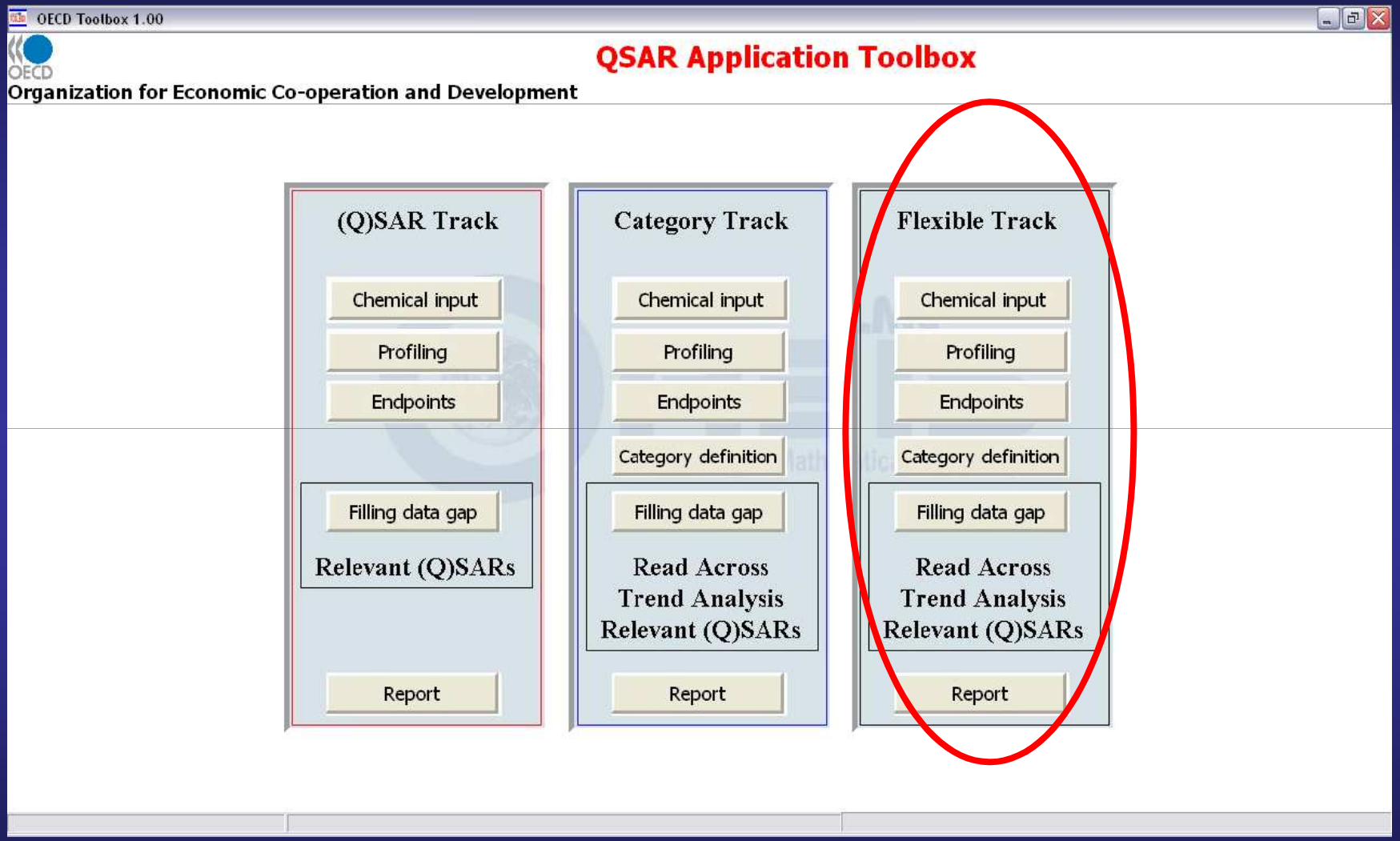
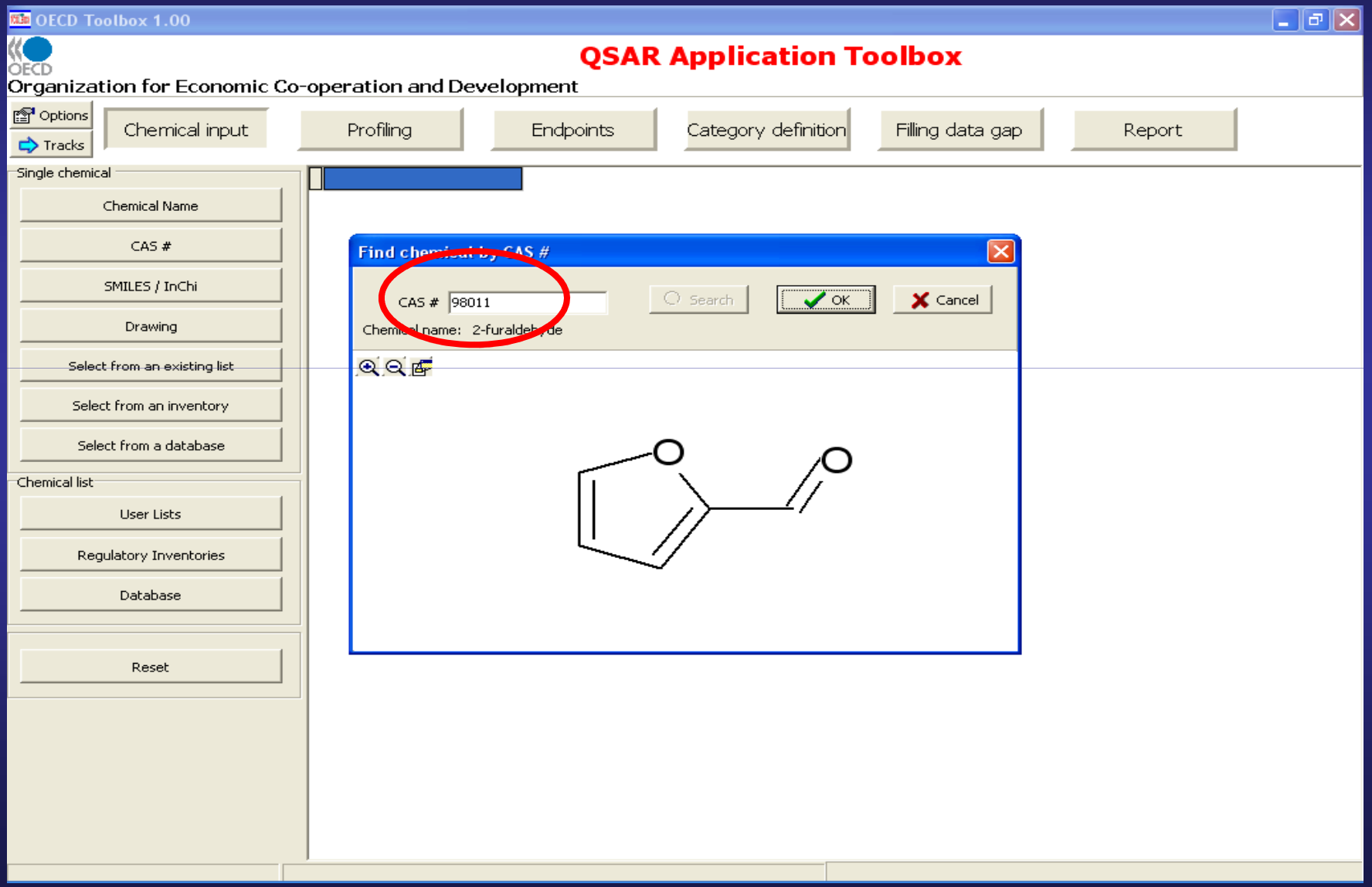
QSAR Application Toolbox – ukázka tvorby QSAR modelu

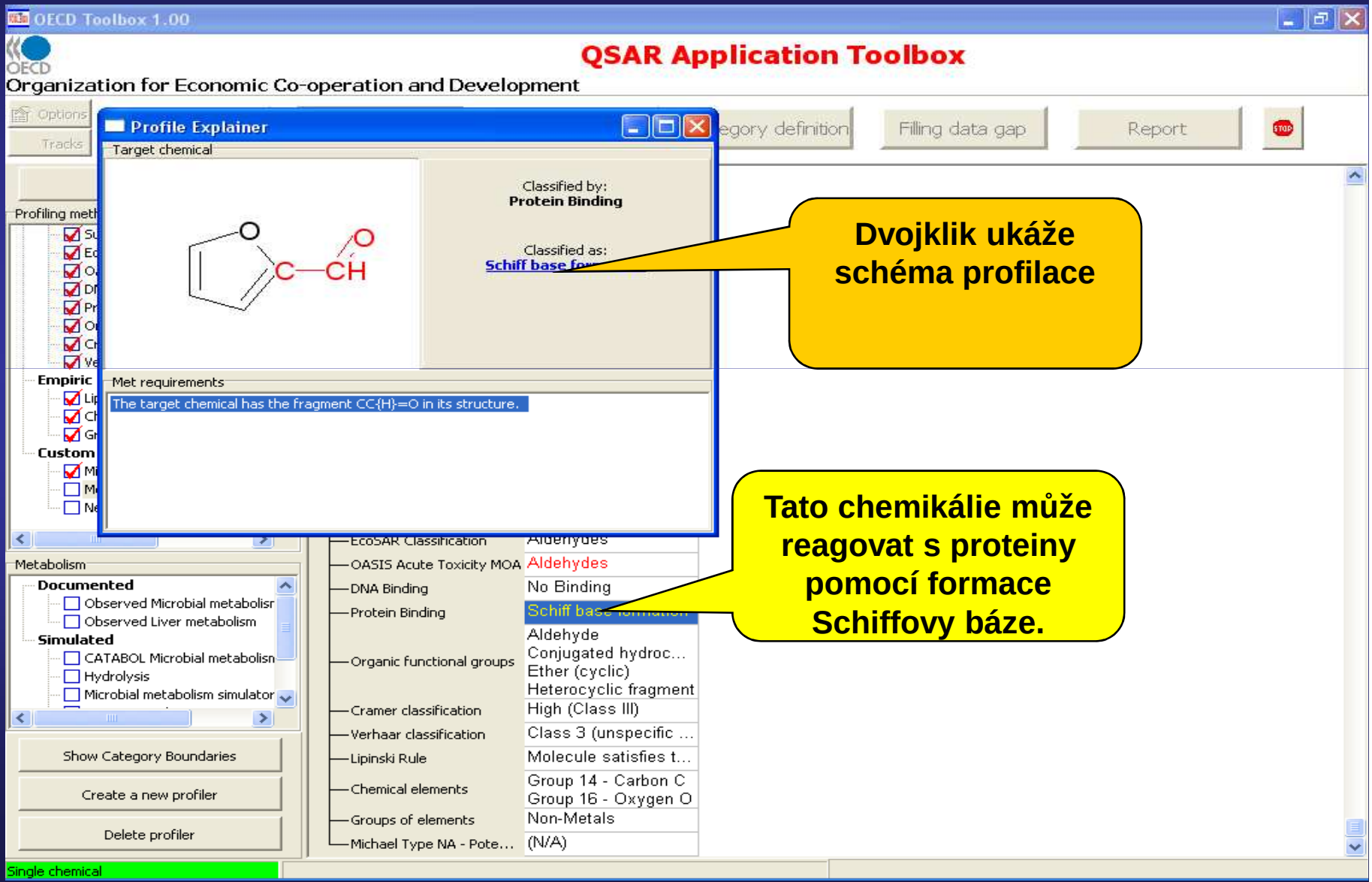
Státní zdravotní ústav, Šrobárova 48, 10042, Praha 10

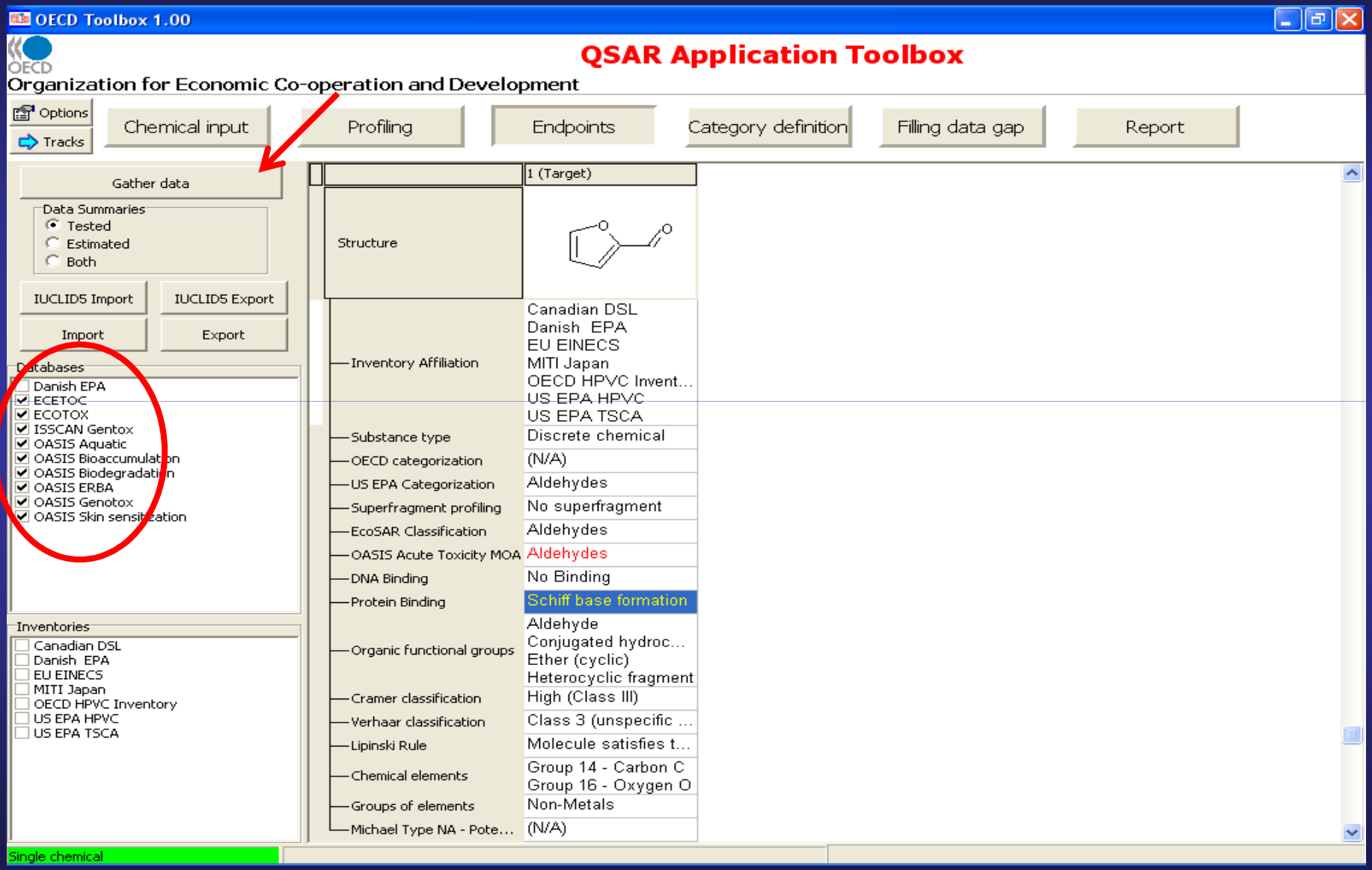
- **Tato presentace demonstruje vytvoření QSAR modelu pro předpověď akutní toxicity aldehydů na prvocích *Tetrahymena pyriformis***
  - **předpověd akutní toxicity cílové chemikálie**
  - **vytvoření QSAR modelu založeného na predikci**
  - **použití modelu na další aldehydy**
  - **export výsledků predikce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


OECD Toolbox 1.00
QSAR Application Toolbox
Organization for Economic Co-operation and Development
(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




OECD Toolbox 1.00
QSAR Application Toolbox
Organization for Economic Co-operation and Development
Profile Explainer
Target chemical
Classified by:
Protein Binding
Classified as:
Met requirements
The target chemical has the fragment CC{H}=O in its structure.
Dvojklik ukáže schéma profilace
Tato chemikálie může reagovat s proteiny pomocí formace Schiffovy báze.
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
OASIS Acute Toxicity MOA
Aldehydes
DNA Binding
No Binding
Protein Binding
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
Group 16 - Oxygen O
Groups of elements
Non-Metals
Michael Type NA - Pote...
(N/A)
Single chemical


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
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
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
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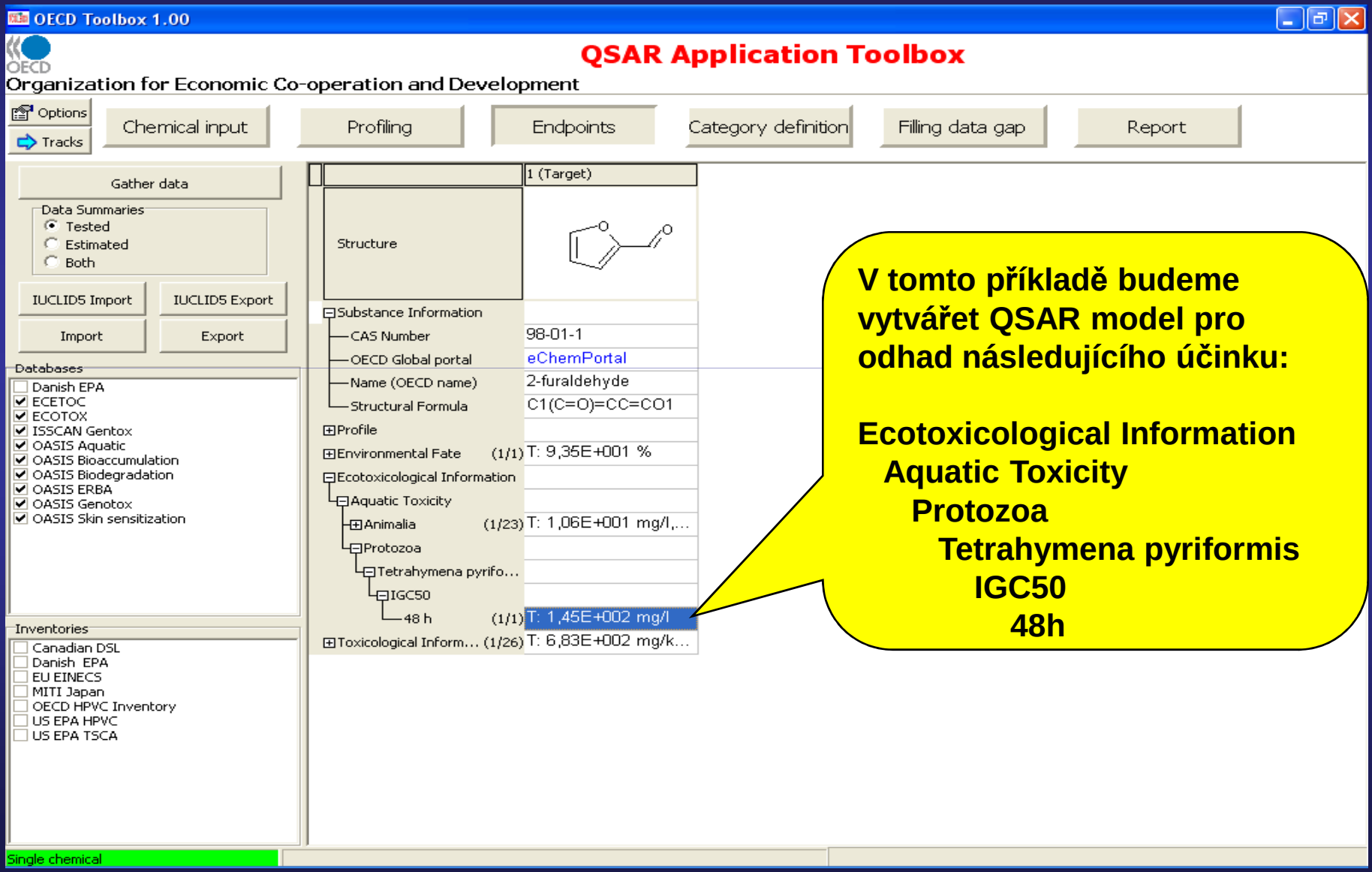
Groups of elements
Non-Metals
Michael Type NA - Pote...
(N/A)
Single chemical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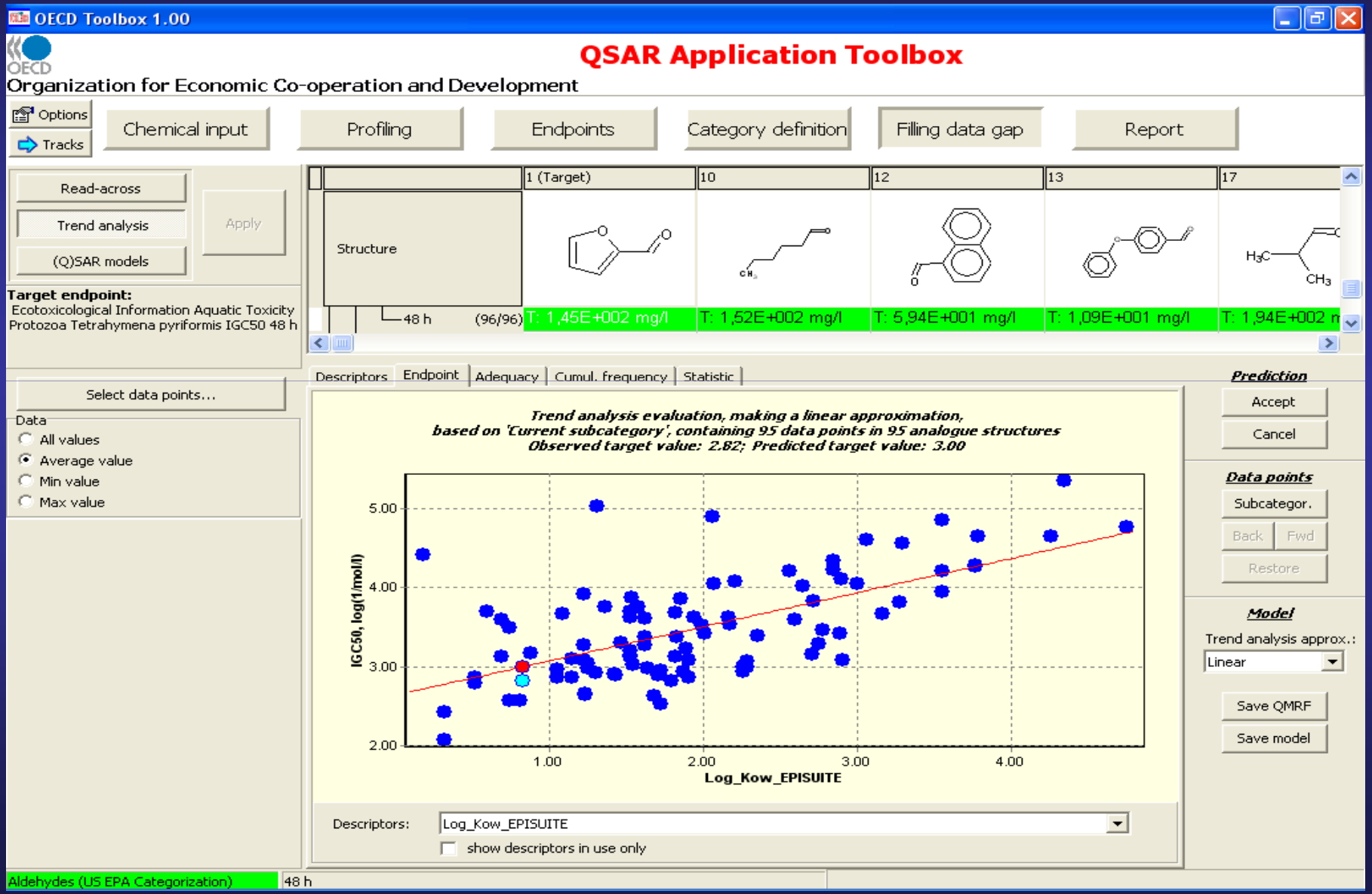
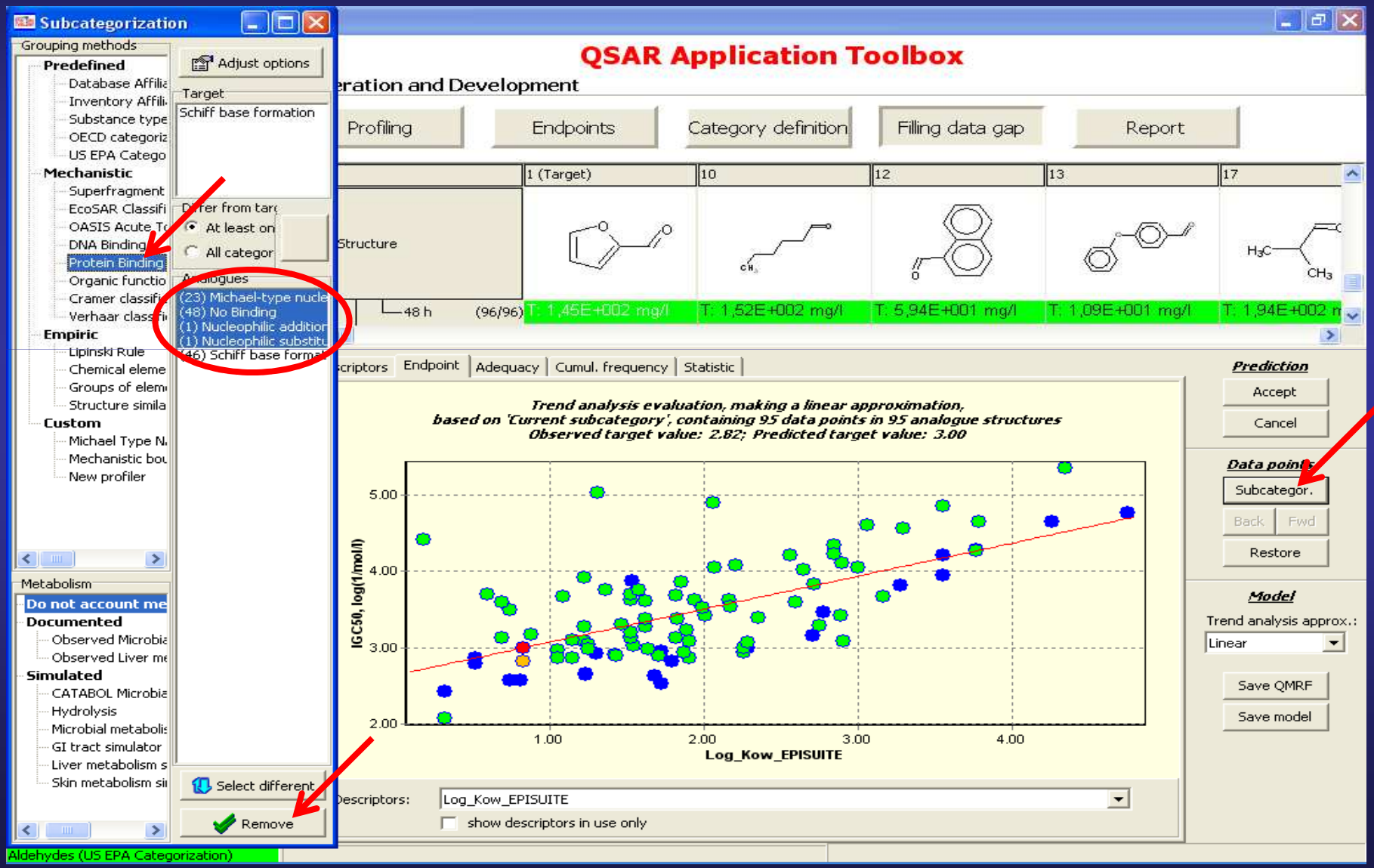
OASIS Skin sensitization
Inventories
Canadian DSL
Danish EPA
EU EINECS
MITI Japan
OECD HPVC Inventory
US EPA HPVC
US EPA TSCA
1 (Target)
Structure
Substance Information
CAS Number 98-01-1
OECD Global portal eChemPortal
Name (OECD name) 2-furaldehyde
Structural Formula C1(C=O)=CC=CO1
Profile
Environmental 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
Single chemical

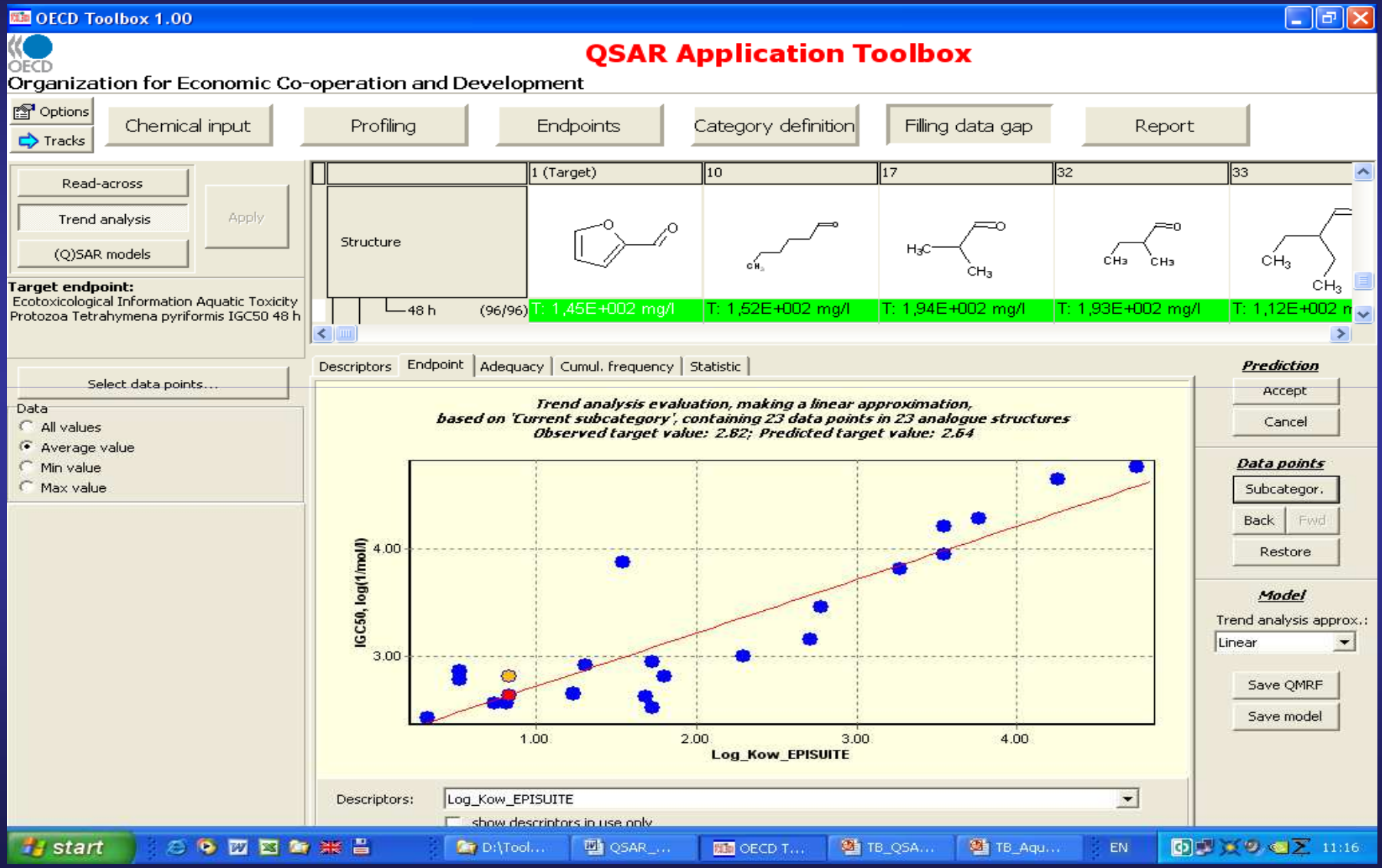
Trendová analýza vybraných aldehydů



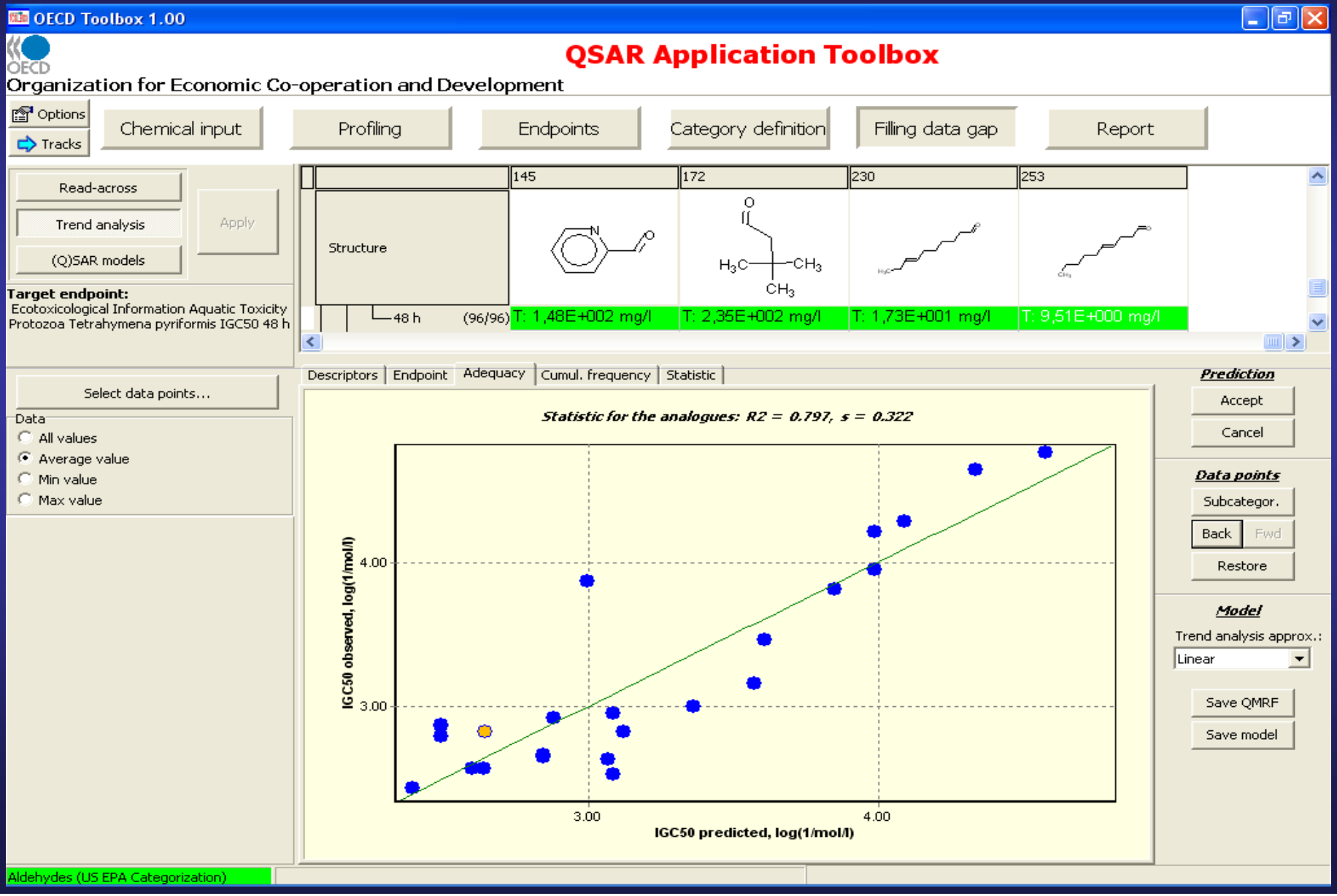
Subkategorizace



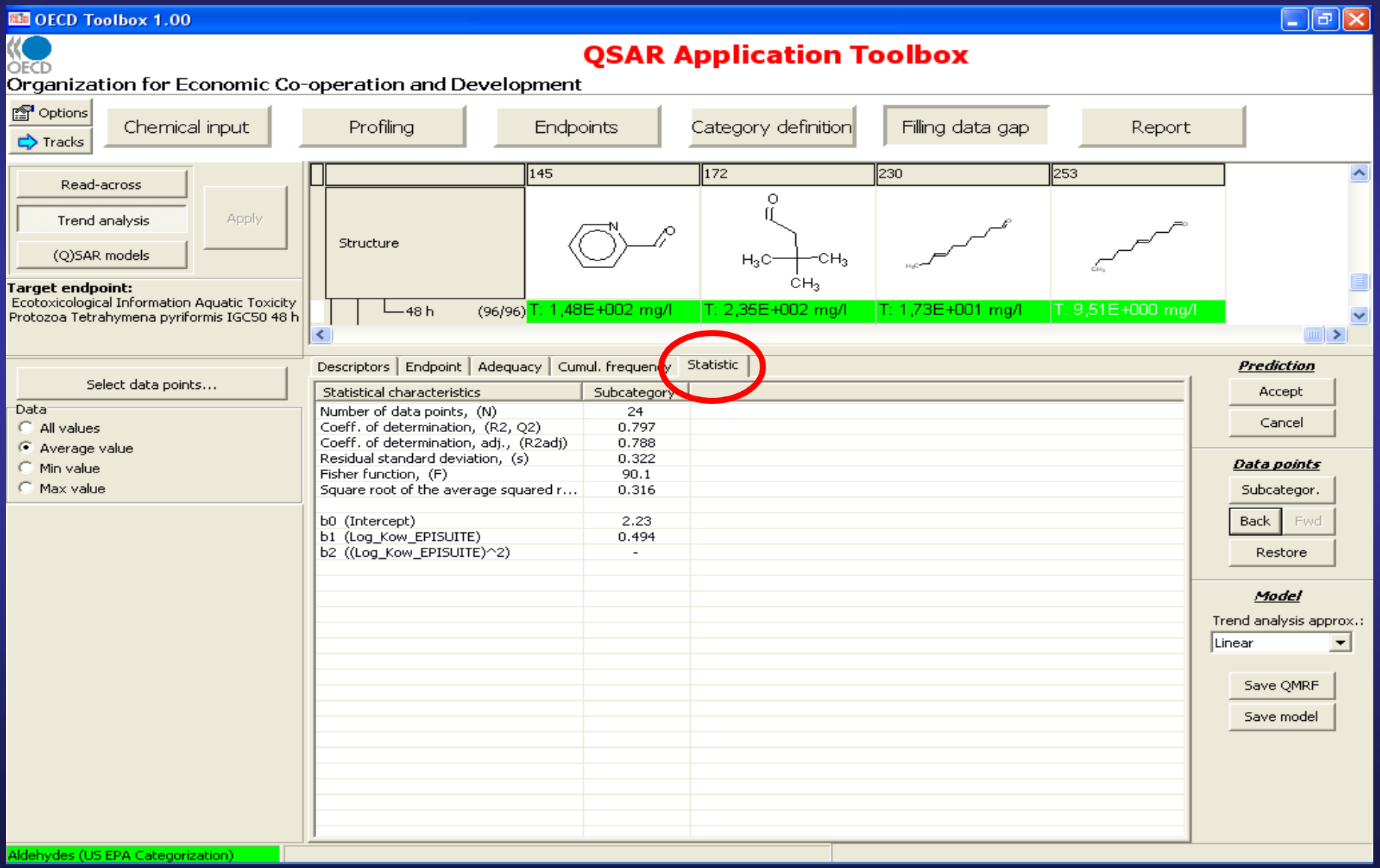
Výsledek po subkategorizaci



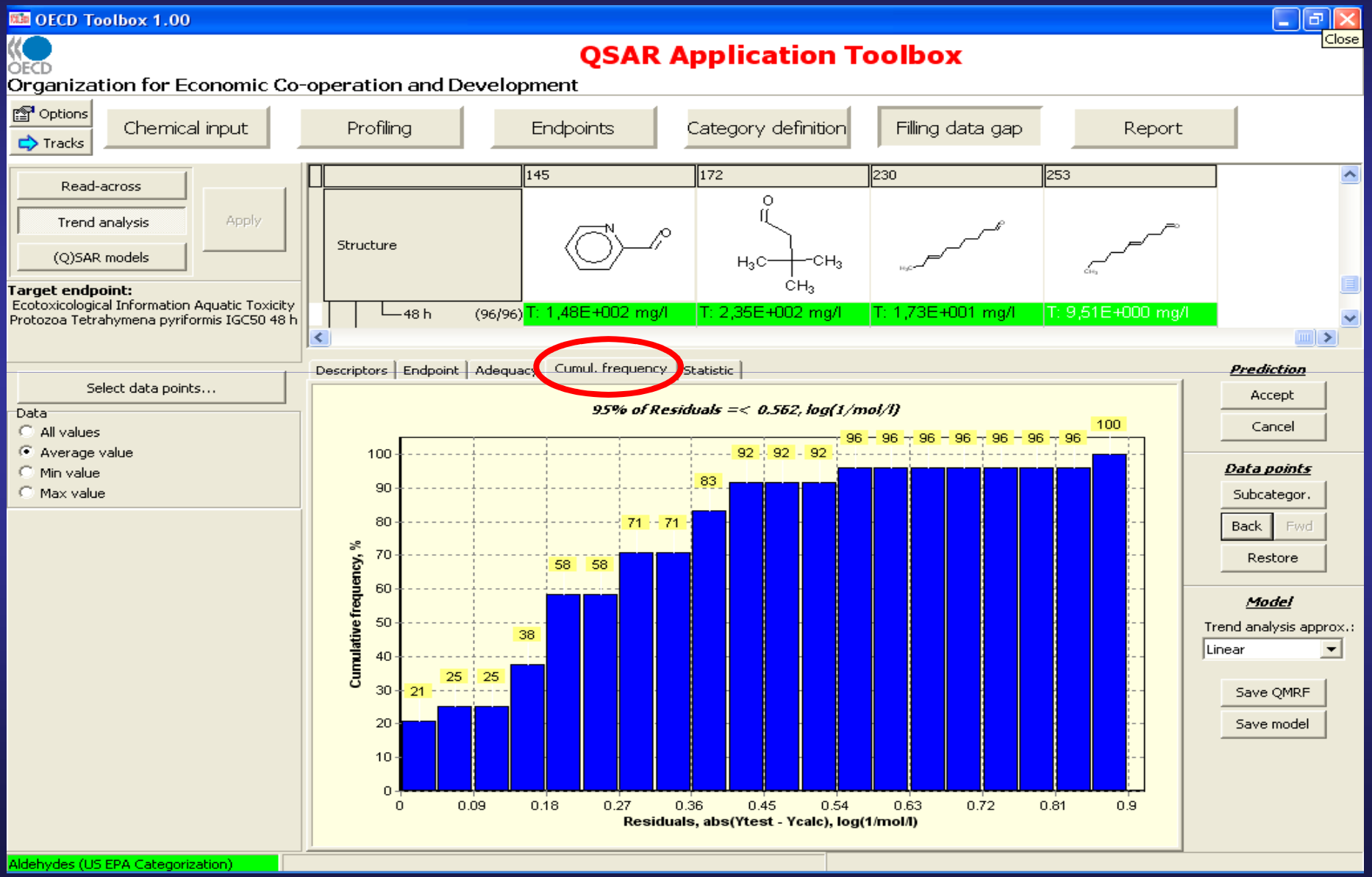
Vyhodnocení QSAR modelu



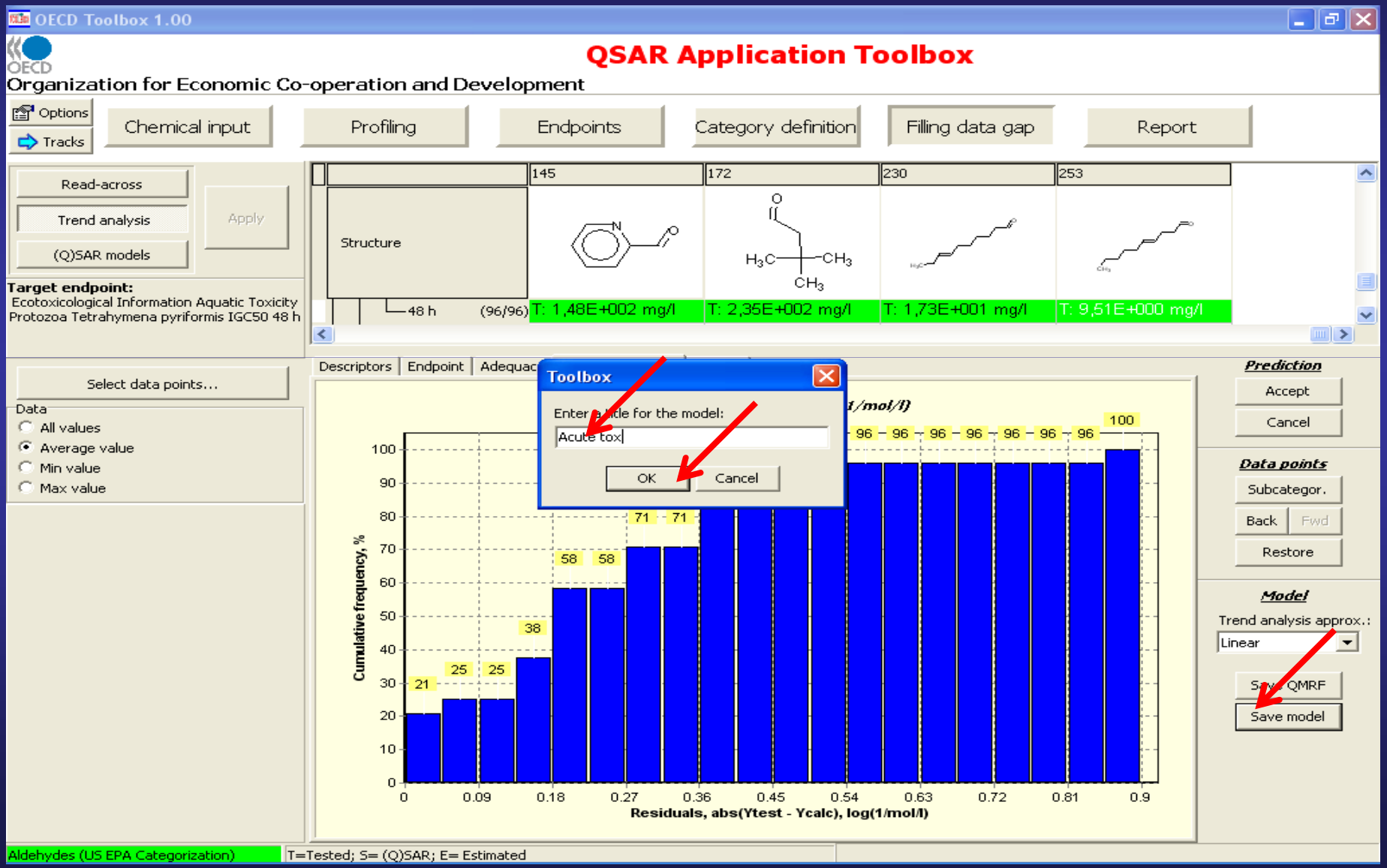
Vyhodnocení QSAR modelu - statistika



Vyhodnocení QSAR modelu



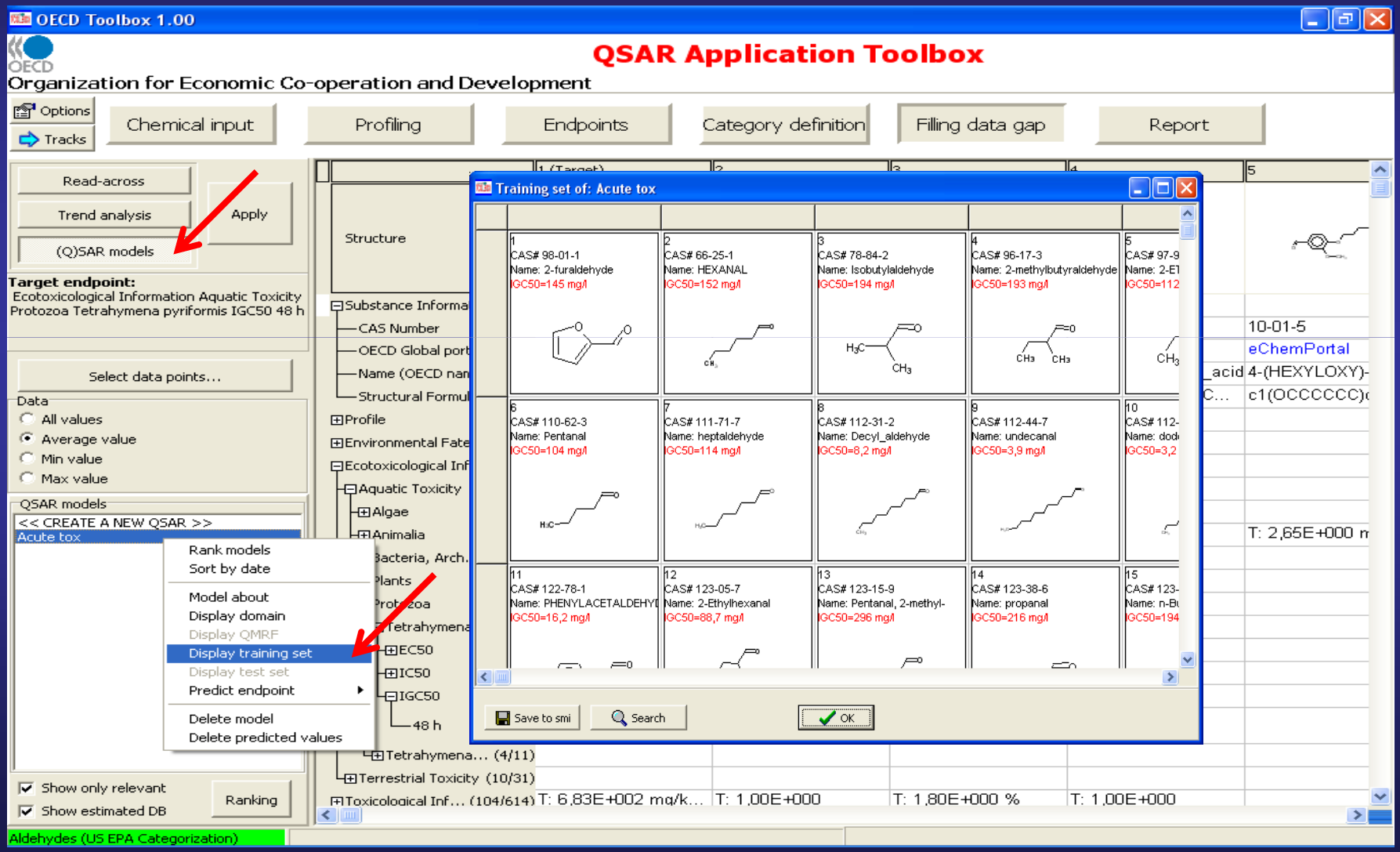
Uložení vytvořeného QSAR modelu



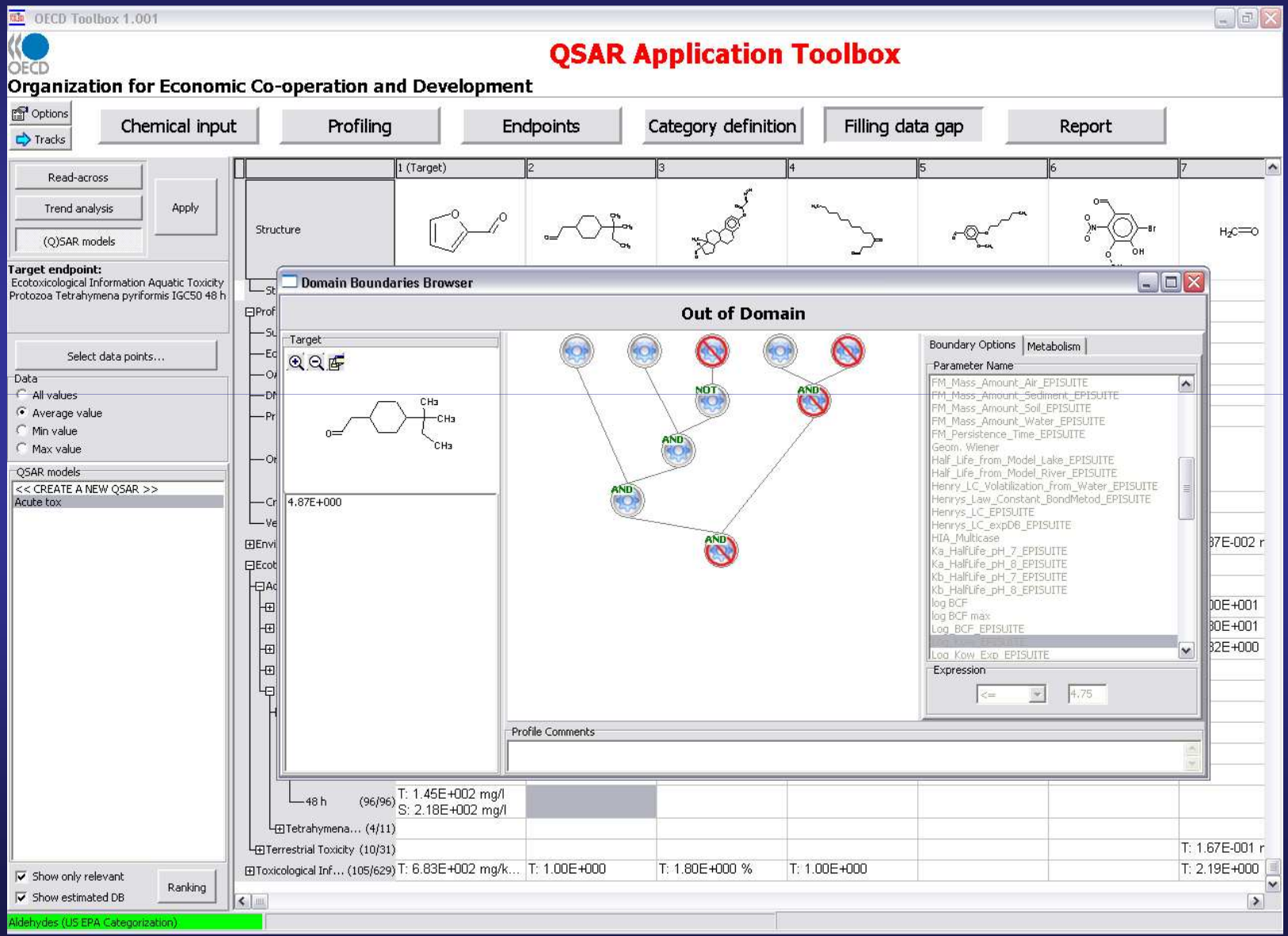
Použití vytvořeného modelu QSAR

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

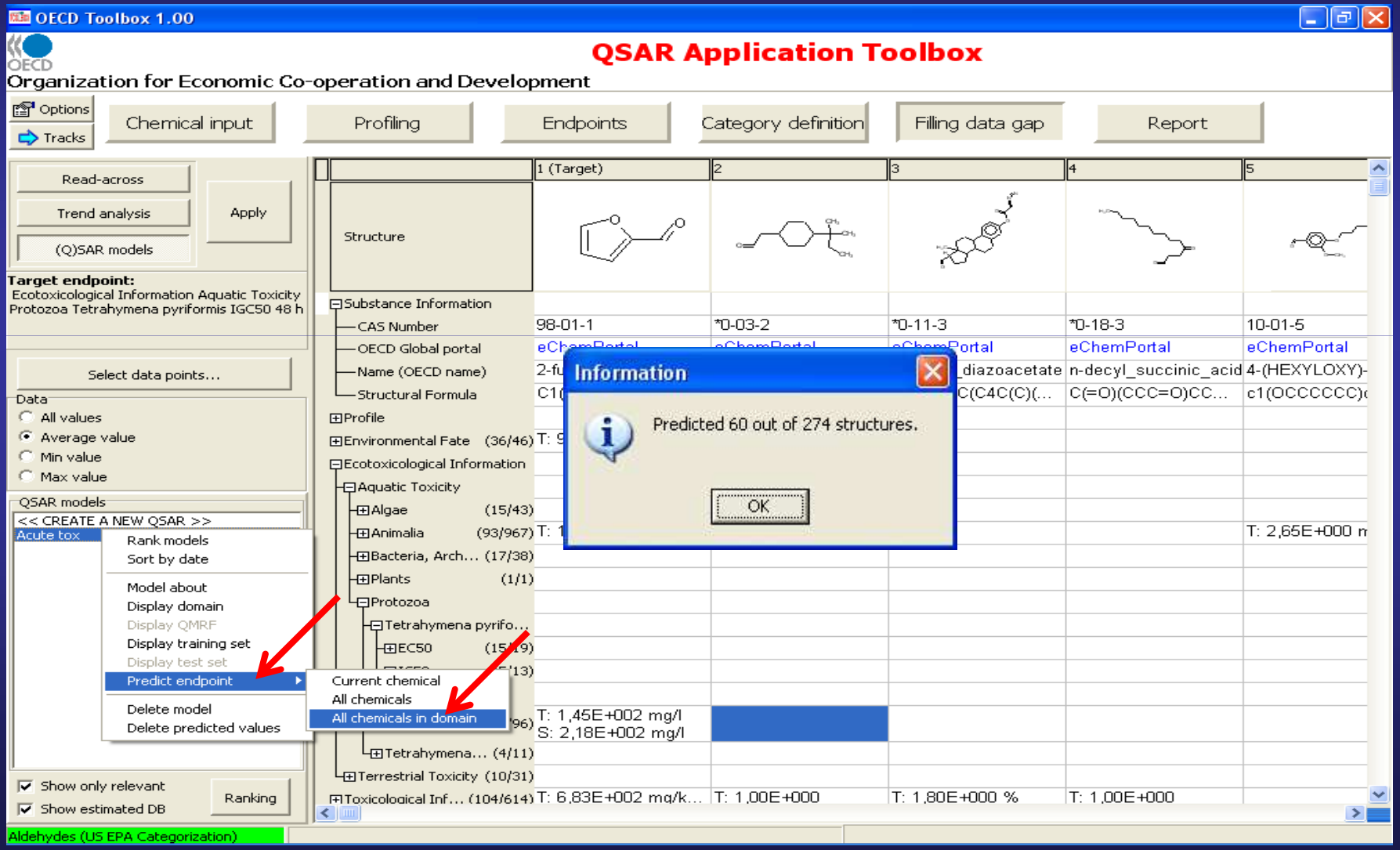
Testovací set



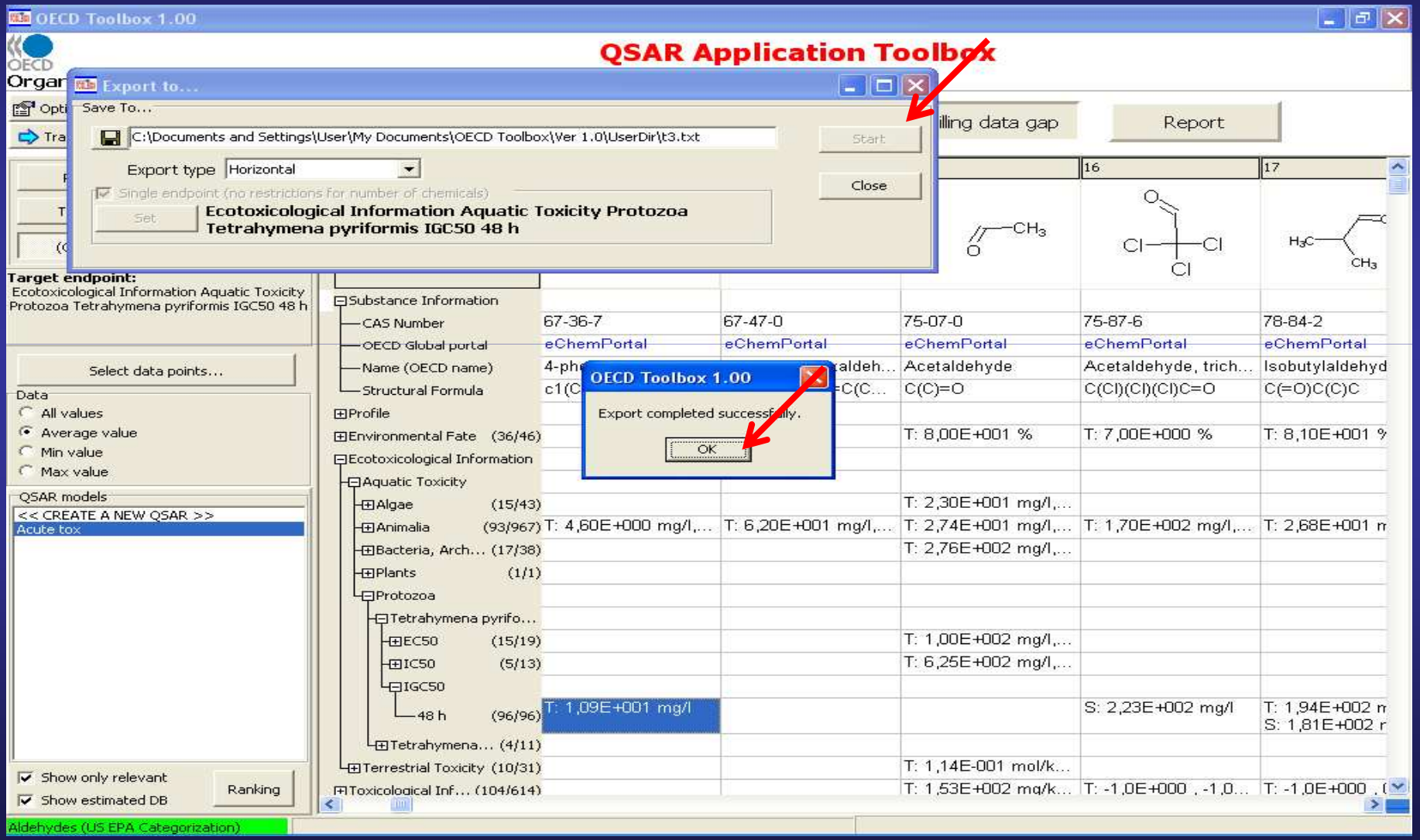
Vizualizace zda je chemikálie v aplikačním rozsahu modelu



Provedení předpovědi účinku



Export výsledků do textového souboru



Ukázka exportovaných výsledků do textového souboru

CAS	NAME	SMILES	Endpoint name	Data	Dimension	SOURCE	
000098-01-1	2-furaldehyde	C1(C=O)=CC=CO1	IGC50	1,45E+02	mg/l	Toxicology methods, 7, 289-309.	
000098-01-1	2-furaldehyde	C1(C=O)=CC=CO1	IGC50	2,18E+02	mg/l	Trend:OECD Toolbox 1.00	
000098-01-1	2-furaldehyde	C1(C=O)=CC=CO1	IGC50	2,18E+02	mg/l	(Q)SAR: Aldehydy	
00000-18-3	n-decyl_succinic_acid	C(=O)(CCC=O)CCCCCCCCCC	IGC50	2,02E+01	mg/l	(Q)SAR: Aldehydy	
000050-00-0	FORMALDEHYDE	C=O	IGC50	1,18E+02	mg/l	(Q)SAR: Aldehydy	
000052-39-1	pregn-4-en-18-al,_11,21-d	C12C(C)(C3C(C4C(C=O)(C(C(=O)CO)CC4)CC3O)CC1)CCC(=O)C=2	IGC50	1,20E+03	mg/l	(Q)SAR: Aldehydy	

Děkuji Vám za pozornost!