

QSAR Application Toolbox – ukázka tvorby QSAR modelu

Státní zdravotní ústav, Šrobárova 48, 10042, Praha 10

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- **Tato presentace demonstruje vytvoření QSAR modelu pro předpověď akutní toxicity aldehydů na prvocích *Tetrahymena pyriformis***
 - předpověď akutní toxicity cílové chemikálie
 - vytvoření QSAR modelu založeného na predikci
 - použití modelu na další aldehydy
 - export výsledků predikce do souboru



QSAR Application Toolbox

The image displays three vertical workflow tracks within a software interface. Each track consists of a sequence of steps represented by buttons. The steps are: Chemical input, Profiling, Endpoints, Filling data gap, and Report. The Flexible Track track includes an additional step, Category definition, between Endpoints and Filling data gap. The Flexible Track track is highlighted with a red oval.

Track	Step 1	Step 2	Step 3	Step 4	Step 5	Step 6	Step 7
(Q)SAR Track	Chemical input	Profiling	Endpoints	Filling data gap	Relevant (Q)SARs	Report	
Category Track	Chemical input	Profiling	Endpoints	Category definition	Filling data gap	Read Across Trend Analysis Relevant (Q)SARs	Report
Flexible Track	Chemical input	Profiling	Endpoints	Category definition	Filling data gap	Read Across Trend Analysis Relevant (Q)SARs	Report

Vybraná chemikálie – Furfural, CAS 98011

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QSAR Application Toolbox
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Options Tracks

Chemical input Profiling Endpoints Category definition Filling data gap Report

Single chemical

Chemical Name
CAS #
SMILES / InChi
Drawing
Select from an existing list
Select from an inventory
Select from a database

Chemical list

User Lists
Regulatory Inventories
Database
Reset

Find chemical by CAS #

CAS # 98011 Search OK Cancel

Chemical name: 2-furaldehyde

The image shows a screenshot of the OECD Toolbox 1.00 software interface. The main window is titled "QSAR Application Toolbox" and features a navigation bar with buttons for "Options", "Tracks", "Chemical input", "Profiling", "Endpoints", "Category definition", "Filling data gap", and "Report". On the left side, there are two main sections: "Single chemical" and "Chemical list". The "Single chemical" section includes buttons for "Chemical Name", "CAS #", "SMILES / InChi", "Drawing", "Select from an existing list", "Select from an inventory", and "Select from a database". The "Chemical list" section includes buttons for "User Lists", "Regulatory Inventories", "Database", and "Reset". A modal dialog box titled "Find chemical by CAS #" is open in the center, showing a search input field with "CAS # 98011" (circled in red), a "Search" button, and "OK" and "Cancel" buttons. Below the search field, the chemical name "2-furaldehyde" is displayed. The chemical structure of 2-furaldehyde is shown as a skeletal structure of a furan ring with an aldehyde group (-CHO) attached to the 2-position.

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OECD
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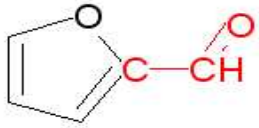
QSAR Application Toolbox

Options Tracks

Category definition Filling data gap Report STOP

Profile Explainer

Target chemical



Classified by:
Protein Binding

Classified as:
Schiff base formation

Met requirements

The target chemical has the fragment CC(H)=O in its structure.

Profiling methods

- S...
- Ec...
- O...
- D...
- Pr...
- O...
- C...
- Ve...

Empirical

- Lip...
- Ch...
- Gr...

Custom

- M...
- M...
- Ne...

Metabolism

Documented

- Observed Microbial metabolism
- Observed Liver metabolism

Simulated

- CATABOL Microbial metabolism
- Hydrolysis
- Microbial metabolism simulator

Show Category Boundaries

Create a new profiler

Delete profiler

Single chemical

EcoSAR Classification	Aldehydes
OASIS Acute Toxicity MOA	Aldehydes
DNA Binding	No Binding
Protein Binding	<u>Schiff base formation</u>
Organic functional groups	Aldehyde
	Conjugated hydroc...
	Ether (cyclic)
	Heterocyclic fragment
Cramer classification	High (Class III)
Verhaar classification	Class 3 (unspecific ...)
Lipinski Rule	Molecule satisfies t...
Chemical elements	Group 14 - Carbon C
Groups of elements	Group 16 - Oxygen O
Michael Type NA - Pote...	Non-Metals
	(N/A)

Dvojklik ukáže schéma profilace

Tato chemikálie může reagovat s proteiny pomocí formace Schiffovy báze.



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- Options
- Tracks
- Chemical input
- Profiling
- Endpoints
- Category definition
- Filling data gap
- Report

Gather data

Data Summaries

- Tested
- Estimated
- Both

IUCLID5 Import

IUCLID5 Export

Import

Export

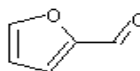
Databases

- Danish EPA
- ECETOC
- ECOTOX
- ISSCAN Genotox
- OASIS Aquatic
- OASIS Bioaccumulation
- OASIS Biodegradation
- OASIS ERBA
- OASIS Genotox
- OASIS Skin sensitization

Inventories

- Canadian DSL
- Danish EPA
- EU EINECS
- MITI Japan
- OECD HPVC Inventory
- US EPA HPVC
- US EPA TSCA

Structure



1 (Target)

Inventory Affiliation

- Canadian DSL
- Danish EPA
- EU EINECS
- MITI Japan
- OECD HPVC Invent...
- US EPA HPVC
- US EPA TSCA

Substance type

Discrete chemical

OECD categorization

(N/A)

US EPA Categorization

Aldehydes

Superfragment profiling

No superfragment

EcoSAR Classification

Aldehydes

OASIS Acute Toxicity MOA

Aldehydes

DNA Binding

No Binding

Protein Binding

Schiff base formation

Organic functional groups

- Aldehyde
- Conjugated hydroc...
- Ether (cyclic)
- Heterocyclic fragment

Cramer classification

High (Class III)

Verhaar classification

Class 3 (unspecific ...

Lipinski Rule

Molecule satisfies t...

Chemical elements

Group 14 - Carbon C

Groups of elements

Group 16 - Oxygen O

Michael Type NA - Pote...

(N/A)

Single chemical



QSAR Application Toolbox

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Options

Chemical input

Profiling

Endpoints

Category definition

Filling data gap

Report

Tracks

Gather data

Data Summaries

- Tested
 Estimated
 Both

IUCLID5 Import

IUCLID5 Export

Import

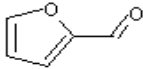
Export

Databases

- Danish EPA
 ECETOC
 ECOTOX
 ISSCAN Gentox
 OASIS Aquatic
 OASIS Bioaccumulation
 OASIS Biodegradation
 OASIS ERBA
 OASIS Genotox
 OASIS Skin sensitization

Inventories

- Canadian DSL
 Danish EPA
 EU EINECS
 MITI Japan
 OECD HPVC Inventory
 US EPA HPVC
 US EPA TSCA

1 (Target)	
Structure	
Substance Information	
— CAS Number	98-01-1
— OECD Global portal	eChemPortal
— Name (OECD name)	2-furaldehyde
— Structural Formula	C1(C=O)=CC=CO1
Profile	
⊕ Environmental Fate	(1/1) T: 9,35E+001 %
Ecotoxicological Information	
⊖ Aquatic Toxicity	
⊕ Animalia	(1/23) T: 1,06E+001 mg/l,...
⊖ Protozoa	
⊖ Tetrahymena pyrifo...	
⊖ IGC50	
— 48 h	(1/1) T: 1,45E+002 mg/l
⊕ Toxicological Inform...	(1/26) T: 6,83E+002 mg/k...

V tomto příkladě budeme vytvářet QSAR model pro odhad následujícího účinku:

Ecotoxicological Information
Aquatic Toxicity
Protozoa
Tetrahymena pyriformis
IGC50
48h

Trendová analýza vybraných aldehydů

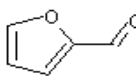

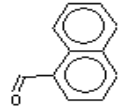
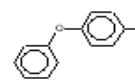
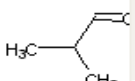
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Options | Tracks | Chemical input | Profiling | Endpoints | Category definition | Filling data gap | Report

Read-across | Trend analysis | (Q)SAR models | Apply

Target endpoint:
Ecotoxicological Information Aquatic Toxicity
Protozoa Tetrahymena pyriformis IGC50 48 h

	1 (Target)	10	12	13	17
Structure					
48 h (96/96)	T: 1,45E+002 mg/l	T: 1,52E+002 mg/l	T: 5,94E+001 mg/l	T: 1,09E+001 mg/l	T: 1,94E+002 mg/l

Select data points...

Data:
 All values
 Average value
 Min value
 Max value

Descriptors: Endpoint | Adequacy | Cumul. frequency | Statistic

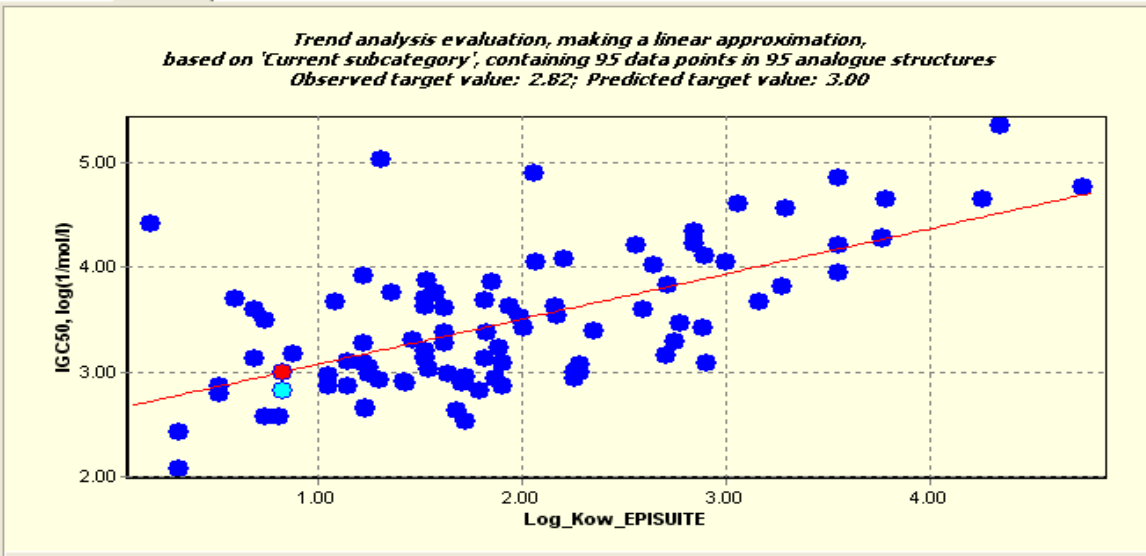
Prediction
Accept | Cancel

Data points
Subcategor. | Back | Fwd | Restore

Model
Trend analysis approx.:
Linear

Save QMRF | Save model

Aldehydes (US EPA Categorization) 48 h



Subkategorizace

Subcategorization

Grouping methods:

- Predefined
 - Database Affili...
 - Inventory Affili...
 - Substance type
 - OECD categoriz...
 - US EPA Catego...
- Mechanistic
 - Superfragment
 - EcoSAR Classifi...
 - OASIS Acute To...
 - DNA Binding
 - Protein Binding**
 - Organic functio...
 - Cramer classifi...
 - Verhaar classifi...
- Empiric
 - Lipinski Rule
 - Chemical eleme...
 - Groups of elem...
 - Structure simila...
- Custom
 - Michael Type N...
 - Mechanistic bou...
 - New profiler

Adjust options

Target: Schiff base formation

Order from target:
 At least on...
 All categor...

Analogues:
 (23) Michael-type nucle...
 (48) No Binding
 (1) Nucleophilic addition
 (1) Nucleophilic substitu...
 (46) Schiff base format...

Metabolism:
Do not account me...
Documented
 Observed Microbi...
 Observed Liver me...
Simulated
 CATABOL Microbi...
 Hydrolysis
 Microbial metaboli...
 GI tract simulator
 Liver metabolism s...
 Skin metabolism si...

Select different
Remove

QSAR Application Toolbox

Generation and Development

Profiling | Endpoints | **Category definition** | Filling data gap | Report

	1 (Target)	10	12	13	17
Structure					
48 h (96/96)	T: 1,45E+002 mg/l	T: 1,52E+002 mg/l	T: 5,94E+001 mg/l	T: 1,09E+001 mg/l	T: 1,94E+002 mg/l

Descriptors | Endpoint | Adequacy | Cumul. frequency | Statistic

Trend analysis evaluation, making a linear approximation, based on 'Current subcategory', containing 95 data points in 95 analogue structures
Observed target value: 2.82; Predicted target value: 3.00

IGC50, log(1/moll)

Log_Kow_EPISUITE

Descriptors: Log_Kow_EPISUITE
 show descriptors in use only

Prediction
Accept
Cancel

Data points
Subcategor...
Back Fwd
Restore

Model
Trend analysis approx.:
Linear
Save QMRF
Save model

Aldehydes (US EPA Categorization)

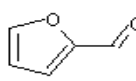
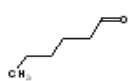
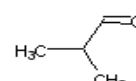
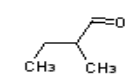
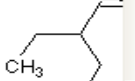
Výsledek po subkategorizaci

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Options Tracks

Chemical input Profiling Endpoints Category definition Filling data gap Report

Structure	1 (Target)	10	17	32	33
Structure					
48 h (96/96)	T: 1,45E+002 mg/l	T: 1,52E+002 mg/l	T: 1,94E+002 mg/l	T: 1,93E+002 mg/l	T: 1,12E+002 mg/l

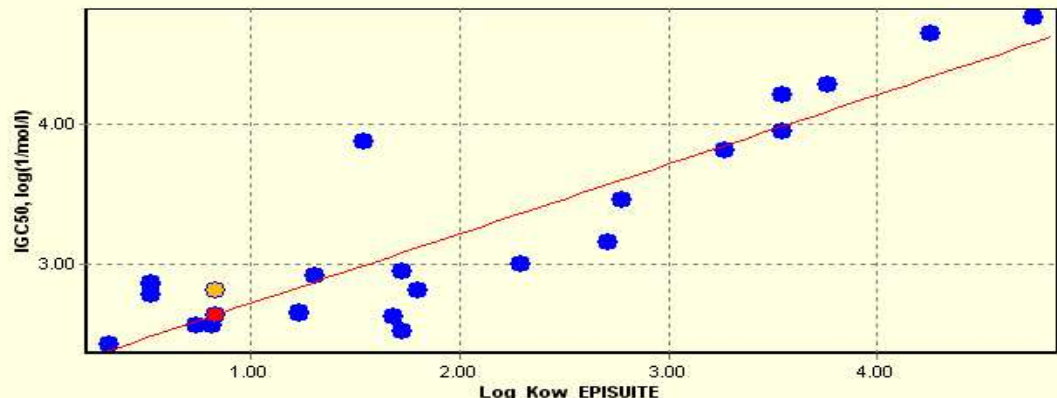
Target endpoint:
Ecotoxicological Information Aquatic Toxicity Protozoa Tetrahymena pyriformis IGC50 48 h

Select data points...

Data
 All values
 Average value
 Min value
 Max value

Descriptors Endpoint Adequacy Cumul. frequency Statistic

Trend analysis evaluation, making a linear approximation, based on 'Current subcategory', containing 23 data points in 23 analogue structures
Observed target value: 2.82; Predicted target value: 2.64



IGC50, log(1/mol/l)

Log_Kow_EPISUITE

Descriptors: Log_Kow_EPISUITE
 show descriptors in use only

Prediction
 Accept
 Cancel

Data points
 Subcategor.
 Back Fwd
 Restore

Model
 Trend analysis approx.:
 Linear
 Save QMRF
 Save model

start

D:\Tool... QSAR... OECD T... TB_QSA... TB_Aqu... EN 11:16

Vyhodnocení QSAR modelu

OECD Toolbox 1.00

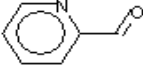
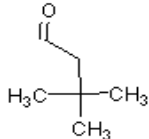

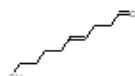
QSAR Application Toolbox
Organization for Economic Co-operation and Development

Options | Chemical input | Profiling | Endpoints | Category definition | Filling data gap | Report

Tracks

Read-across | Trend analysis | (Q)SAR models | Apply

Target endpoint:
Ecotoxicological Information Aquatic Toxicity Protozoa Tetrahymena pyriformis IGC50 48 h

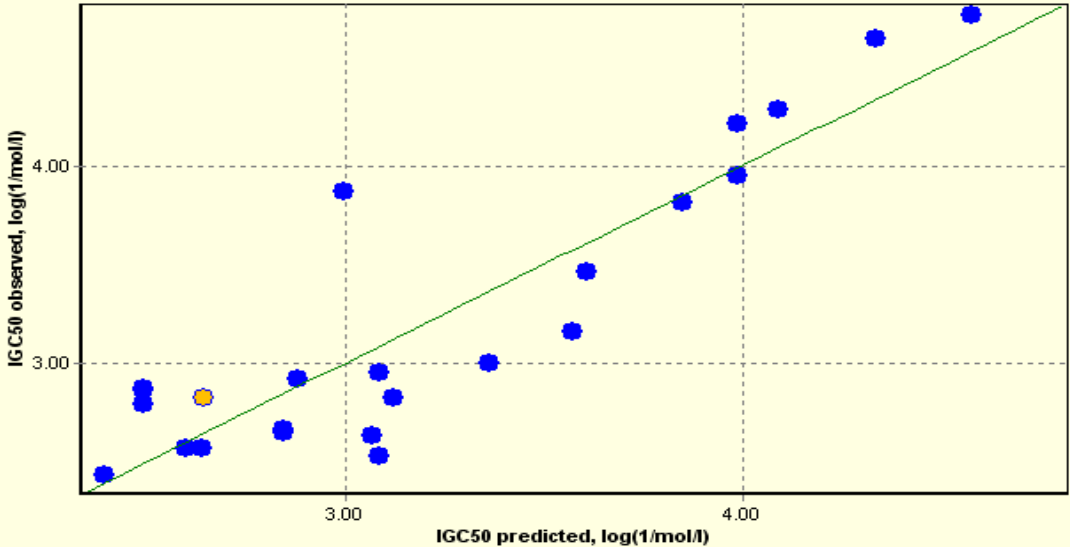
Structure	145	172	230	253
				
48 h (96/96)	T: 1,48E+002 mg/l	T: 2,35E+002 mg/l	T: 1,73E+001 mg/l	T: 9,51E+000 mg/l

Select data points...

Data
 All values
 Average value
 Min value
 Max value

Descriptors | Endpoint | Adequacy | Cumul. frequency | **Statistic**

Statistic for the analogues: $R^2 = 0.797$, $s = 0.322$



IGC50 observed, log(1/mol/l)

IGC50 predicted, log(1/mol/l)

Prediction
 Accept
 Cancel

Data points
 Subcategor. | Back | Fwd | Restore

Model
 Trend analysis approx.:
 Linear

Save QMRF
 Save model

Aldehydes (US EPA Categorization)

Vyhodnocení QSAR modelu - statistika

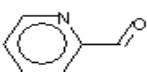
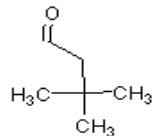
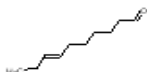

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Options Tracks Chemical input Profiling Endpoints Category definition Filling data gap Report

Read-across Trend analysis (Q)SAR models Apply

Target endpoint:
Ecotoxicological Information Aquatic Toxicity Protozoa Tetrahymena pyriformis IGCS0 48 h

Structure	145	172	230	253
				
48 h (96/96)	T: 1,48E+002 mg/l	T: 2,35E+002 mg/l	T: 1,73E+001 mg/l	T: 9,51E+000 mg/l

Select data points...

Data
 All values
 Average value
 Min value
 Max value

Descriptors	Endpoint	Adequacy	Cumul. frequency	Statistic
Statistical characteristics		Subcategory		
Number of data points, (N)		24		
Coeff. of determination, (R2, Q2)		0.797		
Coeff. of determination, adj., (R2adj)		0.788		
Residual standard deviation, (s)		0.322		
Fisher function, (F)		90.1		
Square root of the average squared r...		0.316		
b0 (Intercept)		2.23		
b1 (Log_Kow_EPISUITE)		0.494		
b2 ((Log_Kow_EPISUITE)^2)		-		

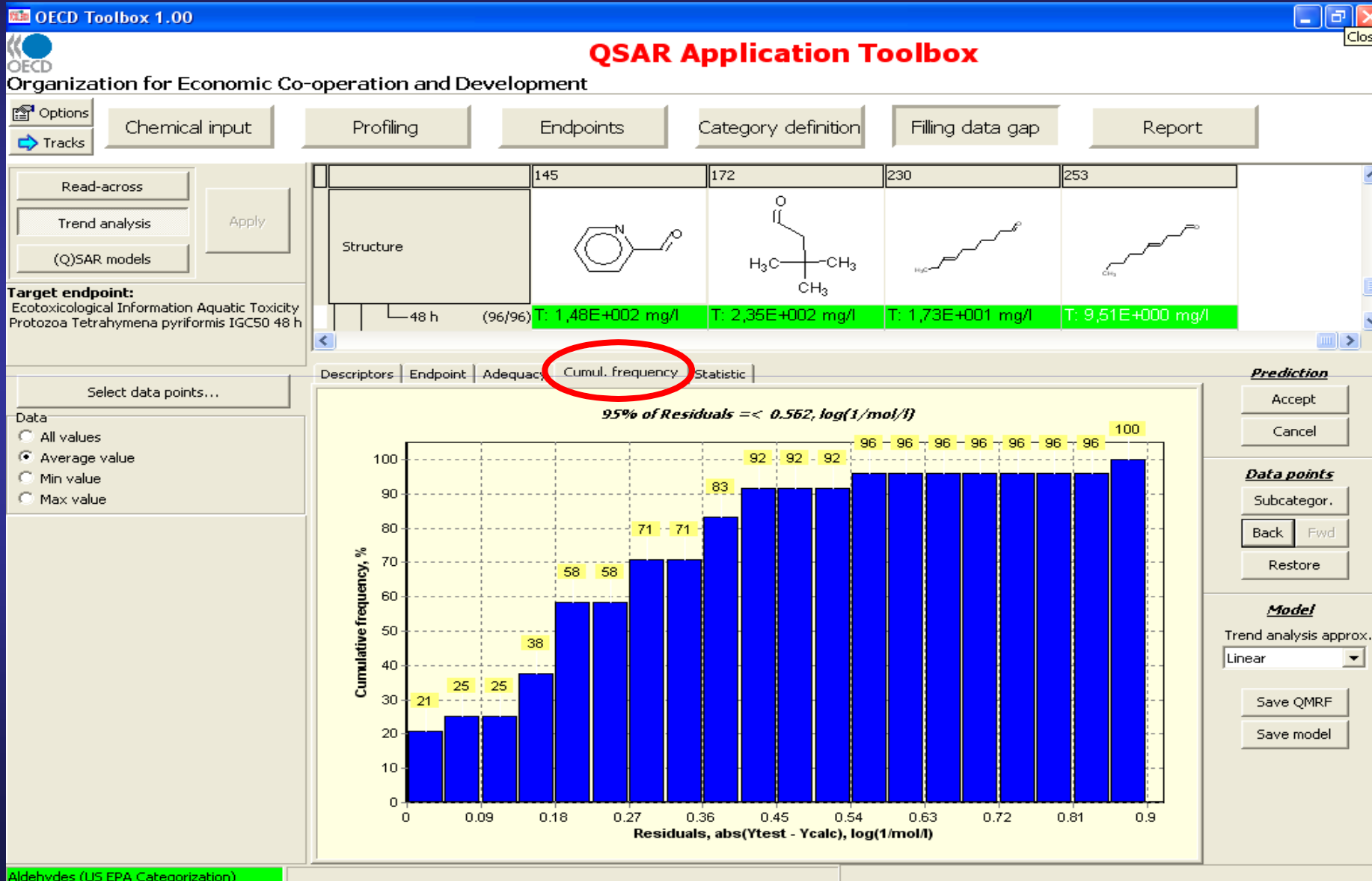
Prediction
Accept Cancel

Data points
Subcategor. Back Fwd Restore

Model
Trend analysis approx.: Linear
Save QMRF Save model

Aldehydes (US EPA Categorization)

Vyhodnocení QSAR modelu



Uložení vytvořeného QSAR modelu

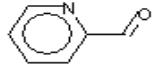
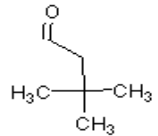

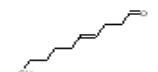
OECD Toolbox 1.00

QSAR Application Toolbox
Organization for Economic Co-operation and Development

Options | Tracks | Chemical input | Profiling | Endpoints | Category definition | Filling data gap | Report

Read-across | Trend analysis | (Q)SAR models | Apply

Target endpoint:
Ecotoxicological Information Aquatic Toxicity Protozoa Tetrahymena pyriformis IGC50 48 h

Structure	145	172	230	253
				
48 h (96/96)	T: 1,48E+002 mg/l	T: 2,35E+002 mg/l	T: 1,73E+001 mg/l	T: 9,51E+000 mg/l

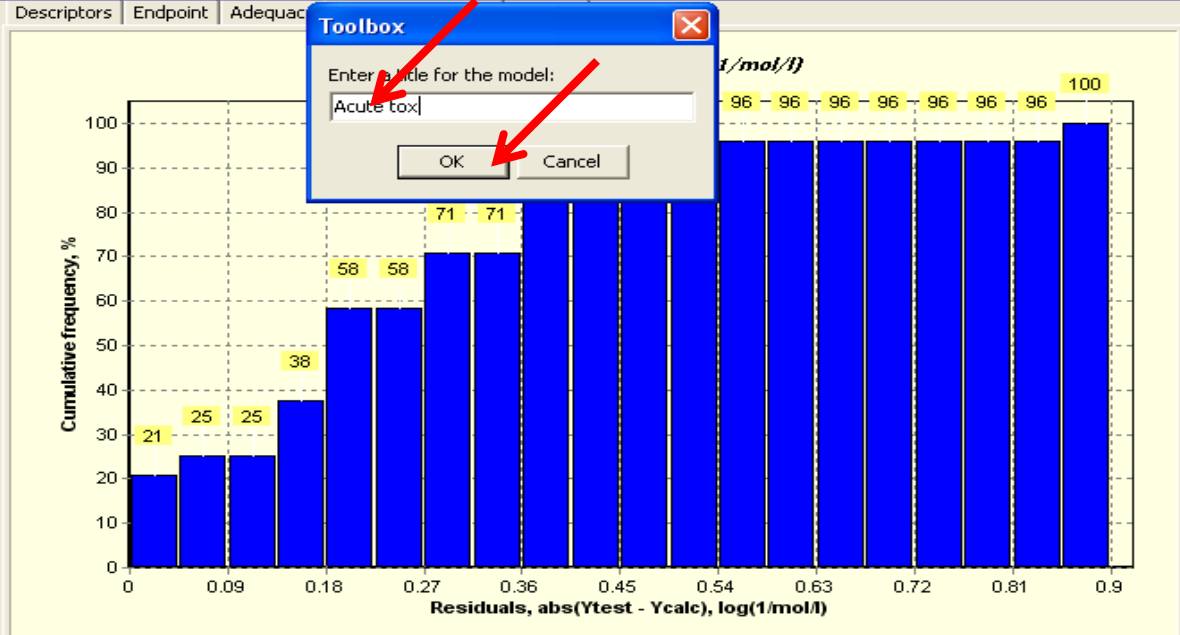
Select data points...
Data:
 All values
 Average value
 Min value
 Max value

Toolbox
Enter a title for the model:
[Acute tox]
OK Cancel

Prediction
Accept
Cancel

Data points
Subcategor.
Back Fwd
Restore

Model
Trend analysis approx.:
Linear
Save QMRF
Save model



Aldehydes (US EPA Categorization) | T=Tested; S= (Q)SAR; E= Estimated

Použití vytvořeného modelu QSAR

- Vytvoření seznamu chemikálii v testovacím setu**
- Vizualizace zda je chemikálie v aplikačním rozsahu modelu**
- Provedení predikce pro chemikálie v matici**

Testovací set

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QSAR Application Toolbox
Organization for Economic Co-operation and Development

Options | Tracks | Chemical input | Profiling | Endpoints | Category definition | Filling data gap | Report

Read-across | Trend analysis | (Q)SAR models | Apply

Target endpoint:
Ecotoxicological Information Aquatic Toxicity
Protozoa Tetrahymena pyriformis IGC50 48 h

Select data points...

Data
 All values
 Average value
 Min value
 Max value

QSAR models
<< CREATE A NEW QSAR >>
Acute tox

- Rank models
- Sort by date
- Model about
- Display domain
- Display QMRF
- Display training set**
- Display test set
- Predict endpoint
- Delete model
- Delete predicted values

Structure

Substance Information
CAS Number
OECD Global port
Name (OECD name)
Structural Formula

Profile
Environmental Fate
Ecotoxicological Information
Aquatic Toxicity
Algae
Animalia
Bacteria, Arch.
Plants
Protozoa
Tetrahymena
EC50
IC50
IGC50
48 h

Terrestrial Toxicity (10/31)
Toxicological Information (104/614) T: 6,83E+002 mg/k... T: 1,00E+000 T: 1,80E+000 % T: 1,00E+000

Aldehydes (US EPA Categorization)

Training set of: Acute tox

1 CAS# 98-01-1 Name: 2-furaldehyde IGC50=145 mg/l <chem>O=Cc1ccoc1</chem>	2 CAS# 66-25-1 Name: HEXANAL IGC50=152 mg/l <chem>CCCCC=O</chem>	3 CAS# 78-84-2 Name: Isobutylaldehyde IGC50=194 mg/l <chem>CC(C)CC=O</chem>	4 CAS# 96-17-3 Name: 2-methylbutyraldehyde IGC50=193 mg/l <chem>CC(C)CC=O</chem>	5 CAS# 97-9 Name: 2-E1 IGC50=112 <chem>CC=O</chem>
6 CAS# 110-62-3 Name: Pentanal IGC50=104 mg/l <chem>CCCCC=O</chem>	7 CAS# 111-71-7 Name: heptaldehyde IGC50=114 mg/l <chem>CCCCCC=O</chem>	8 CAS# 112-31-2 Name: Decyl_aldehyde IGC50=8,2 mg/l <chem>CCCCCCCCC=O</chem>	9 CAS# 112-44-7 Name: undecanal IGC50=3,9 mg/l <chem>CCCCCCCCC=O</chem>	10 CAS# 112-... Name: dodec... IGC50=3,2 <chem>CCCCCCCCC=O</chem>
11 CAS# 122-78-1 Name: PHENYLACETALDEHYDE IGC50=16,2 mg/l <chem>O=Cc1ccccc1</chem>	12 CAS# 123-05-7 Name: 2-Ethylhexanal IGC50=88,7 mg/l <chem>CCCCC(CC)C=O</chem>	13 CAS# 123-15-9 Name: Pentanal, 2-methyl- IGC50=296 mg/l <chem>CC(C)CCCC=O</chem>	14 CAS# 123-38-6 Name: propanal IGC50=216 mg/l <chem>CCC=O</chem>	15 CAS# 123-... Name: n-Bu... IGC50=194 <chem>CCCC=O</chem>

Save to smi | Search | OK

Vizualizace zda je chemikálie v aplikačním rozsahu modelu

OECD Toolbox 1.001

OECD
Organization for Economic Co-operation and Development

Options
Tracks

Chemical input | Profiling | Endpoints | Category definition | Filling data gap | Report

	1 (Target)	2	3	4	5	6	7
Structure							H ₂ C=O
Target							
4.87E+000							
48 h (96/96)	T: 1.45E+002 mg/l S: 2.18E+002 mg/l						
Tetrahymina... (4/11)							
Terrestrial Toxicity (10/31)							T: 1.67E-001 r
Toxicological Inf... (105/629)	T: 6.83E+002 mg/k...	T: 1.00E+000	T: 1.80E+000 %	T: 1.00E+000			T: 2.19E+000

Aldehydes (US EPA Categorization)

Provedení předpovědi účinku

OECD Toolbox 1.00

QSAR Application Toolbox
Organization for Economic Co-operation and Development

Options Tracks

Chemical input Profiling Endpoints Category definition Filling data gap Report

Read-across Trend analysis (Q)SAR models Apply

Target endpoint:
Ecotoxicological Information Aquatic Toxicity Protozoa Tetrahymena pyriformis IGC50 48 h

Select data points...

Data
 All values
 Average value
 Min value
 Max value

QSAR models
<< CREATE A NEW QSAR >>
Acute tox
Rank models
Sort by date
Model about
Display domain
Display QMRF
Display training set
Display test set
Predict endpoint
Delete model
Delete predicted values

Structure

	1 (Target)	2	3	4	5
Structure					
Substance Information					
— CAS Number	98-01-1	*0-03-2	*0-11-3	*0-18-3	10-01-5
— OECD Global portal	eChemPortal	eChemPortal	eChemPortal	eChemPortal	eChemPortal
— Name (OECD name)	2-fu...
— Structural Formula	C10...
Profile					
Environmental Fate (36/46)	T: 9...				
Ecotoxicological Information					
Aquatic Toxicity					
— Algae (15/43)					
— Animalia (93/967)	T: 1...				
— Bacteria, Arch... (17/38)					
— Plants (1/1)					
— Protozoa					
— Tetrahymena pyrifo...					
— EC50 (15/19)					
— EC10 (13/13)					
— EC20 (13/13)					
— EC50 (15/19)	T: 1,45E+002 mg/l S: 2,18E+002 mg/l				
— Tetrahymena... (4/11)					
— Terrestrial Toxicity (10/31)					
Toxicological Inf... (104/614)	T: 6,83E+002 mg/k...	T: 1,00E+000	T: 1,80E+000 %	T: 1,00E+000	

Information
Predicted 60 out of 274 structures.
OK

Aldehydes (US EPA Categorization)

Export výsledků do textového souboru

The screenshot shows the OECD Toolbox 1.00 interface. A dialog box titled "Export to..." is open, showing the save location as "C:\Documents and Settings\User\My Documents\OECD Toolbox\Ver 1.0\UserDir\t3.txt". The export type is set to "Horizontal". The target endpoint is "Ecotoxicological Information Aquatic Toxicity Protozoa Tetrahymena pyriformis IGC50 48 h". A red arrow points to the "Start" button in the dialog box.

Below the dialog box, a success message box is displayed: "OECD Toolbox 1.00 Export completed successfully." with an "OK" button. A red arrow points to the "OK" button.

The background shows a table of results for various chemicals. The table has columns for CAS Number, OECD Global portal, Name (OECD name), Structural Formula, and various toxicity endpoints. The table is partially obscured by the dialog boxes.

CAS Number	OECD Global portal	Name (OECD name)	Structural Formula	Environmental Fate	Ecotoxicological Information
67-36-7	eChemPortal	4-ph...	c1(C...	T: 8,00E+001 %	T: 1,09E+001 mg/l
67-47-0	eChemPortal			T: 6,20E+001 mg/l,...	
75-07-0	eChemPortal	aldehy...	C(C)=O	T: 2,74E+001 mg/l,...	
75-07-6	eChemPortal	Acetaldehyde	C(C)=O	T: 7,00E+000 %	
75-87-6	eChemPortal	Acetaldehyde, trich...	C(Cl)(Cl)(Cl)C=O	T: 1,70E+002 mg/l,...	
78-84-2	eChemPortal	Isobutylaldehyd	C(=O)C(C)C	T: 8,10E+001 %	

Ukázka exportovaných výsledků do textového souboru

CAS	NAME	SMILES	Endpoint name	Data	Dimension	SOURCE
000098-01-1	2-furaldehyde	<chem>C1(C=O)=CC=CO1</chem>	IGC50	1,45E+02	mg/l	Toxicology methods, 7, 289-309.
000098-01-1	2-furaldehyde	<chem>C1(C=O)=CC=CO1</chem>	IGC50	2,18E+02	mg/l	Trend:OECD Toolbox 1.00
000098-01-1	2-furaldehyde	<chem>C1(C=O)=CC=CO1</chem>	IGC50	2,18E+02	mg/l	(Q)SAR: Aldehydy
00000-18-3	n-decyl_succinic_acid	<chem>C(=O)(CCC=O)CCCCCCCC</chem>	IGC50	2,02E+01	mg/l	(Q)SAR: Aldehydy
000050-00-0	FORMALDEHYDE	<chem>C=O</chem>	IGC50	1,18E+02	mg/l	(Q)SAR: Aldehydy
000052-39-1	pregn-4-en-18-al,_11,21-d	<chem>C12C(C)(C3C(C4C(C=O)(C(C(=O)CO)CC4)CC3O)C1)CCC(=O)C=2</chem>	IGC50	1,20E+03	mg/l	(Q)SAR: Aldehydy

Děkuji Vám za pozornost!