A	B	C	D	E	F	G	H	I	J	K
Compound,"Structure","MW","Quality","OT","Synonyms","Links","Source"										
1	(4-Methylcyclohexyl)methanol	128.21	green, fatty, cardboard (details)	0.8 µg/L (details)	2-OCTENAL					
2	(E)-2-decenal	154.25	fishy (details)							
3	(E)-2-hexenal	98.14	(details)	17 µg/L (details)	trans-2-Hexenal					
4	(E)-2-nonenal	140.22	green, fatty, cardboard (details)	0.8 µg/L (details)	trans-2-Nonenal					
5	(E)-2-octenal	126.2	green-leafy, orange (details)	µg/L (details)	trans-2-Octenal					
6	(E)-beta-ionone	192.3	violet, flowery (details)	0.007 µg/L (details)	BETA-IONONE					
7	(E,E)-2,4-heptadienal	110.15	rancid fish, fishy, oily (details)	5 µg/L (details)	2,4-HEPTADIENAL					
8	(E,Z)-2,6-nonadienal	138.21	cucumber-like, grassy (details)	0.08 µg/L (details)	trans-2,cis-6-Nonadienal					
9	(R)-limonene	136.23	citrus (details)		D-Limonene					
10	(Z)-3-hexenol	100.16	grassy(green, sharp) (details)	70 µg/L (details)	cis-3-Hexen-1-ol					
11	(Z)-3-hexenyl acetate	142.2	grassy, green (details)	1 µg/L (details)	cis-3-Hexenyl acetate					
12	124-Tribromo-3-methoxybenzene	344.83	earthy/musty		2,3,6-tribromoanisole					
13	124-Trimethylbenzene	120.19			1,2,4-TRIMETHYLBENZENE					
14	1,3-Dibromo-5-chloro-2-methoxybenzene	300.37			1,3-dibromo-5-chloro-2-methoxybenzene					
15	1,3-Dioxane, 2,5,5-trimethyl	130.18			2,5,5-trimethyl-1,3-dioxane					
16	1,3-Dioxane, 2,5,5-trimethyl	130.18			2,5,5-trimethyl-1,3-dioxane					
17	13-Octadiene	110.2	earthy, mushroom (details)	5600 µg/L (details)	1,3-Octadiene					
18	13-Pentadiene	68.12	petroleum. hydrocarbon. varnish (details)		1,3-PENTADIENE					

Compound	Structure	MW	Quality	OT	Synonyms
(4-Methylcyclohexyl)methanol		128.21	licorice (details)	0.55 µg/L (details)	(4-Methylcyclohexyl)methanol
(E)-2-decenal		154.25	fishy (details)		trans-2-Decenal
(E)-2-hexenal		98.14	(details)	17 µg/L (details)	trans-2-Hexenal
(E)-2-nonenal		140.22	green, fatty, cardboard (details)	0.8 µg/L (details)	trans-2-Nonenal
(E)-2-octenal		126.2	green-leafy, orange (details)	µg/L (details)	trans-2-Octenal
(E)-beta-ionone		192.3	violet, flowery (details)	0.007 µg/L (details)	BETA-IONONE
(E,E)-2,4-heptadienal		110.15	rancid fish, fishy, oily (details)	5 µg/L (details)	2,4-HEPTADIENAL
(E,Z)-2,6-nonadienal		138.21	cucumber-like, grassy (details)	0.08 µg/L (details)	trans-2,cis-6-Nonadienal
(R)-limonene		136.23	citrus (details)		D-Limonene
(Z)-3-hexenol		100.16	grassy(green, sharp) (details)	70 µg/L (details)	cis-3-Hexen-1-ol
(Z)-3-hexenyl acetate		142.2	grassy, green (details)	1 µg/L (details)	cis-3-Hexenyl acetate
124-Tribromo-3-methoxybenzene		344.83	earthy/musty		2,3,6-tribromoanisole
124-Trimethylbenzene		120.19			1,2,4-TRIMETHYLBENZENE
1,3-Dibromo-5-chloro-2-methoxybenzene		300.37			1,3-dibromo-5-chloro-2-methoxybenzene
1,3-Dioxane, 2,5,5-trimethyl		130.18			2,5,5-trimethyl-1,3-dioxane
1,3-Dioxane, 2,5,5-trimethyl		130.18			2,5,5-trimethyl-1,3-dioxane
13-Octadiene		110.2	earthy, mushroom (details)	5600 µg/L (details)	1,3-Octadiene
13-Pentadiene		68.12	petroleum. hydrocarbon. varnish (details)		1,3-PENTADIENE

Column1	Column2	Column3	Column4
(E)-2-octenal,"", "126.2", "green-leafy, orange (details)", "µg/L (details)", "2-OCTENAL		(E)-Oct-2-enal	(E)-2-Octenal
(E)-beta-ionone,"", "192.3", "violet, flowery (details)", "0.007 µg/L (details)", "79-77-6		14901-07-6	4-(2,6,6-Trimethylcyclohex-1-en-1-yl)
(E,E)-2,4-heptadienal,"", "110.15", "rancid fish, fishy, oily (details)", "5 µg/L (details)", "110-15", "2,4-Hepta-2,4-dienal		trans,trans-2,4-Heptadienal	05/03/4313
(E,Z)-2,6-nonadienal,"", "138.21", "cucumber-like, grassy (details)", "0.08 557-48-2		(2E,6Z)-nona-2,6-dienal	Violet leaf aldehyde
(R)-limonene,"", "136.23", "citrus (details)", "D-Limonene	5989-27-5	(R)-(+)-Limonene	(+)-Limonene
(Z)-3-hexenol,"", "100.16", "grassy(green, sharp) (details)", "70 µg/L (details)", "928-96-1		(Z)-Hex-3-en-1-ol	cis-3-Hexenol
(Z)-3-hexenyl acetate,"", "142.2", "grassy, green (details)", "1 µg/L (details)", "3681-71-8		(Z)-3-HEXENYL ACETATE	[(Z)-hex-3-enyl] acetate
1,2,4-Tribromo-3-methoxybenzene,"", "344.83", "earthy/musty", "2,3 95970-19-7		1,2,4-Tribromo-3-methoxybenzene	SCHEMBL6423974
1,2,4-Trimethylbenzene,"", "120.19", "Pseudocumene	95-63-6	Pseudocumol	
1,3-Dibromo-5-chloro-2-methoxybenzene,"", "300.37", "2,6-dibromo-4-chloroanisole		2,6-dibromo-4-chloroanisole	
1,3-Dioxane, 2,5,5-trimethyl,"", "130.18", "2,5,5-trimethyl-1,3-dioxane, 2,5,5-trimethyl-	766-33-6	AI3-19055	
1,3-Dioxane, 2,5,5-trimethyl,"", "130.18", "2,5,5-trimethyl-1,3-dioxane, 2,5,5-trimethyl-	766-33-6	AI3-19055	
1,3-Octadiene,"", "110.2", "earthy, mushroom (details)", "5600 µg/L (details)", "13-Octadiene	1002-33-1	(3E)-octa-1,3-diene	
1,3-Pentadiene,"", "68.12", "petroleum, hydrocarbon, varnish (details)", "13-Pentadiene	trans-Piperylene	Piperylene	
1,4-Dichlorobenzene,"", "147", "almond, sweet (details)", "4.5 µg/L (details)", "106-46-7	p-Dichlorobenzene	paradichlorobenzene	
1,8-cineole (eucalyptol),"", "154.25", "camphor,spicy, cool (details)", "12 cineole	1,8-Cineole	470-82-6	
1-octen-3-ol,"", "128.21", "mushroom like (details)", "0.002 µg/L (details)", "3391-86-4	Oct-1-en-3-ol	1-Vinylhexanol	
1-octen-3-one,"", "126.2", "mushroom like (details)", "0.003 µg/L (details)", "Oct-1-en-3-one	4312-99-6	Vinyl amyl ketone	
1-pentanethiol,"", "104.22", "1-Pentanethiol	110-66-7	n-Amyl mercaptan	
1-penten-3-one,"", "84.12", "pungent, rancid, fishy (details)", "1.24 µg/L (details)", "1-Penten-3-one	1629-58-9	Pent-1-en-3-one	
1-propanethiol,"", "76.16", "0.74 µg/L (details)", "1-Propanethiol	Propane-1-thiol	107-03-9	

Retrieval of CAS number from the Synonyms field

Curation process of CSV data in MS Excel

Column1	CAS
D-glucose,"", "180.16", "sweet taste (details)", "", "D-Glc	2280-44-6
decanal,"", "156.26", "fruity, orange (details)", "3 µg/L(details)", "Decanal	112-31-2
Dibenzyl disulfide,"", "246.4", "", "Dibenzyl disulfide	150-60-7
Dibromoindole,"", "274.94", "(details)", "", "dibromoindole	<chem>C1=CC(=C(C=C1Br)Br)N</chem>
Dichloramine T,"", "240.11", "swimming pool (details)", "", "Dichloramine T	473-34-7
Dicyclopentadiene,"", "132.2", "camphor-like, solvent, chemical (details)", "0.01 µg/L(details)", "77-73-6	
Diethyl sulfide,"", "90.19", "swampy, septic (details)", "µg/L(details)", "Diethyl sulfide	352-93-2
diethyldisulfide,"", "122.3", "swampy, septic (details)", "20 µg/L(details)", "DIETHYL DISULFIDE	110-81-6
Diisopropyl sulfide,"", "118.24", "swampy, septic (details)", "µg/L(details)", "Diisopropyl sulfide	625-80-9
dimethyl disulfide,"", "94.2", "septic, garlic, putrid, decaying vegetation (details)", "4 µg/L(details)", "4	624-92-0
dimethyl sulfide,"", "62.14", "rotten cabbage, decaying vegetation, canned corn (details)", "1 µg	75-18-3
dimethyl trisulfide,"", "126.3", "decaying vegetation, swampy, putrid, garlic (details)", "0.01 µg/	3658-80-8
Dimethylamine,"", "45.08", "", "47", "dimethylamine	124-40-3
Dipropyl sulfide,"", "118.24", "swampy, septic (details)", "1.9 µg/L(details)", "Dipropyl sulfide	111-47-7
Epicubenol,"", "222.37", "sweet/spicy (details)", "µg/L(details)", "Epicubenol	19912-67-5
Epoxy-alpha-ionone,"", "206.28", "", "0.007", "epoxy-alpha-ionone	<chem>CC1=CCCC(C1C=CC(=O)C=O)(C)C</chem>
ethanethiol,"", "62.14", "(details)", "µg/L(details)", "Ethanethiol	75-08-1
ethanethiol,"", "62.14", "", "1", "Ethanethiol	75-08-1
Ethanolamine,"", "61.08", "mild ammonia/ fish (details)", "6.5 µg/L(details)", "Ethanalamine	141-43-5
Ethylbenzene,"", "106.16", "plastic, oily, chemical (details)", "150 µg/L(details)", "ETHYLBENZEN	100-41-4
ethylene glycol,"", "62.07", "sweet taste (details)", "", "ETHYLENE GLYCOL	107-21-1
Galaxolide,"", "258.4", "Perfume, Musk, flowery, soapy (details)", "5 µg/L(details)", "Galaxolide	1222-05-5
geosmine,"", "182.3", "earthy (details)", "0.004 µg/L(details)", "GEOSMIN	19700-21-1
heptanal,"", "114.16", "fatty, oily (details)", "2 µg/L(details)", "Heptanal	111-31-7

Retrieval of CAS number from the Synonyms field.

Adding manually SMILES for the substances with no CAS number available

Curation process of CSV data in MS Excel: data matrix is now ready to be imported as a custom user database in OECD QSAR Toolbox

NAME	MW	QUALITY	OT	unit	Synonym	CAS	SMILES	Endpoint
Cubenol	222,37	woody/earthy	µg/L	µg/L	(-)-Cubenol	21284-22-0		Taste and Odor
Cumene	120,19	shoe polish		µg/L	CUMENE	98-82-8		Taste and Odor
D-glucose	180,16	sweet taste		µg/L	D-Glc	2280-44-6		Taste and Odor
decanal	156,26	fruity, orange	3	µg/L	Decanal	112-31-2		Taste and Odor
Dibenzyl disulfide	246,4			µg/L	Dibenzyl disulfide	150-60-7		Taste and Odor
Dibromoindole	274,94			µg/L	dibromoindole		C1=CC(=C(C=C1)Br)Br	Taste and Odor
Dichloramine T	240,11	swimming pool		µg/L	Dichloramine T	473-34-7		Taste and Odor
Dicyclopentadiene	132,2	camphor-like, s	0,01	µg/L	DICYCLOPENTADIENE	77-73-6		Taste and Odor
Diethyl sulfide	90,19	swampy, septic	µg/L	µg/L	Diethyl sulfide	352-93-2		Taste and Odor
diethyldisulfide	122,3	swampy, septic	20	µg/L	DIETHYL DISULFIDE	110-81-6		Taste and Odor
Diisopropyl sulfide	118,24	swampy, septic	µg/L	µg/L	Diisopropyl sulfide	625-80-9		Taste and Odor
dimethyl disulfide	94,2	septic, garlic, p	4	µg/L	Dimethyl disulfide	624-92-0		Taste and Odor
dimethyl sulfide	62,14	rotten cabbage	1	µg/L	dimethyl sulfide	75-18-3		Taste and Odor
dimethyl trisulfide	126,3	decaying vegeta	0,01	µg/L	Dimethyl trisulfide	3658-80-8		Taste and Odor
Dimethylamine	45,08		47	µg/L	dimethylamine	124-40-3		Taste and Odor
Dipropyl sulfide	118,24	swampy, septic	1,9	µg/L	Dipropyl sulfide	111-47-7		Taste and Odor
Epicubenol	222,37	sweet/spicy	µg/L	µg/L	Epicubenol	19912-67-5		Taste and Odor
Epoxy-alpha-ionone	206,28		0,007	µg/L	epoxy-alpha-ionone		CC1=CCCC(C=C1)O	Taste and Odor
ethanethiol	62,14		1	µg/L	Ethanethiol	75-08-1		Taste and Odor
Ethanolamine	61,08	mild ammonia/	6,5	µg/L	Ethanolamine	141-43-5		Taste and Odor

Import of the Excel database in the Toolbox

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Data Import Export Delete

Gather Import IUCLID6 IUCLID6 Database Inventory

Documents

Data import

Databases

Options 65 Selected

Select All Unselect All Invert

- Bioaccumulation fish CE
- Bioconcentration and lo
- Biodegradation in soil O
- Biodegradation NITE
- Biota-Sediment Accumu
- ECHA REACH

Organise by: ?

Dossiers/Sut

Inventories

Options 0 Selected

Select All Unselect All Invert

- AIIC
- Canada DSL
- COSING

Open file

Used separators

Decimal , Thousands .

☐ Import as inventory

Import to None Import title WaterTop

Preview of file

Apri

Config > Examples

Cerca in Examples

Organizza Nuova cartella

Nome	Ultima modifica
9_aldehydes_IGC50_data_create model	11/01/2019 05
HI_BOD_template	06/11/2018 14
HI_Carcinogenicity_template	06/11/2018 14
HI_Ecotox_template	06/11/2018 14
HI_Multiple_endpoints	06/11/2018 14

Nome file:

All Usable Formats

Apri Annulla

Import of the Excel database in the Toolbox: mapping of the data fields to the Toolbox metadata

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Data Import Export Delete

Gather Import IUCLID6 IUCLID6 Database Inventory

The OECD for Group into Categ
Developer

Documents
Data import

Databases
Options 65 Selected
f Select All Unselect All Invert
Bioaccumulation fish CE
Bioconcentration and lo
Biodegradation in soil
Biodegradation NITE
Biota-Sediment Accumu
ECHA REACH
Organise by: 2
Dossiers/Sut

Inventories
Options 0 Selected
f Select All Unselect All Invert
AIIIC
Canada DSL
COSING
DSSTOX
ECHA PR
EINECS
GEO degradation
HPVC OECD

Importing to WaterTop

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

NAME	MW	QUALITY	OT	unit	Synonym	CAS	SMILES	Endpoint
Chemical Names	Undefined	Undefined	Undefined	Data.Unit	Undefined	CAS	SMILES	Endpoint
4-Methylcyclohexyl)methanol	128,21	licorice	0,55	µg/L	4-Methylcyclohexyl)methanol	34885-03-5		Taste and Odor
(E)-2-decenal	154,25	fishy		µg/L	trans-2-Decenal	3913-81-3		Taste and Odor
(E)-2-hexenal	98,14		17	µg/L	trans-2-Hexenal	6728-26-3		Taste and Odor
(E)-2-nonenal	140,22	green, fatty, cardboard	0,8	µg/L	trans-2-Nonenal	18829-56-6		Taste and Odor
(E)-2-octenal	126,2	green-leafy, orange		µg/L	trans-2-Octenal	2548-87-0		Taste and Odor
(E)-beta-ionone	192,3	violet, flowery	0,007	µg/L	BETA-IONONE	79-77-6		Taste and Odor
(E,E)-2,4-heptadienal	110,15	rancid fish, fishy, oily	5	µg/L	2,4-HEPTADIENAL	5910-85-0		Taste and Odor
(E,Z)-2,6-nonadienal	138,21	cucumber-like, grassy	0,08	µg/L	trans-2,cis-6-Nonadienal	557-48-2		Taste and Odor
(R)-limonene	136,23	citrus		µg/L	D-Limonene	5989-27-5		Taste and Odor
(Z)-3-hexenol	100,16	grassy(green, sharp)	70	µg/L	cis-3-Hexen-1-ol	928-96-1		Taste and Odor
(Z)-3-hexenyl acetate	142,2	grassy, green	1	µg/L	cis-3-Hexenyl acetate	3681-71-8		Taste and Odor
1,2,4-Tribromo-3-methoxybenzene	344,83	earthy/musty		µg/L	2,3,6-tribromoanisole	95970-19-7		Taste and Odor
1,2,4-Trimethylbenzene	120,19			µg/L	1,2,4-TRIMETHYLBENZENE	95-63-6		Taste and Odor
1,3-Dibromo-5-chloro-2-methoxybenzene	300,37			µg/L	1,3-dibromo-5-chloro-2-methoxybenzene	174913-44-1		Taste and Odor
1,3-Dioxane, 2,5,5-trimethyl	130,18			µg/L	2,5,5-trimethyl-1,3-dioxane	766-33-6		Taste and Odor
1,3-Octadiene	110,2	earthy, mushroom	5600	µg/L	1,3-Octadiene	1002-33-1		Taste and Odor
1,3-Pentadiene	68,12	petroleum, hydrocarbon, varnish		µg/L	1,3-PENTADIENE	2004-70-8		Taste and Odor
1,4-Dichlorobenzene	147	almond, sweet	4,5	µg/L	1,4-DICHLOROBENZENE	106-46-7		Taste and Odor
1,8-cineole (eucalyptol)	154,25	camphor,spicy, cool	12	µg/L	Eucalyptol	470-82-6		Taste and Odor
1-octen-3-ol	128,21	mushroom like	0,002	µg/L	1-OCTEN-3-OL	3391-86-4		Taste and Odor
1-octen-3-one	126,2	mushroom like	0,003	µg/L	1-OCTEN-3-ONE	4312-99-6		Taste and Odor

Data Input:

Select the custom WaterTop Database now visible in the database tree

QSAR Toolbox 4.6 [Document 1]

QSAR TOOLBOX



► Input



► Profiling



► Data



► Category definition



► Data Gap Filling



► Report

Document



New



Open



Close



Save

Single Chemical



CAS#



Name



Structure



Composition



Select



ChemIDs



Database



Inventory



List



Substructure (SMART)

Documents

Data import

Select database

Options

1 Selected

f

Select All

Unselect All

Invert

About

Options

▲ Taste and Odor

WaterTOP

▲ Physical Chemical Properties

Bioconcentration and logKow NITE

Chemical Reactivity COLIPA

ECHA REACH

Organise by: ?

☐ Dossiers/Substances

☒ Test materials

Experimental pKa

GSH Experimental RC50

Photosensitivity database

Visualisation of the WaterTop Database (SMILES and chemical formulas have been added automatically during import)

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Document Single Chemical Chemical List Search IUCLID search Target Endpoint

New Open Close Save CAS# Name Structure Composition Select ChemIDs Database Inventory List Substructure (SMARTS) Query Simple Advanced Define

The OECD QSAR Toolbox for Grouping Chemicals into Categories
Developed by LMC, Bulgaria

Documents

- Data import
 - [C: 153;Md: 0;P: 0] Water

Filter endpoint tree...

Structure

☐ Structure info

- Additional Ids
- CAS Number
- CAS-SMILES relation
- Chemical name(s)
- Identity
- Molecular formula
- Predefined substance type
- SMILES

☐ Parameters

- 2D
- 3D

☒ Physical Chemical Properties

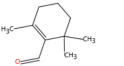
☐ Environmental Fate and Transport

- Bioaccumulation: aquatic
- Bioaccumulation: terrestrial
- Biodegradation
- Photodegradation
- Stability in Water
- Transport and Distribution Between Envir...

☒ Ecotoxicological Information

☐ Human Health Hazards

- Acute Toxicity

1	2	3	4	5	6	7	8
							
EC Number:2070813	EC Number:2039574	EC Number:2145134	EC Number:2050011	EC Number:2010691	EC Number:2222260	EC Number:2330692	EC Number:2242...
432-25-7	112-31-2	1138-52-9	130-89-2	77-92-9	3391-86-4	10028-15-6	4265-25-2
High	High	High	High	High	High	Moderate	High
1-Cyclohexene-1-carb...	1-Decanal	3,5-Bis(1,1-dimethylet...	(87,9R)-6'-methoxycin...	1,2,3-Propanetricarbox...	1-Octen-3-ol	Ozone	2-methyl-1-benz
Sources:9	Sources:17	Sources:12	Sources:10	Sources:26	Sources:15	Sources:15	Sources:5
C10H16O	C10H20O	C14H22O	C20H25ClN2O2	C6H8O7	C8H16O	O3	C9H8O
Mono constituent	Mono constituent	Mono constituent	Multi constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituen
CC1CCCC(C)(C)C=1C=O	CCCCCCCCC=O	CC(C)(C)c1cc(O)cc(c1)...	Cl.COc1ccc2nccc([C@...	OC(=O)CC(O)(CC(O)=...	CCCCC(O)C=C	[O-][O+]=O	Cc1cc2ccccc2o1

QSAR Toolbox 4.6 [Data Import]

Input
Profiling
Data
Category definition
Data Gap Filling
Report

Profiling
Custom profile

Apply
View
New
Delete

The OECD QSAR Toolbox for Grouping Chemicals into Categories

Documents

Data import

[C: 153; M: 0; P: 0] Water

Profiling methods

Options
69 Selected

Select All
Unselect All
Invert

☒ Ultimate biodeg
 ☒ Uncouplers (MITOTOX)
 ☒ Endpoint Specific
 ☒ Acute aquatic toxicity cl
 ☒ Acute aquatic toxicity M
 ☒ Acute Oral Toxicity
 ☒ Aquatic toxicity classifi
 ☒ Bioaccumulation - meta
 ☒ Bioaccumulation - meta
 ☒ Biodegradation fragme
 ☒ Carcinogenicity (genoto

Metabolism/Transformations

Options
0 Selected

Select All
Unselect All
Invert

☒ Documented
 ☐ Observed Mammalian m
 ☐ Observed Microbial met
 ☐ Observed Rat in vivo m
 ☐ Observed rat liver meta
 ☐ Observed Rat Liver S9
 ☒ Simulated
 ☐ Autoxidation simulator
 ☐ Autoxidation simulator (
 ☐ Dissociation simulator
 ☐ Hydrolysis simulator (ac

Filter endpoint tree...

Structure

Hydrolysis half-life (pH 6.5-7.4)

Ionization at pH = 1

Ionization at pH = 4

Ionization at pH = 7.4

Ionization at pH = 9

Protein binding by OASIS

Protein binding by OECD

Protein binding potency Cys (DPRA 13%)

Protein binding potency GSH

Protein binding potency Lys (DPRA 13%)

Toxic hazard classification by Cramer

Ultimate biodeg

Uncouplers (MITOTOX)

Endpoint Specific

Acute aquatic toxicity classification by...

Acute aquatic toxicity MOA by OASIS

Acute Oral Toxicity

Aquatic toxicity classification by ECOS...

Bioaccumulation - metabolism alerts

Bioaccumulation - metabolism half-lives

Biodegradation fragments (BioWIN ML)

Carcinogenicity (genotox and nongenotoxicity)

DART scheme

DNA alerts for AMES, CA and MNT by...

Eye irritation/corrosion Exclusion rules...

Eye irritation/corrosion Inclusion rules...

in vitro mutagenicity (Ames test) alert...

1	2	3	4	5	6	7	8
No value	No value	No value	No value	No value	No value	No value	No value
Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [90.000, 100.000]
Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [90.000, 100.000]	Acidic [0.000, 10.000]	Acidic [90.000, 100.000]	Acidic [0.000, 10.000]
Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [90.000, 100.000]	Acidic [0.000, 10.000]	Acidic [90.000, 100.000]	Acidic [0.000, 10.000]
Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [0.000, 10.000]	Acidic [90.000, 100.000]	Acidic [0.000, 10.000]	Acidic [90.000, 100.000]	Acidic [0.000, 10.000]
Schiff base formation	Schiff base formation	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Schiff Base Formers	Schiff Base Formers	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
DPRA above 21% (DPRA 13%)	DPRA above 21% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)
Moderately reactive (GSH)	Not possible to classify...	Not possible to classify...	Not possible to classify...	Not possible to classify...	Not possible to classify...	Not possible to classify...	Not possible to classify...
DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%)
Low (Class I)	Low (Class I)	Low (Class I)	High (Class III)	Low (Class I)	High (Class III)	High (Class III)	High (Class III)
No data	1 to 10 days	No data	No data	0 to 1 day	1 to 10 days	No data	No data
Undefined	Non concern for unco...	Non concern for unco...	Non concern for unco...	Non concern for unco...	Non concern for unco...	Non concern for unco...	Undefined
Class 3 (unspecific rea...	Class 3 (unspecific rea...	Class 3 (unspecific rea...	Class 3 (unspecific rea...	Class 5 (Not possible t...	Class 3 (unspecific rea...	Class 5 (Not possible t...	Class 1 (narcosis)
Aldehydes	Aldehydes	Phenols and Anilines	Narcotic Amine	Reactive unspecified	Alpha-, Beta-unsaturat...	Reactive unspecified	Basesurface narc...
Not categorized	Not categorized	Not categorized	Not categorized	Not categorized	Not categorized	Not categorized	Not categorized
Vinyl/Allyl Aldehydes	Aldehydes (Mono)	Phenols	Aliphatic Amines	Not Related to an Exis...	Vinyl/Allyl Alcohols	Inorganic Compound	Neutral Organics
-CH2- [cyclic]	-CH2- [linear]	Aromatic alcohol [-OH]	-C=CH [alkenyl hydro...	-CH2- [linear]	-C=CH [alkenyl hydro...	No alert found	Alkyl substituent
Moderate	Fast	Moderate	Fast	Very fast	Fast	Very fast	Fast
-CH2- [cyclic]	-CH2- [linear]	Aromatic alcohol [-OH]	-C=CH [alkenyl hydro...	-CH2- [linear]	-C=CH [alkenyl hydro...	No alert found	Aromatic -CH3
alpha,beta-unsaturate...	Simple aldehyde (Gen...	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Not known precedent...	Not known precedent...	Not known precedent...	Inorganic chemical	Not known precedent...	Not known precedent...	Inorganic chemical	Not known prece...
No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Undefined	Undefined	Group C Melting Point...	Group All Melting Poi...	Group All Melting Poi...	Undefined	Ex	

The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

Developed by LMC, Bulgaria

Data gathering from other Toolbox databases including the imported WaterTop database

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX

Input

Profiling

Data

Category definition

Data Gap Filling

Report

Data

Import

Export

Delete

Gather

Import

IUCLID6

IUCLID6

Database

Inventory

Documents

Data import

[C: 153;Md: 60150;P: 0]

Databases

Options

Select All

Unselect All

Invert

Taste and Odor

WaterTOP

Physical Chemical Properties

Bioconcentration and log K_{ow}

Chemical Reactivity CO₂

ECHA REACH

Organise by

Dossiers/Sut

Inventories

Options

Select All

Unselect All

Invert

ATTC

Canada DSL

COSING

DSSTOX

ECHA PR

EINECS

GEO degradation

USPC

Filter endpoint tree...

Structure

2D

3D

Physical Chemical Properties

Environmental Fate and Transport

Ecotoxicological Information

Aquatic Toxicity

Sediment Toxicity

Terrestrial Toxicity

Human Health Hazards

Acute Toxicity

ADME

Carcinogenicity

Developmental Toxicity / Teratoge...

Genetic Toxicity

In Vitro

In Vivo

Immunotoxicity

Irritation / Corrosion

Neurotoxicity

Photoinduced toxicity

Repeated Dose Toxicity

Sensitisation

ToxCast

Toxicity to Reproduction

Toxicokinetics, Metabolism and Distr...

Taste and Odor

Data analysis: a detailed data matrix is available for each data point

QSAR TOOLBOX

Input

Profiling

Data

Category definition

Data Gap Filling

Report

Gather

Import

IUCLID6

Database

Inventory

Export

Delete

Documents

Data import

[C: 153;Md: 60150;P: 0]

V

Databases

Inventories

f

Select All

Unselect All

Invert

Taste and Odor

Physical Chemical Properties

Environmental Fate and Transport

Ecotoxicological Information

Human Health Hazards

Genetic Toxicity

Immunotoxicity

Irritation / Corrosion

Neurotoxicity

Photoinduced toxicity

Repeated Dose Toxicity

Sensitisation

Toxicity

Toxicity to Reproduction

Toxicokinetics, Metabolism and Distribution

Structure

2D

3D

Organise by

Dossiers/Sub

Inventories

Data import

Taste and Odor

Physical Chemical Properties

Environmental Fate and Transport

Ecotoxicological Information

Human Health Hazards

Genetic Toxicity

Immunotoxicity

Example of filing data gap using QSAR

QSAR toolbox 4.6 [Data import]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Gap Filling Workflow Editor

Trend analysis Read across (Q)SAR Automated Standardized New Import Export Delete

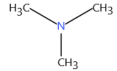
Documents

- Data import
- [C: 153;Md: 60150;P: 1] V

Structure

Filter endpoint tree...

- Solubility in organic solvents / fat sol... 3/12
- Stability in organic solvents and identi... 1/1
- Surface tension 33/60
- Vapour pressure
 - Vapor Pressure 69/69
 - vapour pressure 61/282
- Viscosity 41/130
- Water solubility 82/348
- Environmental Fate and Transport 90/2221
- Ecotoxicological Information
 - Aquatic Toxicity
 - Sediment Toxicity
 - Terrestrial Toxicity
 - Human Health Hazards
 - Acute Toxicity
 - ADME
 - Carcinogenicity
 - Developmental Toxicity / Teratogenicity
 - Genetic Toxicity
 - in Vitro
 - in Vivo
 - Immunotoxicity
 - Irritation / Corrosion
 - Neurotoxicity

36	37	38	39	40
				
	M: 13,5 mN/m			
	M: 1,61E+03 mm Hg	M: 6,4 mm Hg		M: 20,8 mm Hg
	M: 252 Pa	M: 1,09 kPa	Q: 0,424 mm Hg	
	M: 0,177 mPa-s	M: 0,696 mPa-s		
	M: 4,1E+05 mg/L	M: 290 mg/L		M: 1E+06 mg/L
	M: 66 %	M: 8 %		M: 0 %

Details for 5 (Q)SAR models (1 selected)

Checked	#	QSAR name	Endpoint	Provider
☒	1	Selected Vapor Pressure (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA
☐	2	Subcooled liquid Vapor Pressure (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA
☐	3	Vapor Pressure (Antoine Method) (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA
☐	4	Vapor Pressure (Mackay Method) (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA
☐	5	Vapor Pressure (Modified Grain Method) (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA

☐ Show only chemical relevant (Q)SARs
 ☒ Save selection

At this position:

Select a cell with a rigid Automated workflows 7 Standardized workflow8

Example of filing data gap using QSAR: a vapour pressure value example

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Gap Filling Workflow Editor

Documents

Data import

[C: 153;Md: 60150;P: 0]

Filter endpoint tree...

Structure

Physical Chemical Properties

- Autoflammability / Self-ignition te... 52/99 M: 165 °C
- Boiling point 88/279 M: 2,8 °C
- Chemical reactivity 40/95
- Density 60/206 M: 6,27E+05 mg/L
- Dissociation Constant (pKa) 43/742 M: 4,24
- Explosive properties 1/1
- Flammability 16/26 M: Category 1 (flamm...
- Flash point 57/149 M: -12,2 °C M: 31 °C
- Melting / freezing point 96/243 M: -117 (-117÷-117) °C M: -31 °C
- Oxidation reduction potential
- Oxidising properties 1/1
- Particle size 5/12
- Partition Coefficient: 84/270 M: <-3,5 M: ca.0,35
- Solubility in organic solvents / fat sol... 3/12
- Stability in organic solvents and identi... 1/1
- Surface tension 33/60 M: 13,5 mN/m
- Vapour pressure 78/350 M: 252 Pa M: 1,09 kPa
- Viscosity 41/130 M: 0,177 mPa.s M: 0,696 mPa.s
- Water solubility 82/348 M: 4,1E+05 mg/L M: 290 mg/L

Environmental Fate and Transport

Ecotoxicological Information

- Aquatic Toxicity AW SW 104/24068 M: 0,59 mg/L M: 6E-05 mg/L
- Sediment Toxicity 2/21
- Terrestrial Toxicity 67/5182 M: 0,175 % M: 1,15E+03 mg/kg b...

Human Health Hazards

- Acute Toxicity 81/1071 M: 4,84 mg/L M: 11,8 mg/L M: 1,15E+03 mg/kg

Details for 5 (Q)SAR models (1 selected)

Checked	#	QSAR name	Endpoint	Provider
☒	1	Selected Vapor Pressure (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA
☐	2	Subcooled liquid Vapor Pressure (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA
☐	3	Vapor Pressure (Antoine Method) (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA
☐	4	Vapor Pressure (Mackay Method) (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA
☐	5	Vapor Pressure (Modified Grain Method) (EPISUITE)	vapour pressure	United States Environmental Protection Agency (EPA), USA

☐ Show only chemical relevant (Q)SARs ☒ Save selection

Check all Uncheck all Predict Predict all Predict all in domain Gap-filling

Cancel

☐ Surface tension

☒ Vapour pressure ⁵

☐ Viscosity

☐ Water solubility ²

☐ Environmental Fate and Transport

☐ Ecotoxicological Information

☐ Human Health Hazards

- ☐ Acute Toxicity ⁶
- ☐ ADME
- ☐ Carcinogenicity ¹⁸
- ☐ Developmental Toxicity / Teratogenicity ⁵
- ☐ Genetic Toxicity ⁶⁸
- ☐ Immunotoxicity
- ☐ Irritation / Corrosion ⁶
- ☐ Neurotoxicity
- ☐ Photoinduced toxicity ¹
- ☐ Repeated Dose Toxicity ⁴

☐ Hide positions without (Q)SARs

OK Cancel

Trend analysis illustration

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Gap Filling Workflow Editor

Trend analysis Read across (Q)SAR Automated Standardized New Import Export Delete

Documents

- Data import
 - [C: 153;Md: 60150;P: 1]

Filter endpoint tree...

Structure

- vapour pressure
- Viscosity
- Water solubility
- Environmental Fate and Transport
- Ecotoxicological Information
 - Aquatic Toxicity AW SW
 - Sediment Toxicity
 - Terrestrial Toxicity
- Human Health Hazards
 - Acute Toxicity
 - ADME
 - Carcinogenicity
 - Developmental Toxicity / Teratoge
 - Genetic Toxicity
 - in Vitro
 - in Vivo
 - Immunotoxicity
 - Irritation / Corrosion
 - Neurotoxicity
 - Photoinduced toxicity
 - Repeated Dose Toxicity
 - Sensitisation AW SW A
 - ToxCast
 - Toxicity to Reproduction
 - Toxicokinetics, Metabolism and Dis

Possible data inconsistency

Metadata

- Endpoint
 - ☒ vapour pressure (60 chemicals; 281 data)
- Native scale/unit
 - ☒ Pa (26 chemicals; 71 data)
 - ☒ Torr (1 chemicals; 2 data)
 - ☒ bar (2 chemicals; 4 data)
 - ☒ hPa (35 chemicals; 143 data)
 - ☒ kPa (13 chemicals; 32 data)
 - ☒ mbar (2 chemicals; 2 data)
 - ☒ mm Hg (12 chemicals; 12 data)
 - ☒ no endpoint given (1 chemicals; 1 data)
 - ☒ psi (4 chemicals; 14 data)

Required unit/scale

Select scale/unit to use

- ☒ Pa [71 native data and 209 converted]
- ☐ Torr [2 native data and 278 converted]
- ☐ bar [4 native data and 276 converted]
- ☐ hPa [143 native data and 137 converted]

Converted data

- 2 from scale/unit Torr
- 4 from scale/unit bar
- 143 from scale/unit hPa
- 32 from scale/unit kPa
- 2 from scale/unit mbar

Chemicals 60/60; Data 280/281

OK Cancel

Chemical structure: CCCCC=O and c1ccncc1

Endpoint	Value
24 mm Hg	
M: 1E+06 mg/L	
M: 0 %	
M: 0,01 mg/L	
M: 2 mmol	
5E+03 mg/kg	M: 11,3 mg/L
M: 24,4 mg/kg bdwt/d	
M: 10 mg/kg bdwt/d	
M: Negative	
M: negative	
M: Category 1 (irrevers	
M: 1 mg/kg bdwt/d	
M: 1,3E+03 µM	
M: 25 mg/kg bdwt/d	

Trend analysis illustration

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Gap Filling Workflow Editor

Trend analysis Read across (Q)SAR Automated Standardized New Import Export Delete

The OECD QSAR Toolbox for Grouping Chemicals into Categories

Developed by LMC, Bulgaria

Documents

- Data import
 - [C: 153;Md: 60150;P: 1] Wa
 - [C: 88;Md: 33543;P: 1] I
 - [C: 88;Md: 33543;P: 1] I
 - [C: 88;Md: 33543;P: 1] I
 - [C: 88;Md: 33543;P: 1] I
 - [C: 88;Md: 33543;P: 1] I

Filter endpoint tree...

Structure

Taste and Odor 87/89

Profiling

- Predefined
 - Database Affiliation
 - Inventory Affiliation
 - OECD HPV Chemical Categories
 - Substance type
 - US-EPA New Chemical Categories
- General Mechanistic
 - Biodec BioHC half-life (Biowin)

	30	31	34	37	38	39	40	41
Structure								
M: 0.0004 mg/L	M: 1 mg/L	M: 0.0002 mg/L	M: 0.00021 mg/L	M: 0.065 mg/L	M: 0.005 mg/L	M: 1,1 mg/L	M: 0.00124 mg/L	
ECOTOX	Aquatic ECETOC	WaterTOP	Acute Oral toxicity DB	Acute Oral toxicity DB	Acute Oral toxicity DB	Acute Oral toxicity DB	Aquatic OASIS	
DSSTOX	AIIC	Does not belong to an...	AIIC	AIIC	Canada DSL	AIIC	AIIC	
Not categorized	Not categorized	Tertiary Amines	Not categorized	Not categorized	Not categorized	Not categorized	Not categorized	
Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	Discrete chemical	
Neutral Organics	Not categorized	Not categorized	Aliphatic Amines	Not categorized	Aldehydes (Acute toxi...	Not categorized	Not categorized	
No value	No value	No value	No value	1 to 10 days	No value	No value	No value	

Data Gap Filling Settings

☒ Only endpoint relevant

At this position:

- QSARs 2
- Automated workflows 0
- Standardized workflow0

In nodes below:

- QSARs 0
- Automated workflows 0
- Standardized workflow0

Descriptors

Prediction

Adequacy

Cumulative frequency

Residuals

Statistics

Trend analysis prediction for undefined endpoint, based on 87 values

Predicted: 1.01 mg/L

Model equation: undefined endpoint = $1E3 (\pm 2,15E3) + 0,639 (\pm 3,54) \cdot \text{Vapor Pressure (Mackay method), } \mu\text{g/L}$

Select / filter data

Gap filling approach

Descriptors / data

Model/QSAR

Calculation options

Visual options

Information

Miscellaneous

✓ Accept prediction

Save as a user defined OSAR model

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX



► Input



► Profiling



► Data



► Category definition



► Data Gap Filling



► Report



The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

Developed by LMC, Bulgaria

nd analysis Read across (Q)SAR

Documents

- Data import
 - [C: 153;Md: 60150;P: 1] Wa
 - [C: 88;Md: 33543;P: 1] f
 - [C: 88;Md: 33543;P: 1] f
 - [C: 88;Md: 33543;P: 1] f
 - [C: 88;Md: 33543;P: 1] f
 - [C: 88;Md: 33543;P: 1] f

Filter endpoint tree

Structure

Taste and Odor

Profiling

Predefined

Databas

Inventor

OECD H

Substan

US-EPA

General Me

Biodea

Data Gap Filling Settings

☒ Only endpoint relevant

At this position:

QSARs 2
Automated workflows 0
Standardized workflow 0

In nodes below:

QSARs 0

Descriptors

Prediction

Adequacy

Cumulative frequ

Residuals

Wizard pages

QSAR Identity

General information

Defining the
endpoint – OECD
Principle 1

Defining the
algorithm – OECD
Principle 2

Applicability domain
– OECD Principle 3

Training set and
statistics – OECD
Principle 4

External validation
and predictivity –
OECD Principle 4

Mechanistic
interpretation –
OECD Principle 5

Miscellaneous

QSAR Title/Caption

Version

Other related models

Software implementing the
model

WaterTop TandO

1.0

Automatically populated by the system

40	41
mg/L	M: 1,1 mg/L
mg/L	M: 0,00124 mg/L
Acute Oral toxicity DB	Acute Oral toxicity DB
DSL	AIIC
Not categorized	Not categorized
Discrete chemical	Discrete chemical
es (Acute toxi...	Not categorized
No value	No value

Select / filter data

Gap filling approach

Descriptors / data

Model/QSAR

Show domain

Save model

Export in Excel as a data matrix

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Reports Export

Prediction Data Matrix Category QMRF SMI File SDF File CAS List Data Matrix

Documents

Data import

- [C: 153;Md: 60150;P: 2] V
- [C: 88;Md: 33543;P: 2] I
- [C: 88;Md: 33543;P: 2] I
- [C: 88;Md: 33543;P: 2] I
- [C: 88;Md: 33543;P: 2] I
- [C: 88;Md: 33543;P: 2] I

Filter endpoint tree...

Structure

vapour pressure 61/282 M: 4,5 mm Hg M: 30 hPa M: 1 mm Hg M: 0,3 kPa

Viscosity 41/130 M: 0,737 mPa·s M: 0,53 mPa·s

Water solubility 82/348 M: ca.50 mg/L M: 1,5E+04 mg/L M: 1,13E+04 mg/L M: 57 mg/L M: 10,8 mg/L M: 1,25 mg/L

Environmental Fate and Transport 90/2221 M: 2 % M: 40 % M: 0 % M: 0 % M: 2,77 log(L/kg) M: <10 %

Ecotoxicological Information

Aquatic Toxicity AW SW 104/24068 M: 1÷2 mg M: 3,5 mg

Sediment Toxicity 2/21

Terrestrial Toxicity 67/5182 M: 60,1÷601 mg/L M: 1E+03

Human Health Hazards

Acute Toxicity 81/1071 M: 9,5 mg/L M: 0,819

ADME 10/25

Carcinogenicity 28/596 M: 125 ppm (nominal) M: Negat

Developmental Toxicity / Teratoge... 45/968 M: Positive M: 50 mg

Genetic Toxicity

in Vitro 87/2624 M: Negative M: Positiv

in Vivo 46/355 M: ambiguous M: Equiv

Immunotoxicity 4/4

Irritation / Corrosion 63/1478 M: not irritating M: GHS c

Neurotoxicity 7/94

Photoinduced toxicity

Repeated Dose Toxicity 69/16526 M: 154 mg/kg bdwt/d M: ≥90,3

Sensitisation AW SW AOP 56/505 M: not sensitising M: 424 µ

ToxCast 36/486

Toxicity to Reproduction 61/715 M: 100 ppm M: 50 mg

Toxicokinetics. Metabolism and Distr... 11/94 M: 0,48 % M: ca.0,1 %

Matrix export

Select All Unselect All

Filter

- ☒ Structure info
- ☒ Parameters
- ☒ Physical Chemical Properties
- ☒ Environmental Fate and Transport
- ☒ Ecotoxicological Information
- ☒ Human Health Hazards
- ☒ Taste and Odor
- ☒ Profiling

☐ Export detailed metadata ☐ Distribute profiling results

☐ Remove empty columns ☐ Filter points by metadata

☐ Do not multiply chemical ID

Export

Export in Excel/CSV as a data matrix

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX

Input

Profiling

Data

Category definition

Data Gap Filling

Report

Reports

Export

Prediction

Data Matrix

Category

QMRF

SMI File

SDF File

CAS List

Data Matrix

Documents

Data import

- [C: 153;Md: 60150;P: 2] I
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- [C: 88;Md: 33543;P: 2] I

Filter endpoint tree...

- Structure
- vapour pressure
- Viscosity
- Water solubility
- Environmental Fate and Transport
- Ecotoxicological Information
 - Aquatic Toxicity
 - Sediment Toxicity
 - Terrestrial Toxicity
- Human Health Hazards
 - Acute Toxicity
 - ADME
 - Carcinogenicity
 - Developmental Toxicity / Teratoge...
 - Genetic Toxicity
 - in Vitro
 - in Vivo
 - Immunotoxicity
 - Irritation / Corrosion
 - Neurotoxicity
 - Photoinduced toxicity
 - Repeated Dose Toxicity
 - Sensitisation
 - ToxCast
 - Toxicity to Reproduction
 - Toxicokinetics. Metabolism and Distr...

	15	16	17	18	19	20
Structure						
vapour pressure	61/282	M: 4,5 mm Hg	M: 30 hPa	M: 1 mm Hg	M: 0,3 kPa	
Viscosity	41/130	M: 0,737 mPa·s	M: 0,53 mPa·s			
Water solubility	82/348	M: ca.50 mg/L	M: 1,5E+04 mg/L	M: 1,13E+04 mg/L	M: 57 mg/L	
Environmental Fate and Transport	90/2221	M: 2 %	M: 40 %	M: 0 %	M: 0 %	
Ecotoxicological Information						
Aquatic Toxicity	104/24068	M: 1+2 mg	M: 3,5 mg			
Sediment Toxicity	2/21					
Terrestrial Toxicity	67/5182	M: 60,1+601 mg/L	M: 1E+03			
Human Health Hazards						
Acute Toxicity	81/1071	M: 9,5 mg/L	M: 0,819			
ADME	10/25					
Carcinogenicity	28/596	M: 125 ppm (nominal)	M: Negat			
Developmental Toxicity / Teratoge...	45/968	M: Positive	M: 50 mg			
Genetic Toxicity						
in Vitro	87/2624	M: Negative	M: Positiv			
in Vivo	46/355	M: ambiguous	M: Equiv			
Immunotoxicity	4/4					
Irritation / Corrosion	63/1478	M: not irritating	M: GHS c			
Neurotoxicity	7/94					
Photoinduced toxicity						
Repeated Dose Toxicity	69/16526	M: 154 mg/kg bdwt/d	M: ≥90,3			
Sensitisation	56/505	M: not sensitising	M: 424 µl			
ToxCast	36/486					
Toxicity to Reproduction	61/715	M: 100 ppm	M: 50 mg			
Toxicokinetics. Metabolism and Distr...	11/94		M: 0,48 %		M: ca.0.1 %	

Matrix export

Select All Unselect All

Filter

☒ Structure info

☒ Parameters

☒ Physical Chemical Properties

☒ Environmental Fate and Transport

☒ Ecotoxicological Information

☒ Human Health Hazards

☒ Taste and Odor

☒ Profiling

☐ Export detailed metadata

☐ Distribute profil

☐ Remove empty columns

☐ Filter points by

☐ Do not multiply chemical ID

Wizard pages

Data matrix

Options

The section provides detailed information about the Data Matrix chemicals, including parameters, profiles and experimental data. The information will be provided in a separate MS Excel file.

☒ Include profiles

☒ Select profiles to report

☒ Include measured and predicted data

☒ Select experimental data to report

☒ Include predictions

Cancel Create report

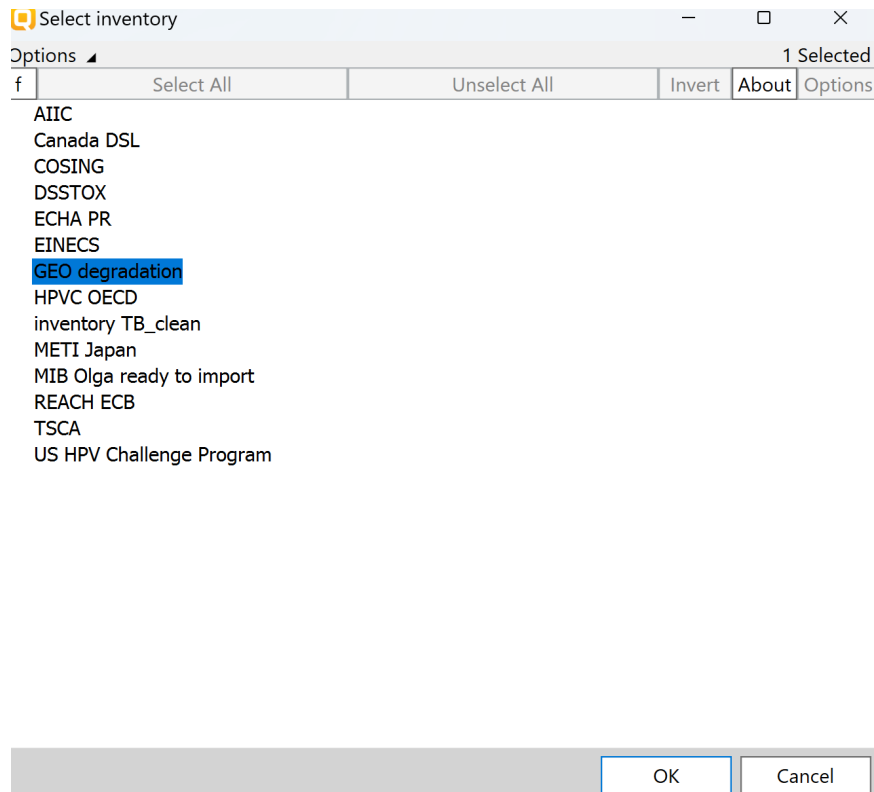
1				Chemical #2			Chemical #3			Composition #4			Ch
2	Substance identity												
3	Structure												
4	CAS number			112-31-2			1138-52-9			130-89-2			
5	Chemical name			Decanal			3,5-Di-tert-butylphenol			Quinine * HC1			
6	Other identifier												
7	SMILES			CCCCCCCCC=O			CC(C)(C)c1cc(O)cc(c1)C(C)(C)C			Cl.COc1ccc2nccc([C@@H](O)[C@@H]3C[C@H](O)C3)cc2			OC(=O)C
376	Aquatic Toxicity	EC100					7	mg/L	Test organisms (species): Daphnia magna Endpoint: EC100 Duration: 24 h Reference source: Water Res.23(4): 495-499 Author: Kuhn,R., M. Pattard, K.D. Pernak, and A. Winter Title: Results of the Harmful Effects of Selected Water Pollutants (Anilines, Phenols, Aliphatic Compounds) to Daphnia magna Database: ECOTOX				

Import of degradation data of Geosmin and MIB as a custom inventory

	smiles	name	CAS
MIB	CC1(C)C2CCC1(C)C(C)(O)C2	2-Methylisoborneol	2371-42-8
	CC1=CC2CC[C@]1(C)C2(C)C	1,2,7,7-Tetramethyl-bicyclo[2.2.1]hept-2	72540-93-3
I	CC1(C)C2CC[C@]1(C)C(=O)C2	1,6,7,7-Tetramethyl-bicyclo[2.2.1]hept-5-en-2-ol	
II	CC1=CC2CC(O)[C@@]1(C)C2(C)C	1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-ol	76-22-2
V	CC1(C)C2CC(=O)[C@@]1(C)CC2=O	1,7,7-Trimethyl-bicyclo[2.2.1]heptane-2,	4230-32-4
✓	CC1(C)C2CC[C@]1(C)C(=O)C2=O	1,7,7-Trimethyl-bicyclo[2.2.1]heptane-2,	2767-84-2
✓I	CC1(C)C2CC(=O)[C@@]1(C)C(=O)C2	1,7,7-Trimethyl-bicyclo[2.2.1]heptane-2,6-dione	
✓II	CCc1cc(C)oc1C	3-Ethyl-2,5-dimethyl-furan	10599-62-9
✓III	CC\C=C\CC1(C)COC1=O	4-Methyl-3-pent-2-enyl-dihydro-furan-2-one	chemsketcl
X	CC1CCC(C=O)=CC1(C)C	2,3,4,5-Tetramethyl-cyclopent-2-enone	54458
✗	CC1=CC[C@H](CC=O)C1(C)C	(2,2,3-Trimethyl-cyclopent-3-enyl)-acetate	4501-
✗I	CC1CCC(C=O)=CC1(C)C	3,3,4-Trimethyl-cyclohex-1-enecarbaldehyde	
✗II	CC(C)\C=C\C=C(/C)C	2,6-Dimethyl-hepta-2,4-diene	4634-
✗III	CCCC(C)\C=C\C	4-Methyl-hept-2-ene	3404-
✗IV	CC1(C)C2CCC1(C)C(=C)C2		4423-94-3
✗V	CC1(C)C2CCC(C)(C2)C1=C		
✗VI	CC1=CC2CCC1(C)C2(C)C		
✗VII	CC1(C)C2CCC1(C)C(=O)O2		
✗VIII	CC1(C)C2(C)CCC1(O)CC2=O		
✗IX	CC1(C)C2CCC1(CC2=O)C(O)=O		

Name	SMILES	Identity
GEOSMIN	C[C@H]1CCCC[C@]2(C)CCCC[C@@]12O	Geosmine
8a-Hydroxy-4a-methyl-octahydro-naphthalene	CC12CCCC[C@]1(O)CC(=O)CC2	IV
4a-Methyl-4,4a,5,6,7,8-hexahydro-3H-naphthalene	CC12CCCCC1=CC(=O)CC2	V
8,8a-Dimethyl-decahydro-naphthalene-1,4-dione	CC1CCCC2CCCC(O)C12C	VI
2-Ethyl-cyclohexanone	CCC1CCCCC1=O	VII
7a-Methyl-1,4,5,6,7,8-hexahydro-inden-1-one	O=C1CC2CCCCC2=C1	VIII
2,4-Dimethyl-cyclopentane-1,3-dione	CC1CCCC1(C)CO	IX
(1,2-Dimethyl-cyclopentyl)-methanol	CC1CC(=O)C(C)C1=O	X
1-(1-Methyl-cyclohexyl)-ethanone	CC(=O)C1(C)CCCCC1	XII
5-Isopropenyl-2-methyl-cyclohexanol	C[C@H]1CC[C@@H](C[C@H]1O)C(C)=C	XIII
1-Isopropyl-4-methyl-cyclohexane	CC1CCC(CC1)C(C)C	XIV
3-(2,6,6-Trimethyl-cyclohex-2-enyl)-propan-2-one	CC1=CCCC(C)C(C)C1C=C\C=C=O	XV
1-(2-Methoxy-cyclohexyl)-propan-2-one	COC1CCCCC1CC(C)=O	XVI
Cyclohexanone	O=C1CCCCC1	XVII
2,2-Dimethyl-cyclohexanone	CC1(C)CCCCC1=O	XVIII
3,5-Dimethyl-cyclohex-3-enecarbaldehyde	CC1CC(CC(C)=C)C=O	XIX
2,2,6-Trimethyl-cyclohexanone	CC1CCCC(C)(C)C1=O	XX
5-Acetyl-3,3-dimethyl-cyclohexanone	CC1CC(CC(=O)C)C(C)=O	XXI
3,5,5-Trimethyl-cyclohex-2-enone	CC1CC(C)(C)CC(=O)C=1	XXII
2-Ethyl-hex-2-enal	CCC\C=C(/CC)C=O	XXIII
Octanoic acid	CCCCCCCC(O)=O	XXIV
2,4,5,6-Tetramethyl-hepta-1,3,6-triene	CC(C(C)=C)C/C=C/C(C)=C	XXV

Import of degradation data of Geosmin and MIB as a custom inventory



Geosmin and its degradation products: profiling results

[illegible]

Geosmin and its degradation products: data collection results

QSAR Toolbox 4.6 [Data import]

QSAR TOOLBOX

Input Profiling Data Category definition Data Gap Filling Report

Data Import Export Delete

Gather Import IUCLID6 Database Inventory

The OECD QSAR Tool for Grouping Chemicals into Categories
Developed by LMC, B

Filter endpoint tree...

Documents

- Data import
 - [C: 153;Md: 60150;P: 2] We
 - [C: 88;Md: 33543;P: 2] I
 - [C: 88;Md: 33543;P: 2] I
 - [C: 88;Md: 33543;P: 2] I
 - [C: 88;Md: 33543;P: 2] I
 - [C: 23;Md: 617;P: 0] GEO

Databases

Options 65 Selected

Select All Unselect All Invert

☒ Taste and Odor
☒ Water/Top
☒ Physical Chemical Properties
☒ Bioconcentration and log
☒ Chemical Reactivity CO
☒ ECHA REACH

Organise by: Dossiers/Substances

Inventories

Options 0 Selected

Select All Unselect All Invert

☐ AIIC
☐ Canada DSL
☐ COSING
☐ DSTOX
☐ ECHA PR
☐ EINECS
☐ GEO degradation
☐ HPVC OECD
☐ Inhouse TP class

Structure

	10	11	12	13	14	15	16	17
CAS Number	No CAS number	78-59-1	No CAS number	2408-37-9	No CAS number	No CAS number	No CAS number	645-62-5
CAS-SMILES relation	Not applicable	High	Not applicable	High	Not applicable	Not applicable	Not applicable	Low
Chemical name(s)	2,4,5,6-Tetramethyl-he...	1-cyclohexen-3-one, 1...	5-Isopropenyl-2-meth...	2,2,6-Trimethyl-cyclo...	5-Acetyl-3,3-dimethyl...	1-(1-Methyl-cyclohexy...	7a-Methyl-1,4,5,6,7a...	2-Ethyl-2-he...
Identity	Sources:1	Sources:38	Sources:1	Sources:9	Sources:1	Sources:1	Sources:1	Sources:2
Molecular formula	C11H18	C9H14O	C10H18O	C9H16O	C9H14O2	C9H16O	C9H12O	C8H14O
Predefined substance type	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono constituent	Mono consti
SMILES	CC(C(C)=C)C(C)=C/C(C...	CC1CCC(C)(C)C(=O)C=1	C[C@H]1CC[C@H](C)[C...	CC1CCCC(C)(C)C1=O	CC1CC(C(C(=O)C)C(C)...	CC(=O)C1(C)CCCCC1	O=C1CC2CCCCC2=C1	CCC/C=C/C(C)C
Parameters								
Physical Chemical Properties	4/77	M: 8.54 mmol/L		M: -31.8 °C				
Environmental Fate and Transport	2/30	M: 1 %						
Ecotoxicological Information	2/247	M: 0.65 mg/L						
Human Health Hazards								
Acute Toxicity	1/33	M: 7 mg/L						
ADME								
Carcinogenicity	1/12	M: 1.21E+03 mg/kg b...						
Developmental Toxicity / Teratogeni...	2/11	M: 150 ppm						
Genetic Toxicity								
in Vitro	5/94	M: Positive		M: Negative				
in Vivo	1/5	M: negative						
Immunotoxicity								
Irritation / Corrosion	1/29	M: Category 2 (irritat...						
Neurotoxicity								
Photoinduced toxicity								
Repeated Dose Toxicity	2/43	M: 102 mg/kg bdwt/d						
Sensitisation	2/9	M: GH5 criteria not met						
ToxCast	1/12	M: 0.205 mg/L						
Toxicity to Reproduction	2/15	M: 65 mg/kg bdwt/d						

Data points

Datapoints	#	Value	
Toxicity in Vitro; in Vitro Mammalian Chromosome Aberration Test; in vitro cytogenetic / chromosome aberration study in mammalian cells; Undefined Test organisms (species); No S9 Info; No Strain	1	M: Positive (Chromosome aberration I (Oasis))	Positive (C (Oasis))
Human Health Hazards; Genetic Toxicity in Vitro; Bacterial Reverse Mutation Assay (e.g. Ames Test); Gene mutation; Salmonella typhimurium; With or Without; No Strain Information	2	M: Negative (Gene mutation I)	Negat
Human Health Hazards; Genetic Toxicity in Vitro; Bacterial Reverse			

☐ Hierarchical mode Find

Thank you very much!



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ENVIRONMENT AND HEALTH