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

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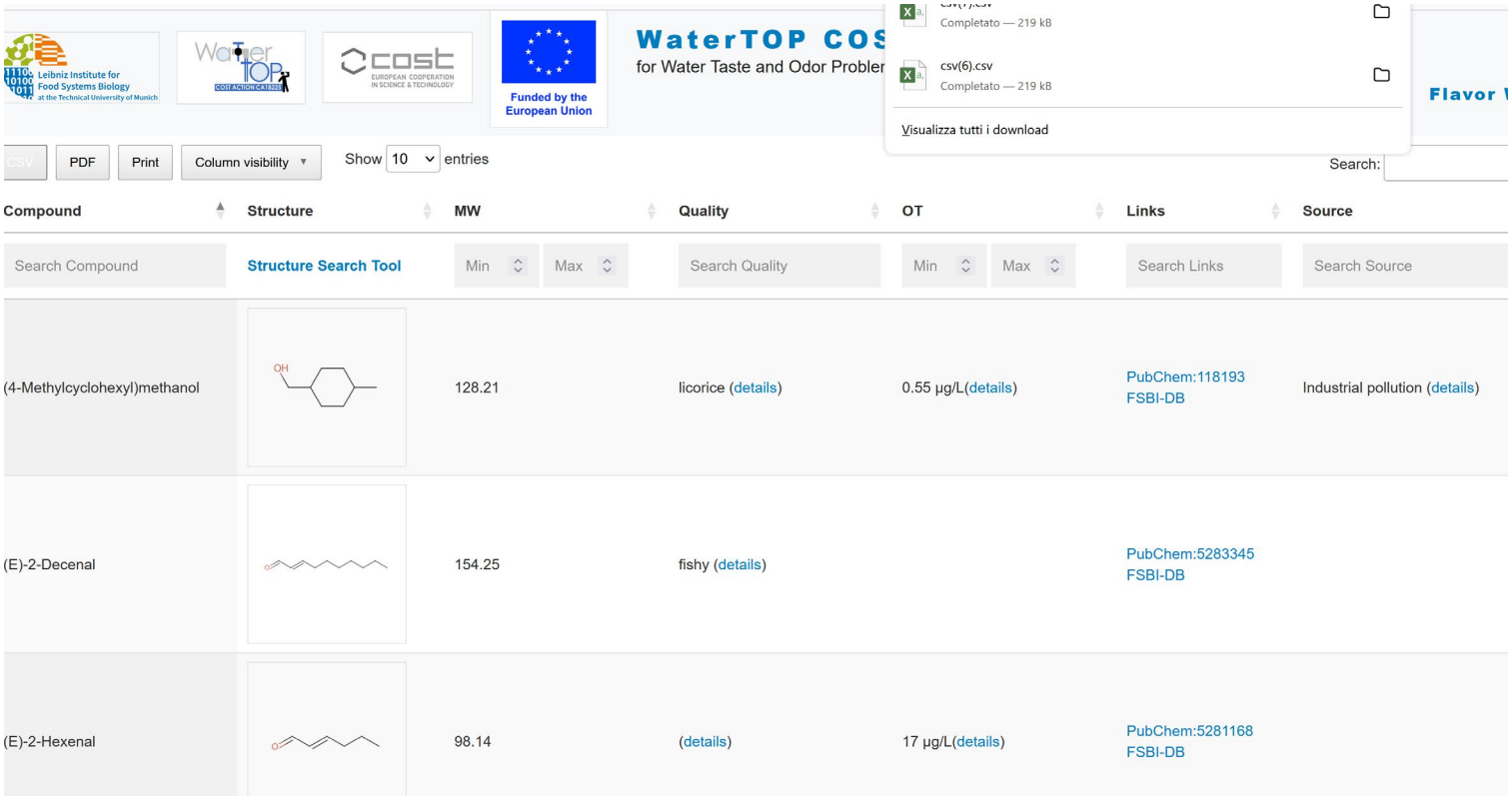
Data Management in the OECD QSAR Toolbox:

- 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



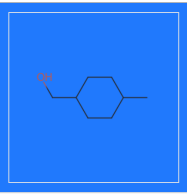
WaterTop database https://fsbi-db.de/waterTop/

Importance of chemical identifiers: SMILES and CAS number

CSV PDF Print Column visibility Show 10 entries Searc

Compound	Structure	MW	Quality	OT
Search Compound	Structure Search Tool	Min Max	Search Quality	Min Max

Search Synonyms Search Links Search

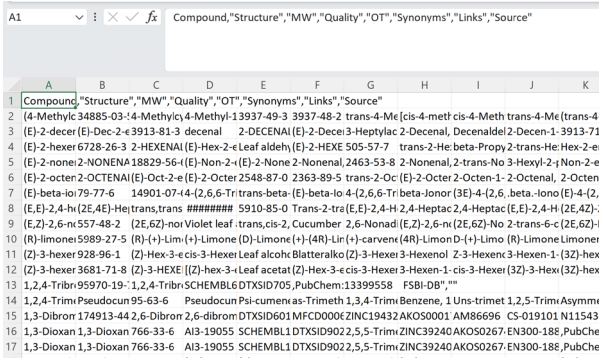
(4-Methylcyclohexyl)methanol		128.21	licorice (details)	0.55 µg/L(details)

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;AI3-28423;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	Structur	MW	Quality	OT	Synonyms
(4-Methylcyclohexyl)methanol		128.21	licorice (details)	0.55 µg/L(details)	(4-Methylcyclohexyl)metha
(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 (de	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 (detai	5 µg/L(details)	2,4-HEPTADIENAL
(E,Z)-2,6-nonadienal		138.21	cucumber-like, grassy (deta	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) (detai	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-me
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(detail	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,	(2E,4E)-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(deta	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-methoxyben	SCHEMBL6423974
1,2,4-Trimethylbenzene,"","120.19","","","1,2,4-TRIMETHYLBENZENE	95-63-6	Pseudocumene	Pseudocumol
1,3-Dibromo-5-chloro-2-methoxybenzene,"","300.37","","","1,3-dibror	174913-44-1	2,6-Dibromo-4-chloroanisole	2,6-dibromo-4-chloro-anisole
1,3-Dioxane, 2,5,5-trimethyl-,"","130.18","","","2,5,5-trimethyl-1,3-dio	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-dio	1,3-Dioxane, 2,5,5-trimethyl-	766-33-6	AI3-19055
1,3-Octadiene,"","110.2","earthy, mushroom (details)","5600 µg/L(det	Octadiene	1002-33-1	(3E)-octa-1,3-diene
1,3-Pentadiene,"","68.12","petroleum, hydrocarbon, varnish (details)","'	trans-1,3-Pentadiene	trans-Piperylene	Piperylene
1,4-Dichlorobenzene,"","147","almond, sweet (details)","4.5 µg/L(detai	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	Pentane-1-thiol	110-66-7	n-Amyl mercaptan
1-penten-3-one,"","84.12","pungent, rancid, fishy (details)","1.24 µg/L(	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	Propanethiol	107-03-9

Retrieval of CAS number from the Synonyms field

Curation process of CSV data in MS Excel

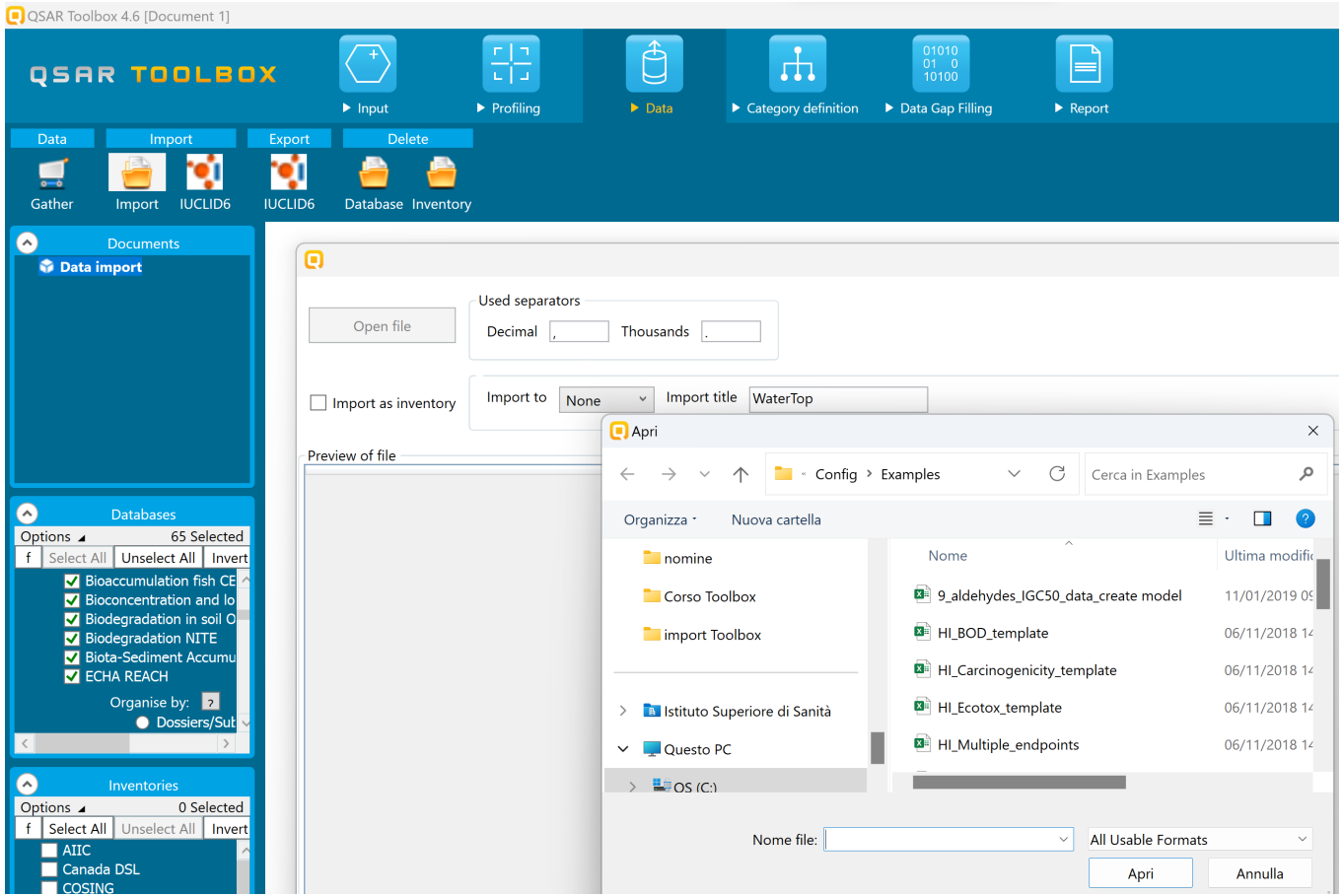
Column1	CAS
D-glucose,"","180.16","sweet taste (details)","","D-Glc	2280-44-6
decanal,"","156.26","fruity, orange (details)","3 µg/L(details)","Decanal	112-31-2
Dibenzyl disulfide,"","246.4","","","Dibenzyl disulfide	150-60-7
Dibromoindole,"","274.94","(details)","","dibromoindole	C1=CC(=C(C=C1Br)Br)N
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, septtic (details)","µg/L(details)","Diisopropyl sulfide	625-80-9
dimethyl disulfide,"","94.2","septic, garlic, pudrid, decaying vegetation (details)","4 µg/L(detai	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	CC1=CCCC(C1C=CC(=O)C=O)(C)C
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)","Ethanolamine	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,"","114.19","fishy, oily (details)","3 µg/L(details)","Heptanal	111-71-7

Retrieval of CAS number from the Synonyms field.
Adding manually SMILES for the substances with no CAS number available

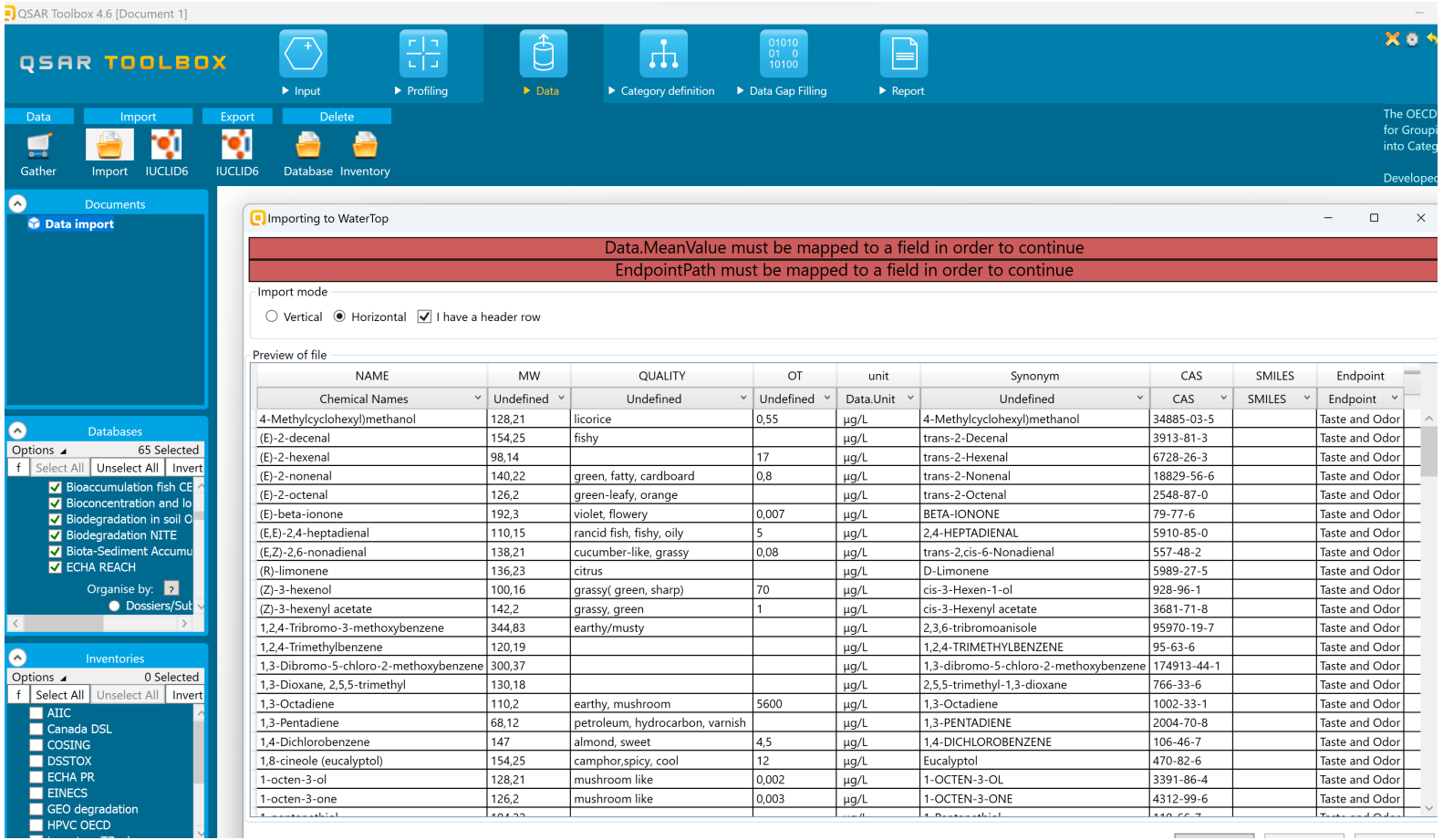
Curation process of CSV data in MS Excel: data matrix is now ready to be imported as a custom user database in OECD QSAR Toolbox

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

Import of the Excel database in the Toolbox

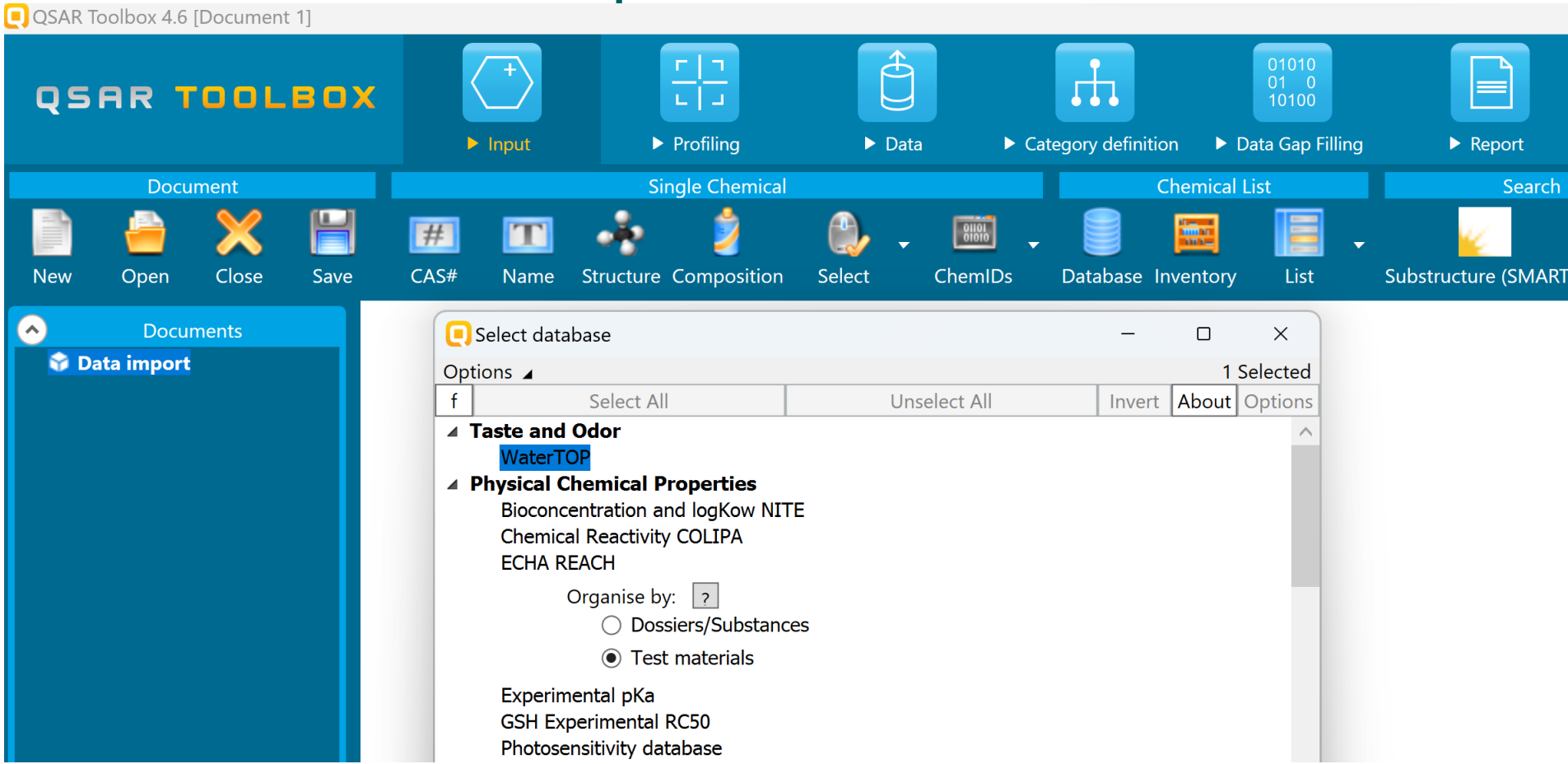


Import of the Excel database in the Toolbox: mapping of the data fields to the Toolbox metadata

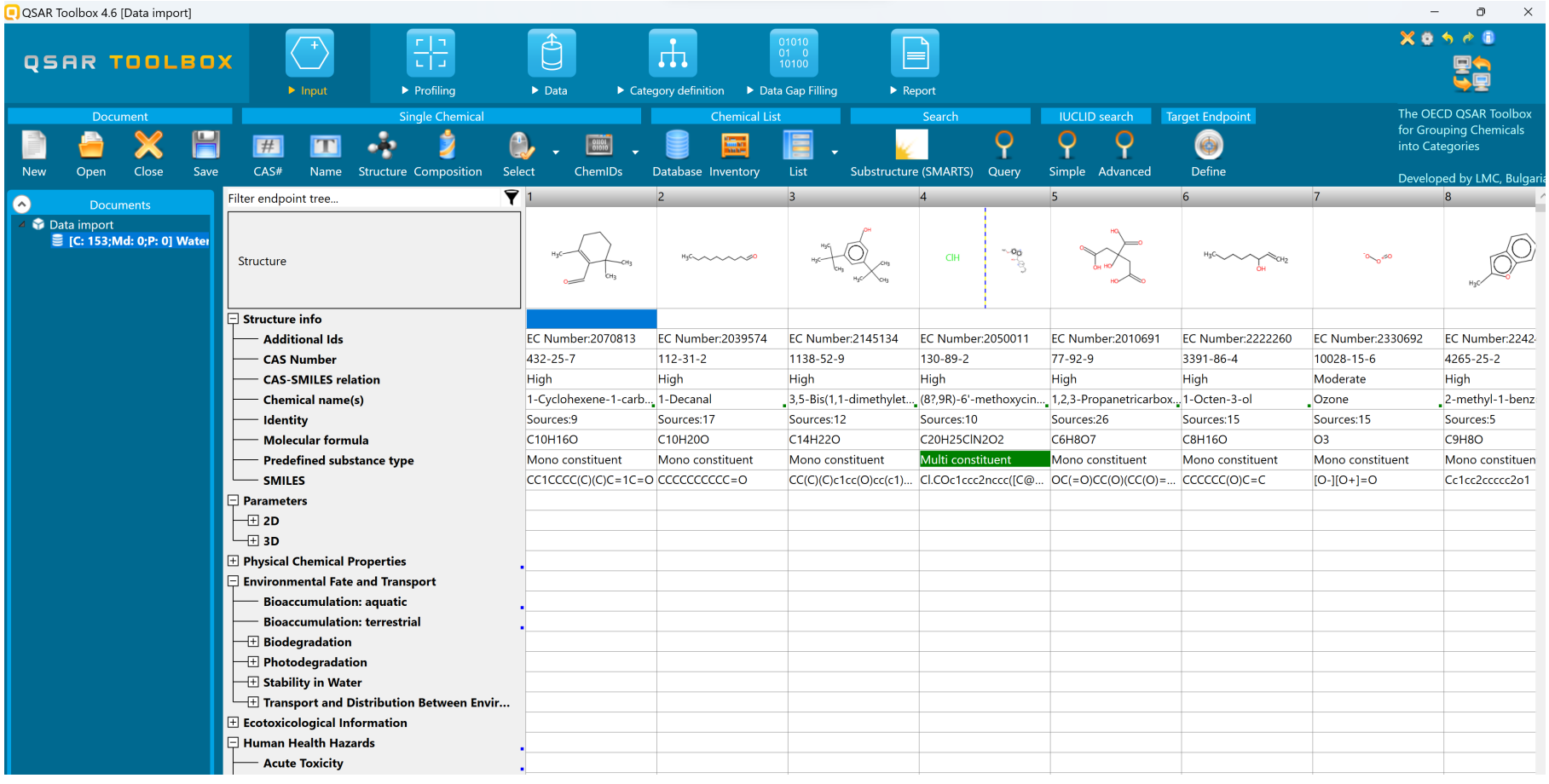


NAME	MW	QUALITY	OT	unit	Synonym	CAS	SMILES	Endpoint
Chemical Names	Undefined	Undefined	Undefined	Data.Unit	Undefined	CAS	SMILES	Endpoint
4-Methylcyclohexyl)methanol	128,21	licorice	0,55	µg/L	4-Methylcyclohexyl)methanol	34885-03-5		Taste and Odor
(E)-2-decenal	154,25	fishy		µg/L	trans-2-Decenal	3913-81-3		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

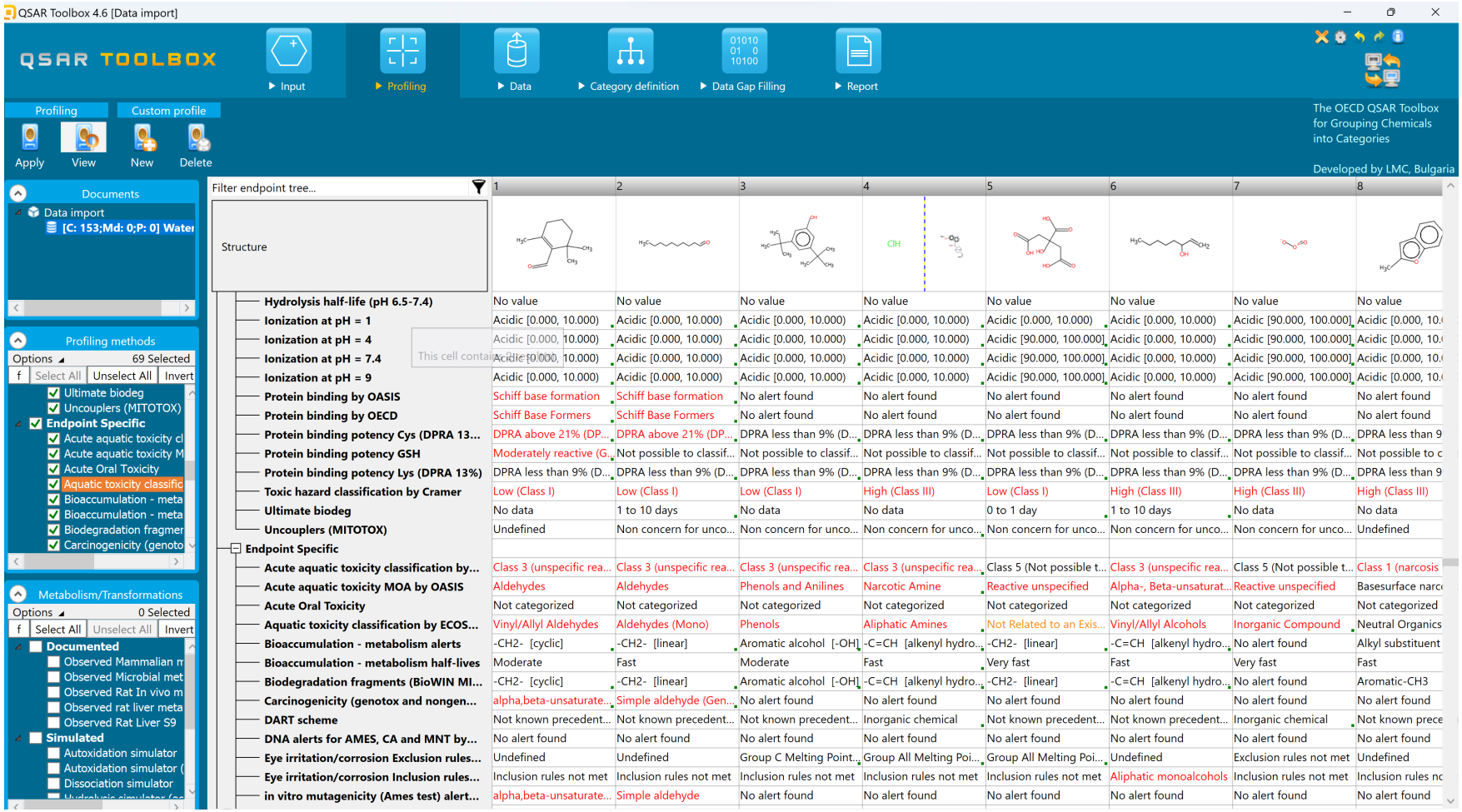
Data Input:
Select the custom WaterTop Database now visible in the database tree



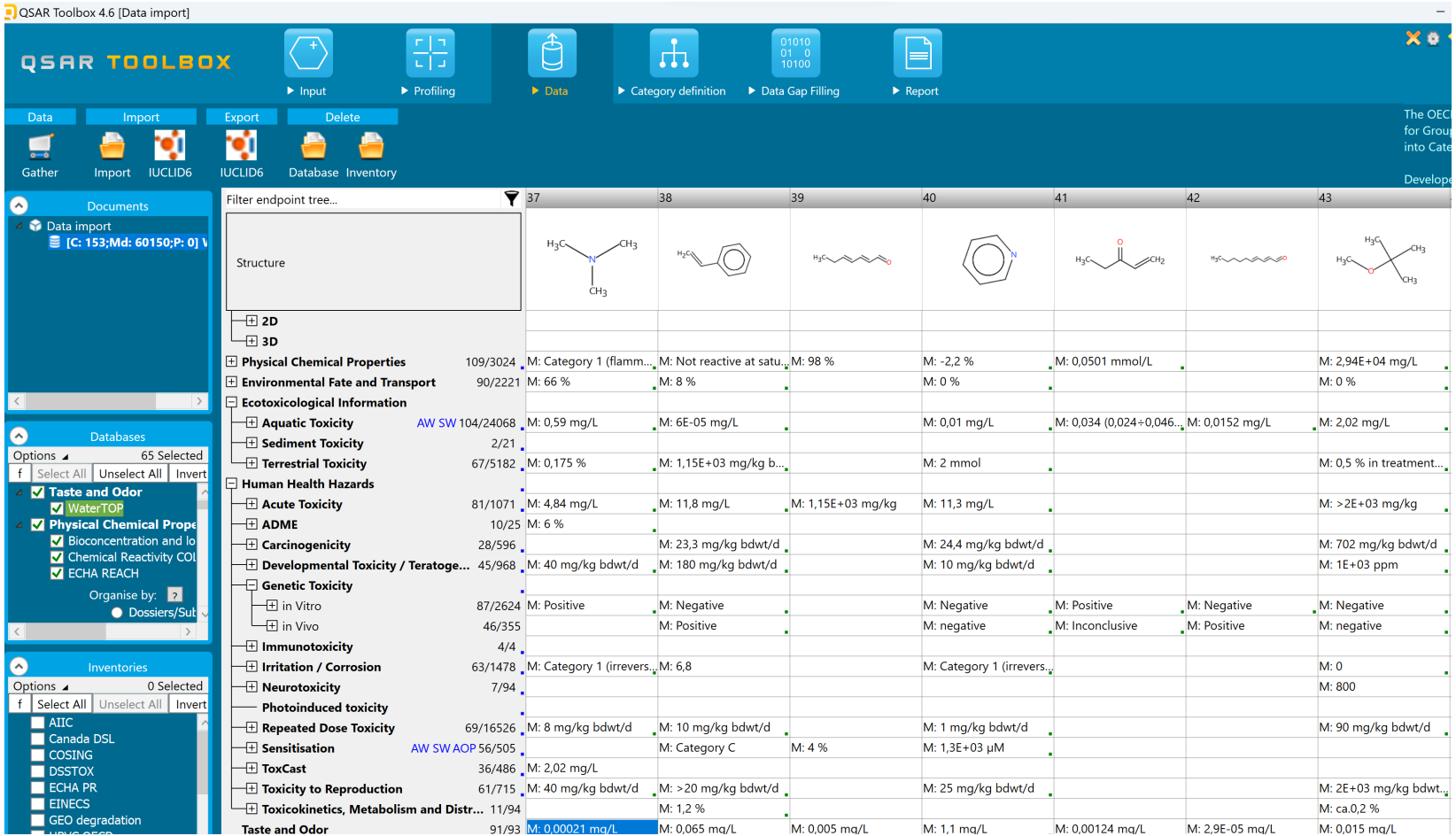
Visualisation of the WaterTop Database (SMILES and chemical formulas have been added automatically during import)



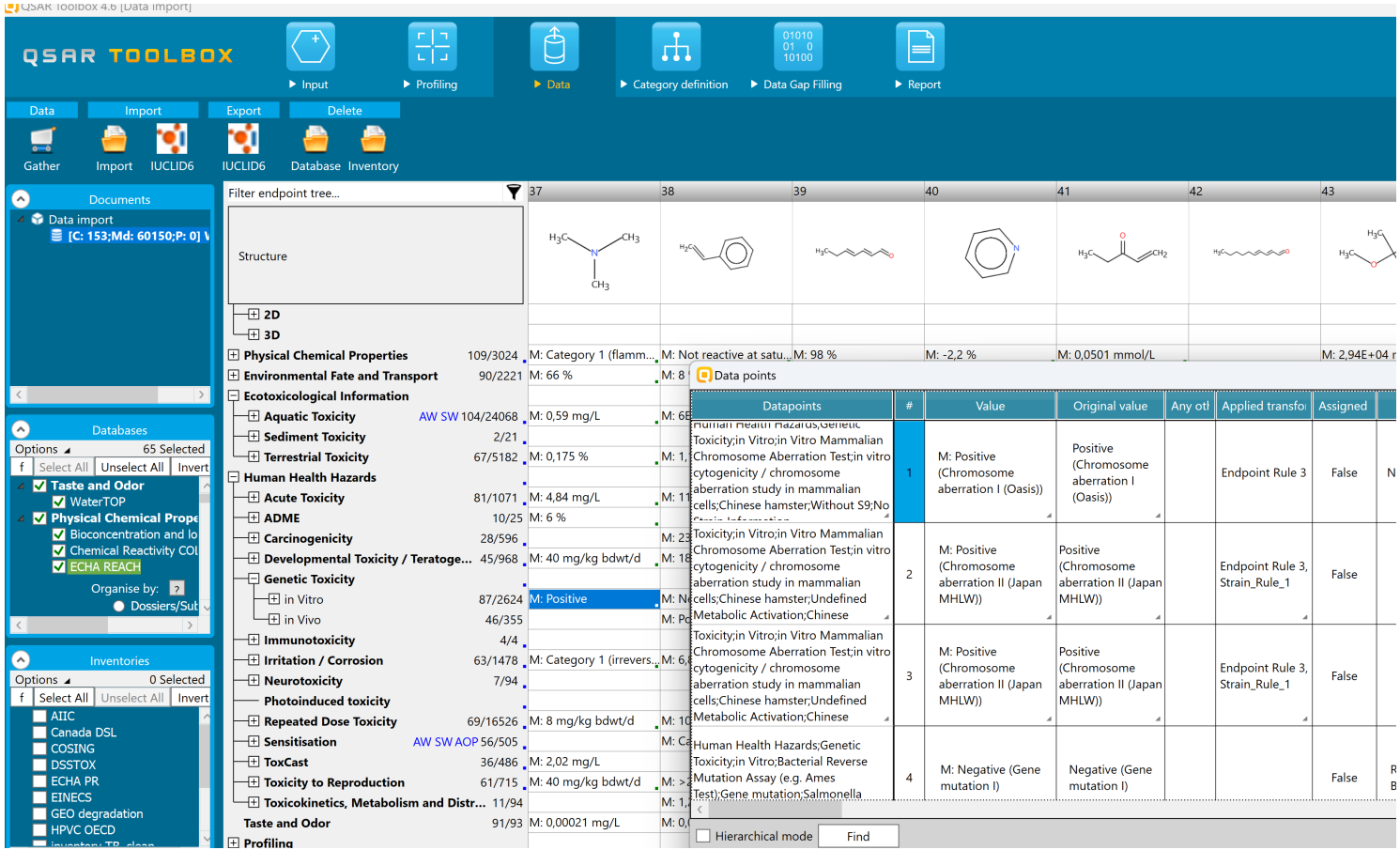
Profiling: visualisation of possible toxicological alerts



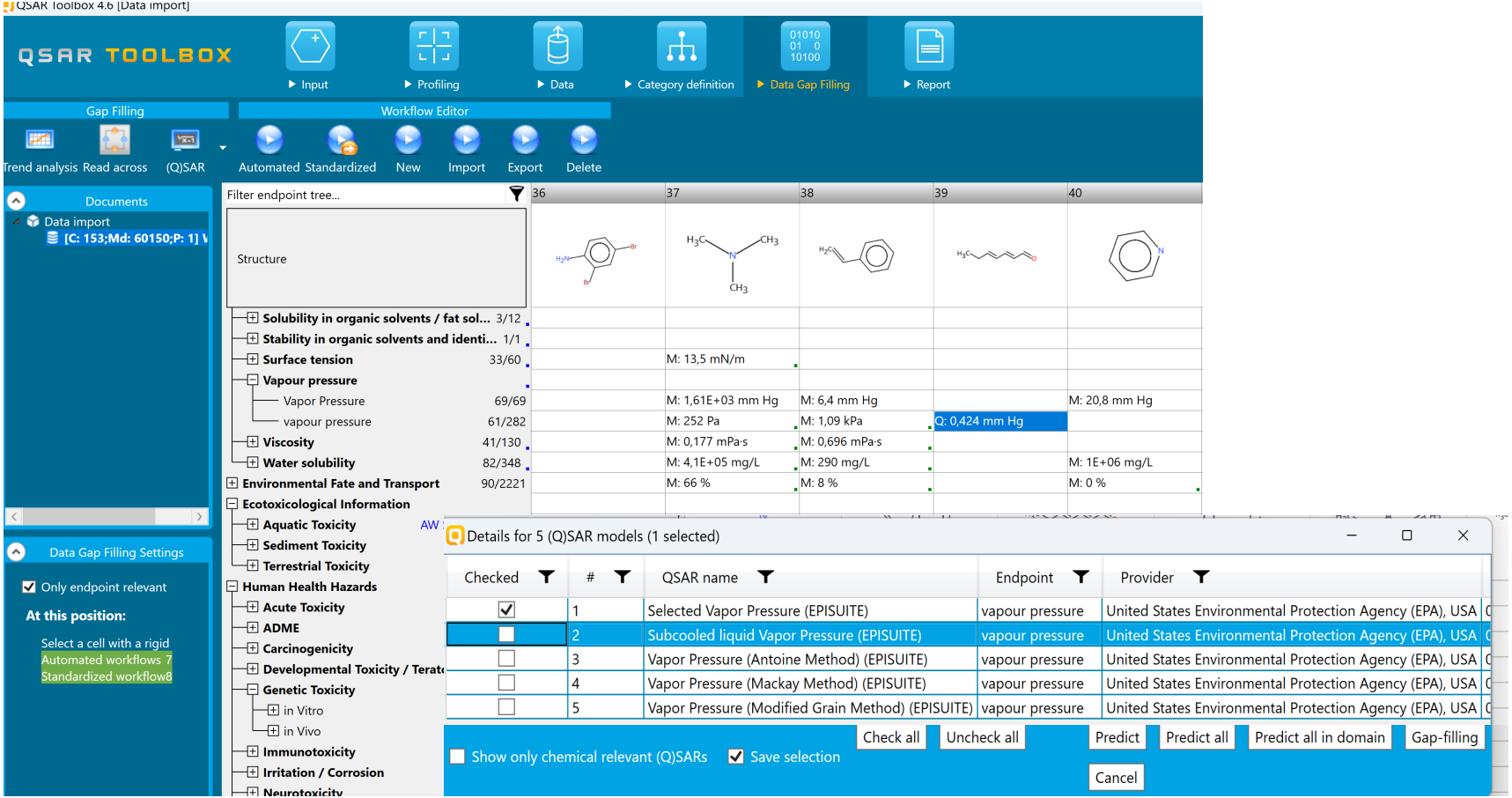
Data gathering from other Toolbox databases including the imported WaterTop database



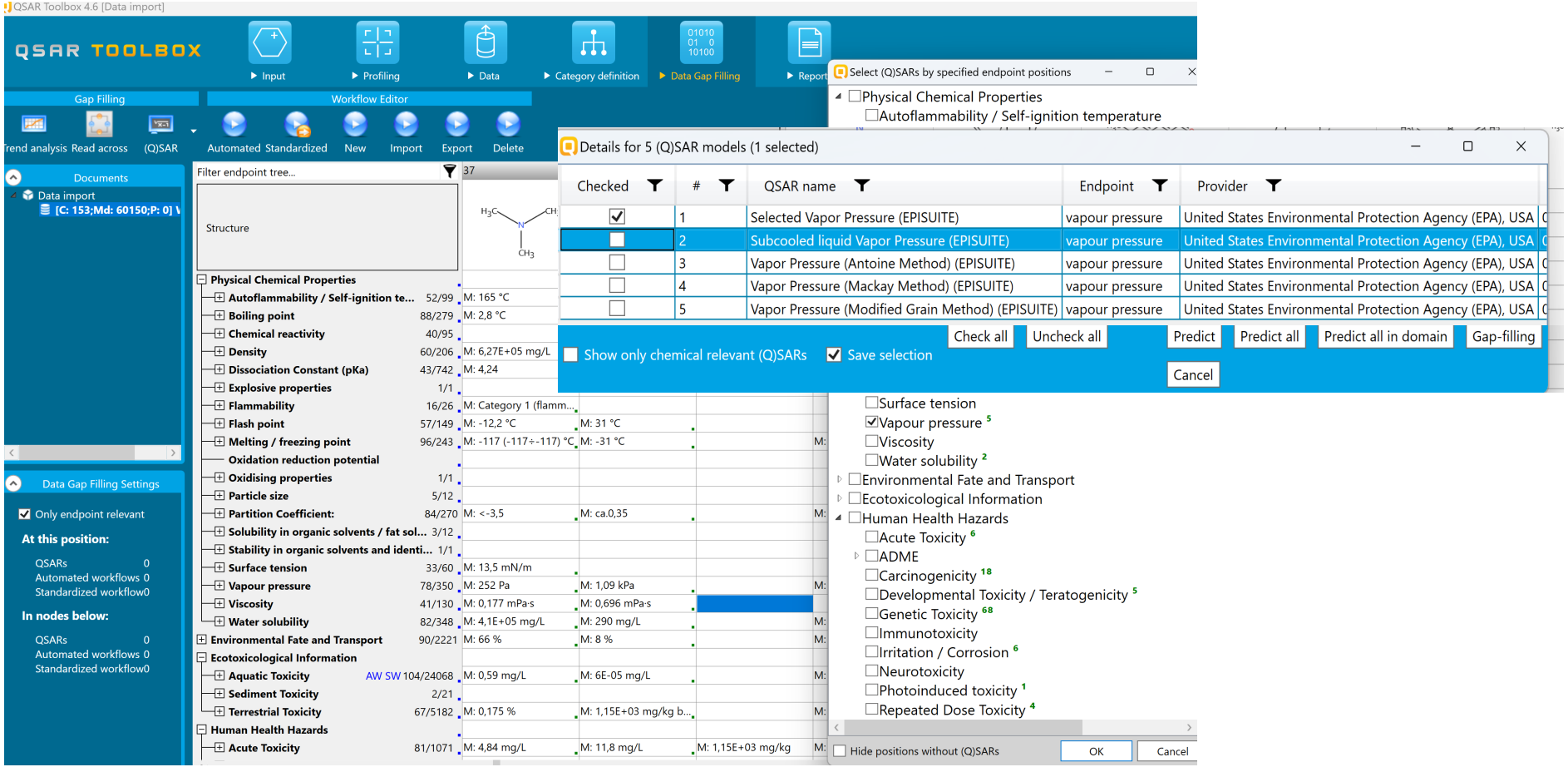
Data analysis: a detailed data matrix is available for each data point



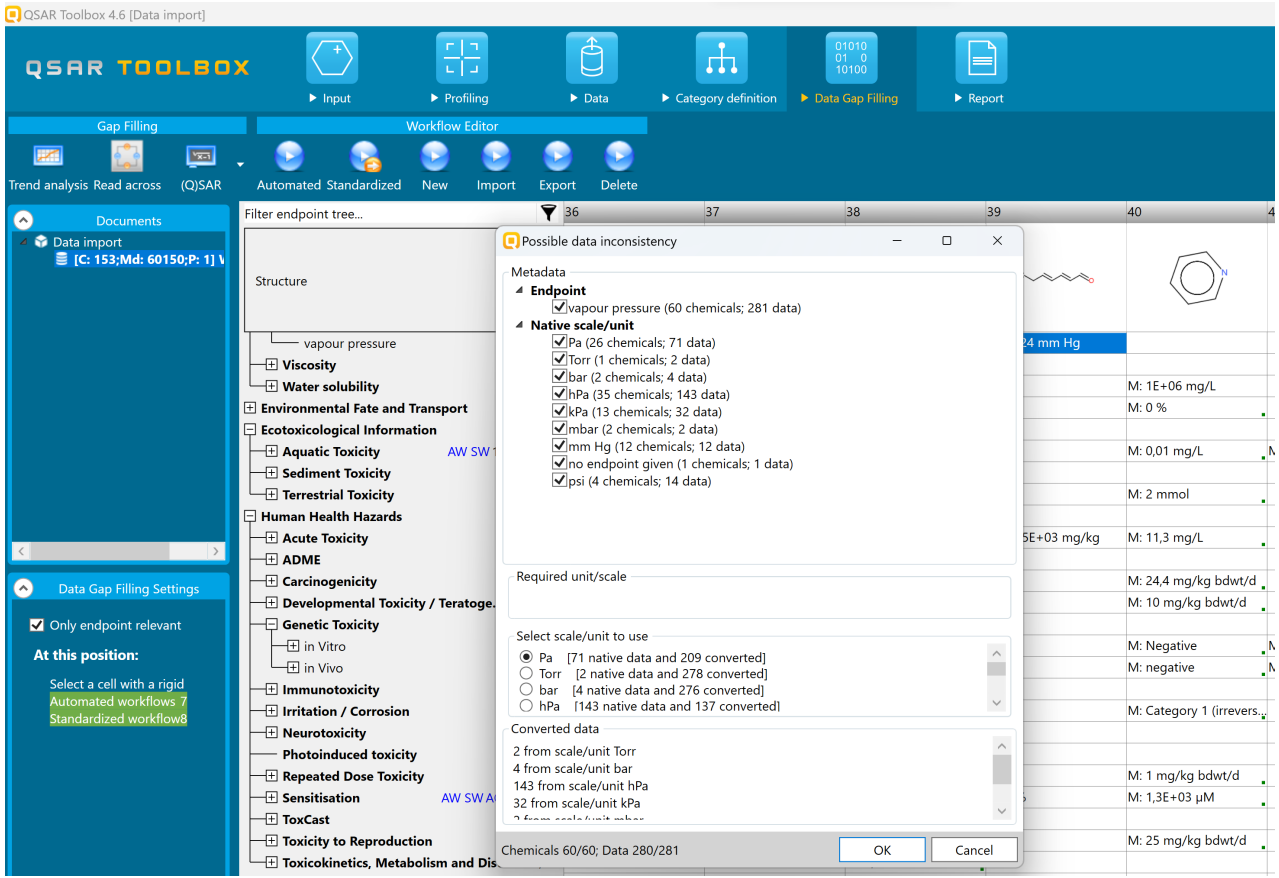
Example of filing data gap using QSAR



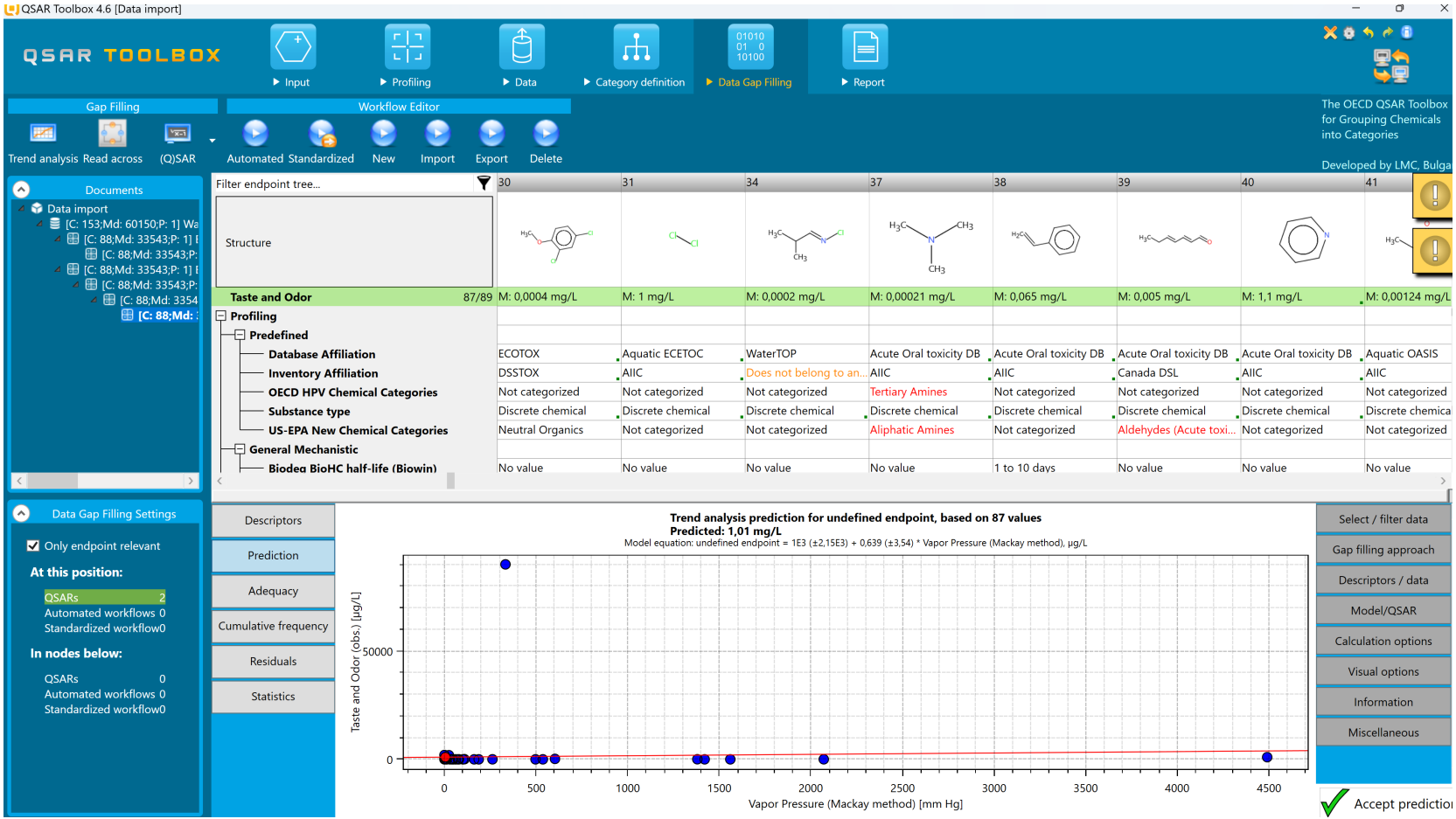
Example of filing data gap using QSAR: a vapour pressure value example



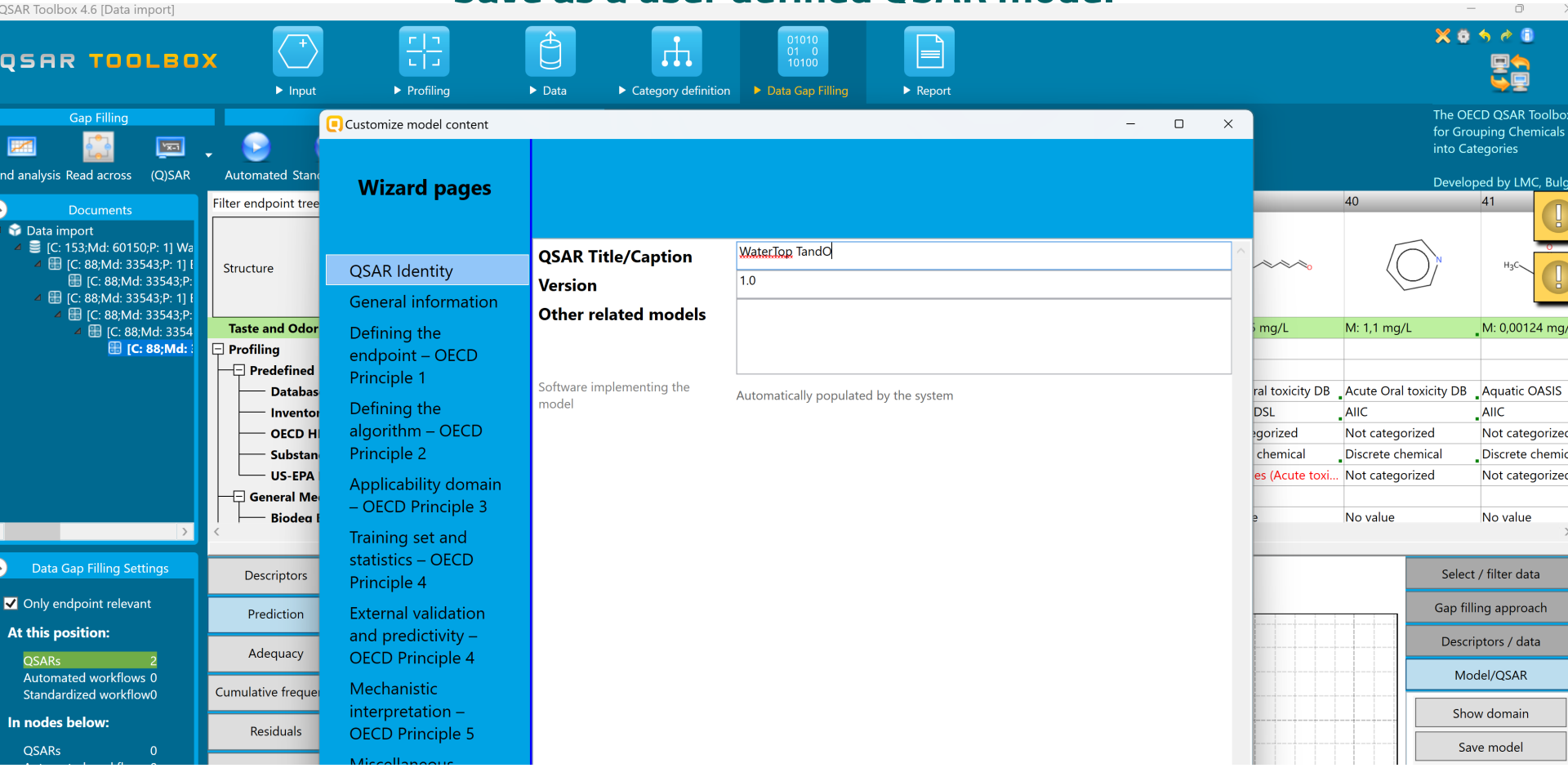
Trend analysis illustration



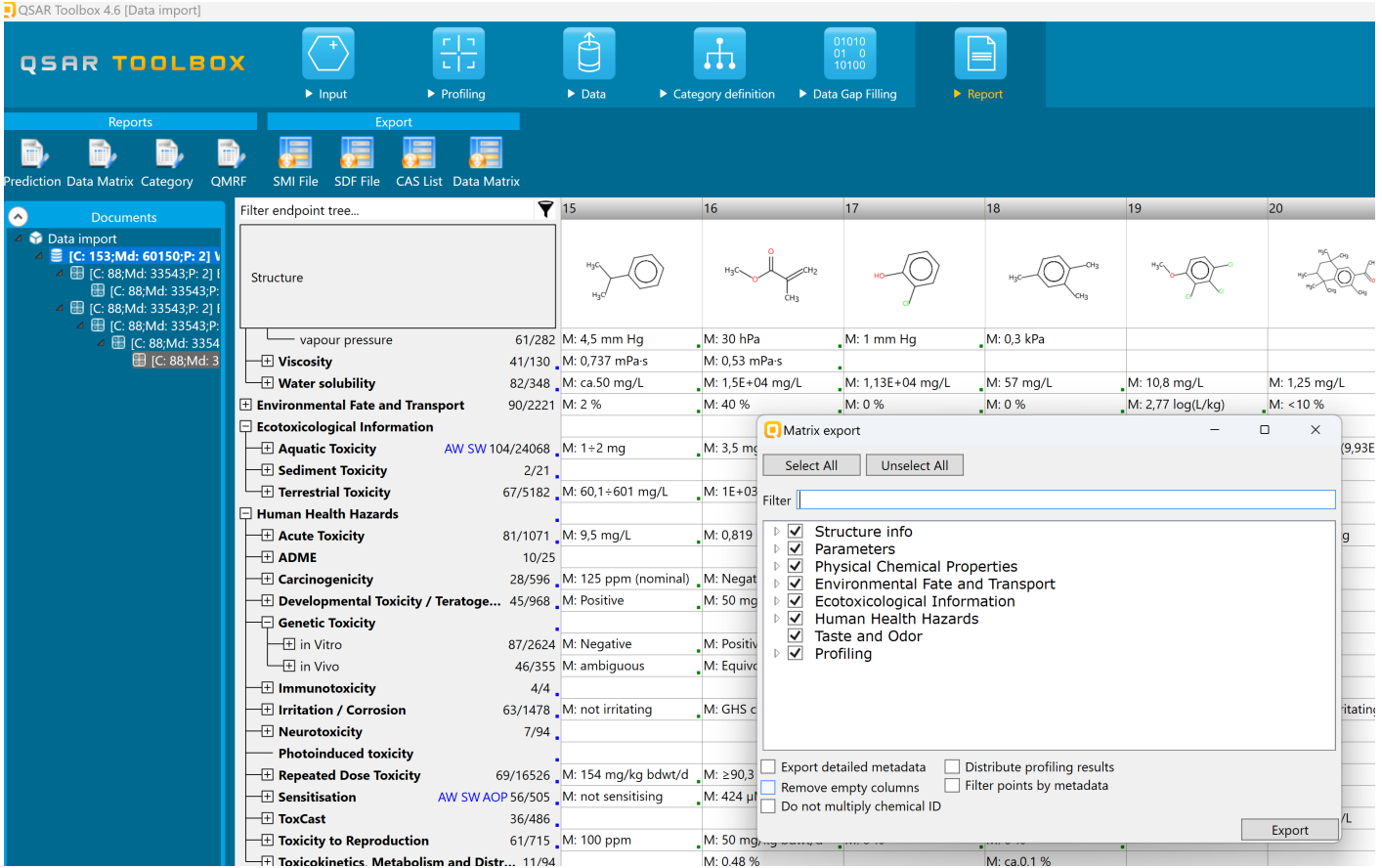
Trend analysis illustration



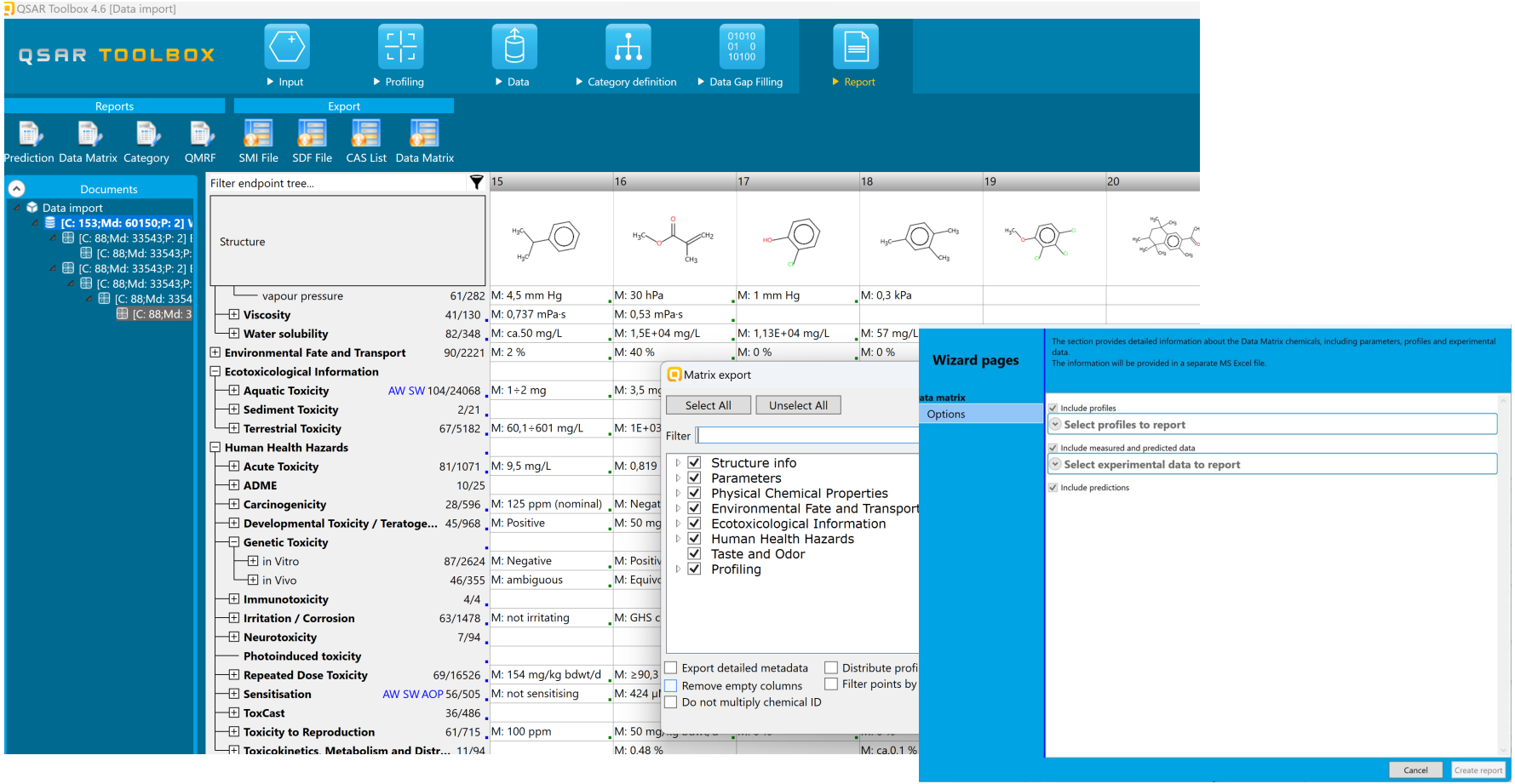
Save as a user defined QSAR model



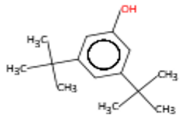
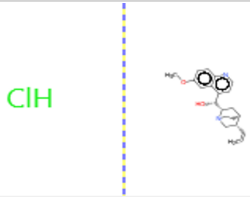
Export in Excel as a data matrix



Export in Excel/CSV as a data matrix



Export in Excel/CSV as a data matrix

		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	CCCCCCCCCC=O	CC(C)(C)c1cc(O)cc(c1)C(C)(C)C	Cl.COc1ccc2nccc([C@@H](O)[C@@H]3C[C@	OC(=O)CC(

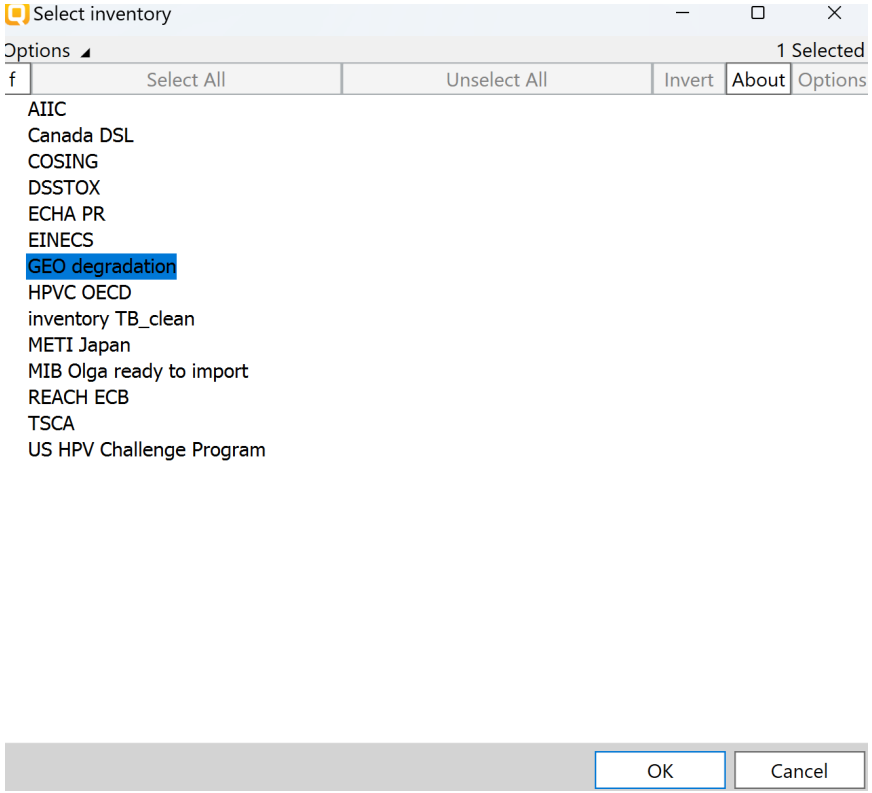
	Aquatic Toxicity	EC100	7	mg/L	Test organisms (species): Daphnia magna Endpoint: EC100 Duration: 24 h Reference source: Water Res.23(4): 495-499 Author: Kuhn,R., M. Pattard, K.D. Pernak, and A. Winter Title: Results of the Harmful Effects of Selected Water Pollutants (Anilines, Phenols, Aliphatic Compounds) to Daphnia magna Database: ECOTOX	
376							

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

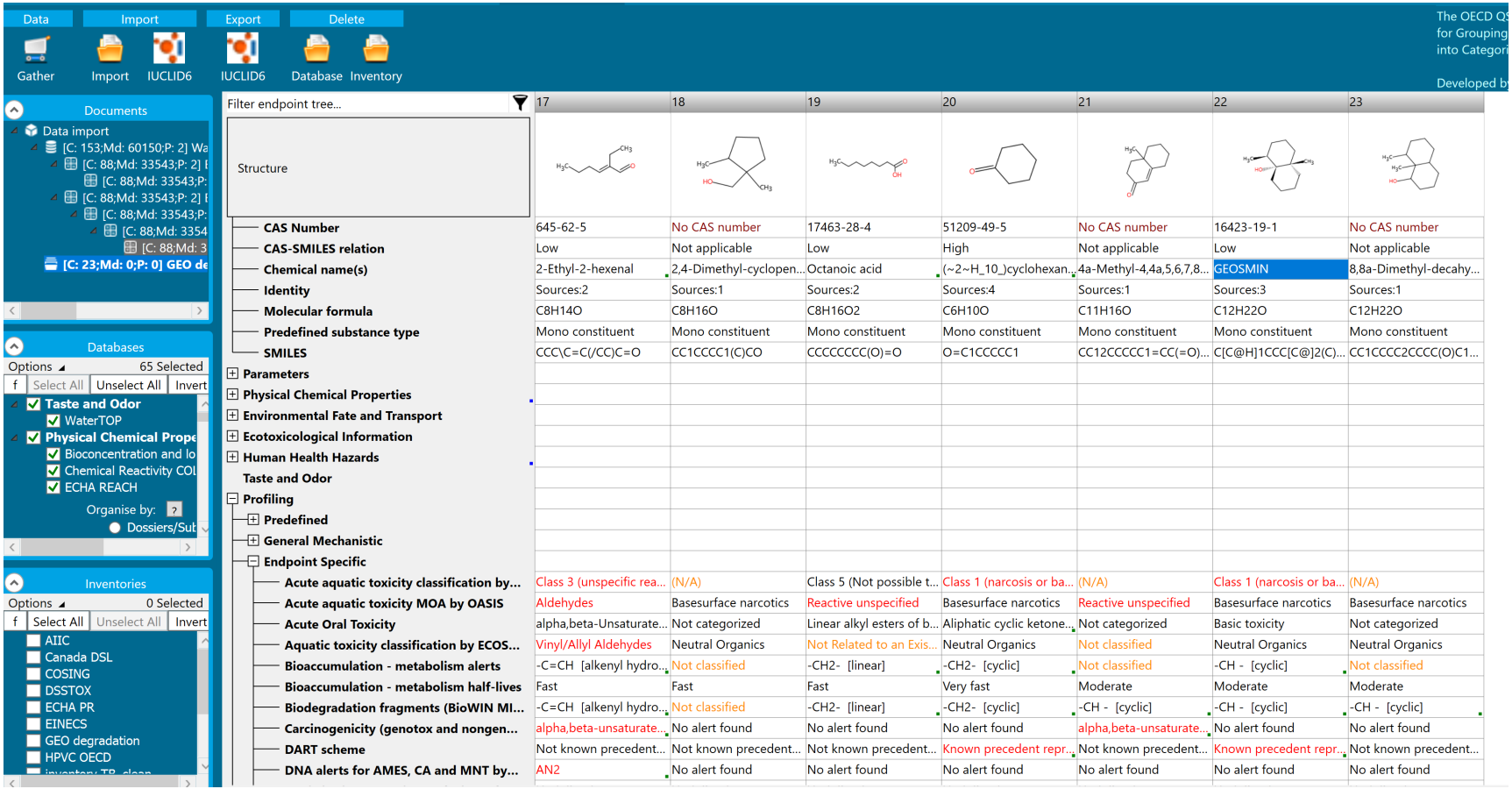
	smiles	name	CAS
VIIB	CC1(C)C2CCC1(C)C(C)(O)C2	2-Methylisoborneol	2371-42-8
	CC1=CC2CC[C@@]1(C)C2(C)C	1,2,7,7-Tetramethyl-bicyclo[2.2.1]hept-2	72540-93-3
I	CC1(C)C2CC[C@]1(C)C(=O)C2	1,6,7,7-Tetramethyl-bicyclo[2.2.1]hept-5-en-2-ol	
II	CC1=CC2CC(O)[C@@]1(C)C2(C)C	1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-o	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
V	CC1(C)C2CC[C@]1(C)C(=O)C2=O	1,7,7-Trimethyl-bicyclo[2.2.1]heptane-2,	2767-84-2
VI	CC1(C)C2CC(=O)[C@@]1(C)C(=O)C2	1,7,7-Trimethyl-bicyclo[2.2.1]heptane-2,6-dione	
VII	CCc1cc(C)oc1C	3-Ethyl-2,5-dimethyl-furan	10599-62-9
VIII	CC\C=C\CC1C(C)COC1=O	4-Methyl-3-pent-2-enyl-dihydro-furan-2-one	chemsketch
X	CC1CCC(C=O)=CC1(C)C	2,3,4,5-Tetramethyl-cyclopent-2-enone	5445
X	CC1=CC[C@@H](CC=O)C1(C)C	(2,2,3-Trimethyl-cyclopent-3-enyl)-aceta	4501-
XI	CC1CCC(C=O)=CC1(C)C	3,3,4-Trimethyl-cyclohex-1-enecarbaldehyde	
XII	CC(C)\C=C\C=C(/C)C	2,6-Dimethyl-hepta-2,4-diene	4634-
XIII	CCCC(C)\C=C\C	4-Methyl-hept-2-ene	3404-
XIV	CC1(C)C2CCC1(C)C(=C)C2		
XV	CC1(C)C2CCC(C)(C2)C1=C		
XVI	CC1=CC2CCC1(C)C2(C)C		
XVII	CC1(C)C2CCC1(C)C(=O)O2		
XVIII	CC1(C)C2(C)CCC1(O)CC2=O		
XIX	CC1(C)C2CCC1(CC2=O)C(O)=O		

CAS	Name	SMILES	Identity
16423-19-1	GEOSMIN	C[C@H]1CCC[C@]2(C)CCCC[C@@]12O	Geosmine
	8a-Hydroxy-4a-methyl-octahydro-napht	CC12CCCC[C@@]1(O)CC(=O)CC2	IV
	4a-Methyl-4,4a,5,6,7,8-hexahydro-3H-na	CC12CCCCC1=CC(=O)CC2	V
	8,8a-Dimethyl-decahydro-naphthalen-1-	CC1CCCC2CCCC(O)C12C	VI
4423-94-3	2-Ethyl-cyclohexanone	CCC1CCCCC1=O	VII
	7a-Methyl-1,4,5,6,7,7a-hexahydro-inden	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
99-82-1	1-Isopropyl-4-methyl-cyclohexane	CC1CCC(CC1)C(C)C	XIV
	3-(2,6,6-Trimethyl-cyclohex-2-enyl)-prop	CC1=CCCC(C)(C)C1\C=C\C=O	XV
	1-(2-Methoxy-cyclohexyl)-propan-2-one	COC1CCCCC1CC(C)=O	XVI
51209-49-5	Cyclohexanone	O=C1CCCCC1	XVII
1333-44-4	2,2-Dimethyl-cyclohexanone	CC1(C)CCCCC1=O	XVIII
27939-60-2	3,5-Dimethyl-cyclohex-3-enecarbaldehy	CC1CC(CC(C)=C1)C=O	XIX
2408-37-9	2,2,6-Trimethyl-cyclohexanone	CC1CCCC(C)(C)C1=O	XX
	5-Acetyl-3,3-dimethyl-cyclohexanone	CC1CC(CC(=O)C1)C(C)=O	XXI
78-59-1	3,5,5-Trimethyl-cyclohex-2-enone	CC1CC(C)(C)CC(=O)C=1	XXII
645-62-5	2-Ethyl-hex-2-enal	CCC\C=C(/CC)C=O	XXIII
17463-28-4	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

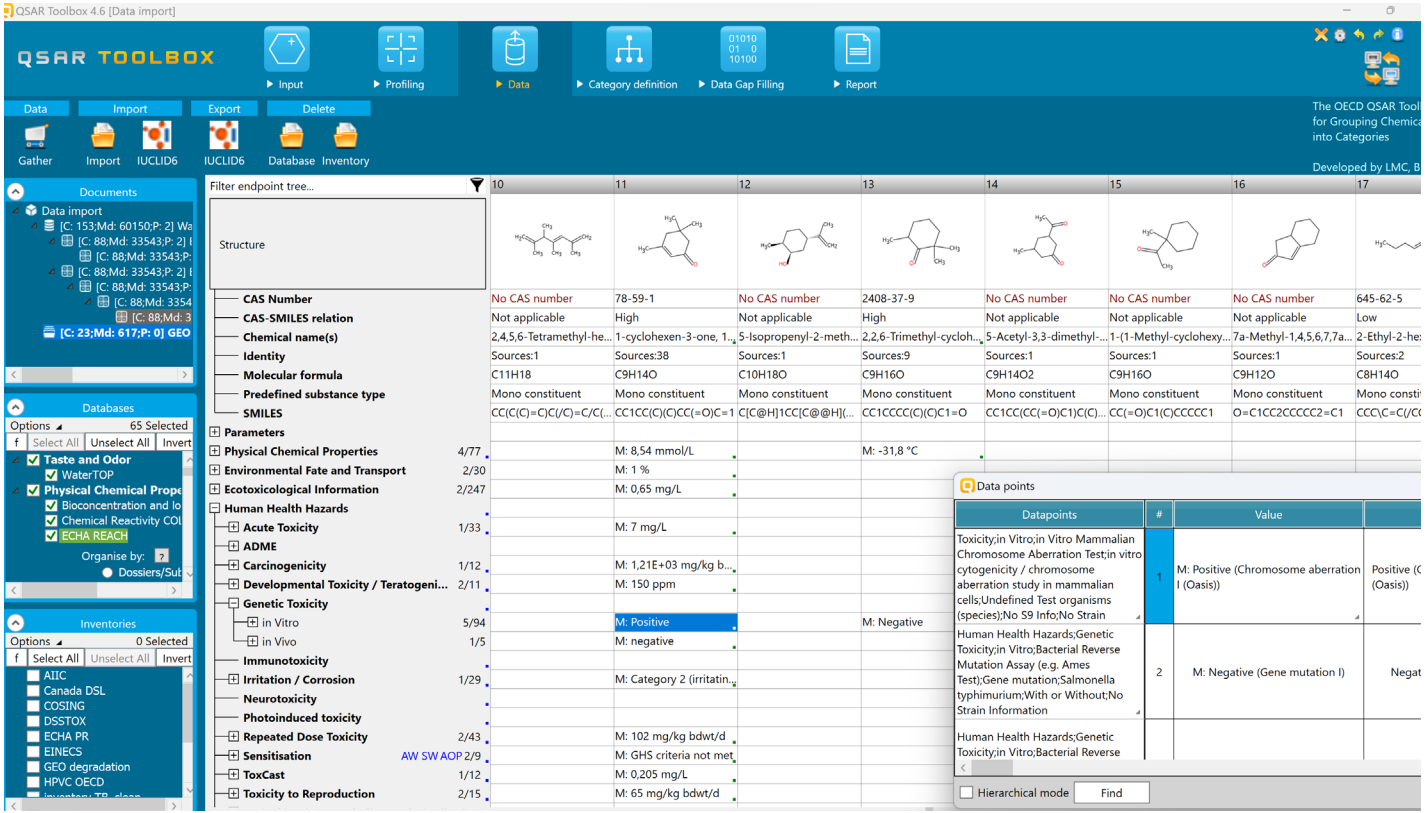
Import of degradation data of Geosmin and MIB as a custom inventory



Geosmin and its degradation products: profiling results



Geosmin and its degradation products: data collection results



Thank you very much!