QSAR Application Toolbox

Workflow

Laboratory of Mathematical Chemistry,
Bourgas University “Prof. Assen Zlatarov”
Bulgaria

Outlook

Description
General scheme and workflow
Basic functionalities
Forming categories

Laboratory of Mathematical Chemistry

Philosophy

- Toolbox helps registrants and authorities to
  - ✓ Use the methodologies to group chemicals into categories and
  - ✓ Refine and expand the categories approach
  - ✓ Provide a mechanistic transparency of the formed categories
  - ✓ Fill data gaps by read-across, trend analysis and (Q)SARs
  - ✓ Ensure uniform application of read-across
  - ✓ Support the regulatory use of (Q)SAR approach
  - ✓ Improve the regulatory acceptance of (Q)SAR methods

Philosophy

- (Q)SAR Toolbox is a central tool for non-test data in ECHA and OECD

- ECHA and OECD coordinate the Toolbox development

Description

- Toolbox is not a QSAR model and hence can not be compared with other QSAR models

- Training sets (categories) for each prediction are defined dynamically as compared to other (Q)SAR model which have rigid training sets

- Each estimated value can be individually justified based on:
  - ✓Category hypothesis (justification) and consistency
  - ✓Quality of measured data and
  - ✓Computational method used for grouping and data gap filling

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Description

- It is developed under the continuing peer review of:
  - ✓ Member state countries,
  - ✓ Regulatory agencies
  - ✓ Chemical industry and NGOs

- The predictions are getting acceptance by toxicologists and regulators due to the:
  - ✓International peer review process for developing the system and
  - ✓Mechanistic transparency of the results

- The system is freely available and maintained in the public domain by OECD

History

Phase I - The first version (2005 - 2008)

- Emphasizes technological proof-of-concept
- Released in 2008
- Developed by LMC

Phase II (2008 - 2012)

- More comprehensive Toolbox which fully implements the capabilities of the first version
- Second version was released in 2010
- Developed by LMC, subcontractors: LJMU, Lhasa Ltd and TNO
- Third version was released in 2012
- Maintenance 2013 - v. 3.2 – in January 2014
- Version 3.3.1 was released in December 2014
- Version 3.3.2 was released in February 2015
- Version 3.3.3 is expected to be released in June 30, 2015

Phase III (2013 – 2019 + 4 years maintenance)

- Significant focus on streamlining + new IT platform
- Knowledge and data rationalization and curation
- Implementation of Ontology, ADME
- Implementation of AOPs
- Version 4.0 will be released in spring of 2016
- Developed by LMC, subcontractors: LJMU and Lhasa Ltd

Main Government Donators

- OECD
- European chemicals agency
- US EPA
- Environment Canada
- Health Canada
- NITE Japan
- NIES Japan
- Danish EPA
- UBA Germany
- NICNAS Australia
- DEWNA Australia
- ISS Italy

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Main Industry Donators

- L’Oreal
- DuPont
- Givaudan
- Dow chemicals
- BASF
- ExxonMobil
- 3M
- Firmenich SV
- SRC, Syracuse
- Unilever

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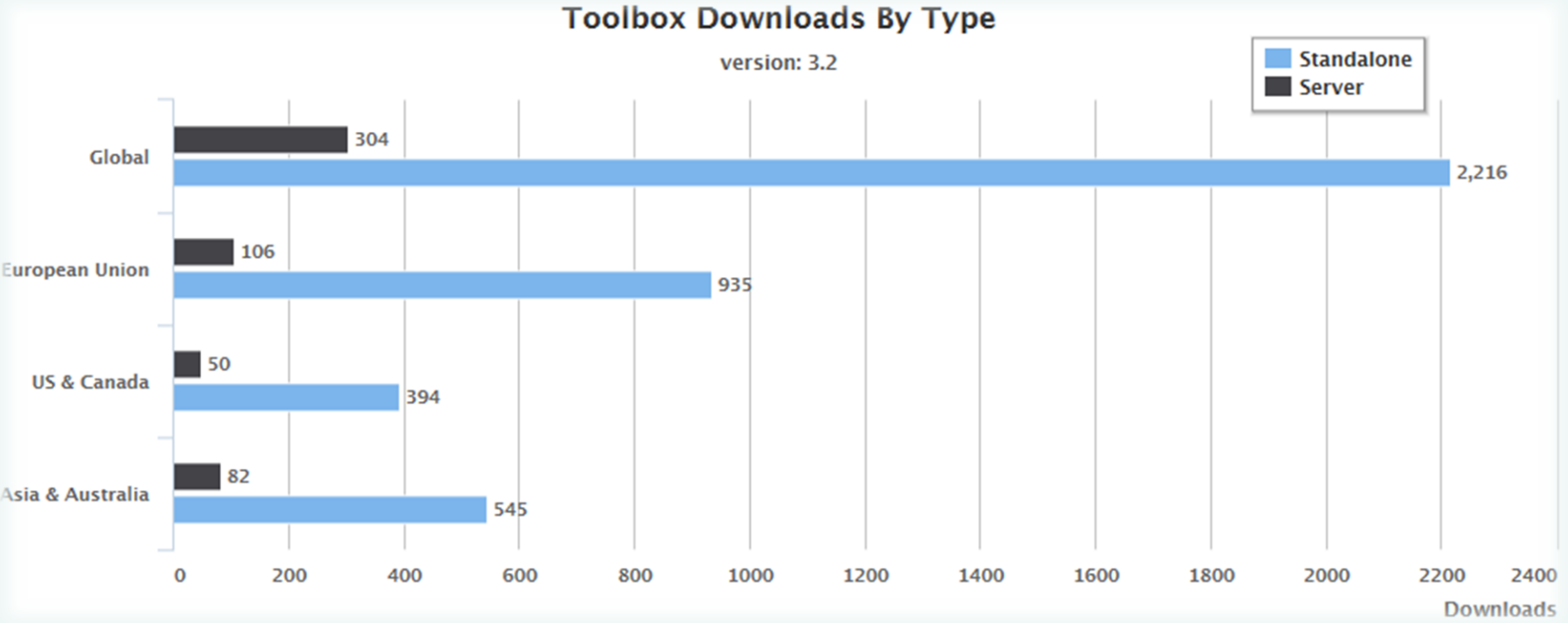
Download statistics of QSAR Toolbox by registered users worldwide



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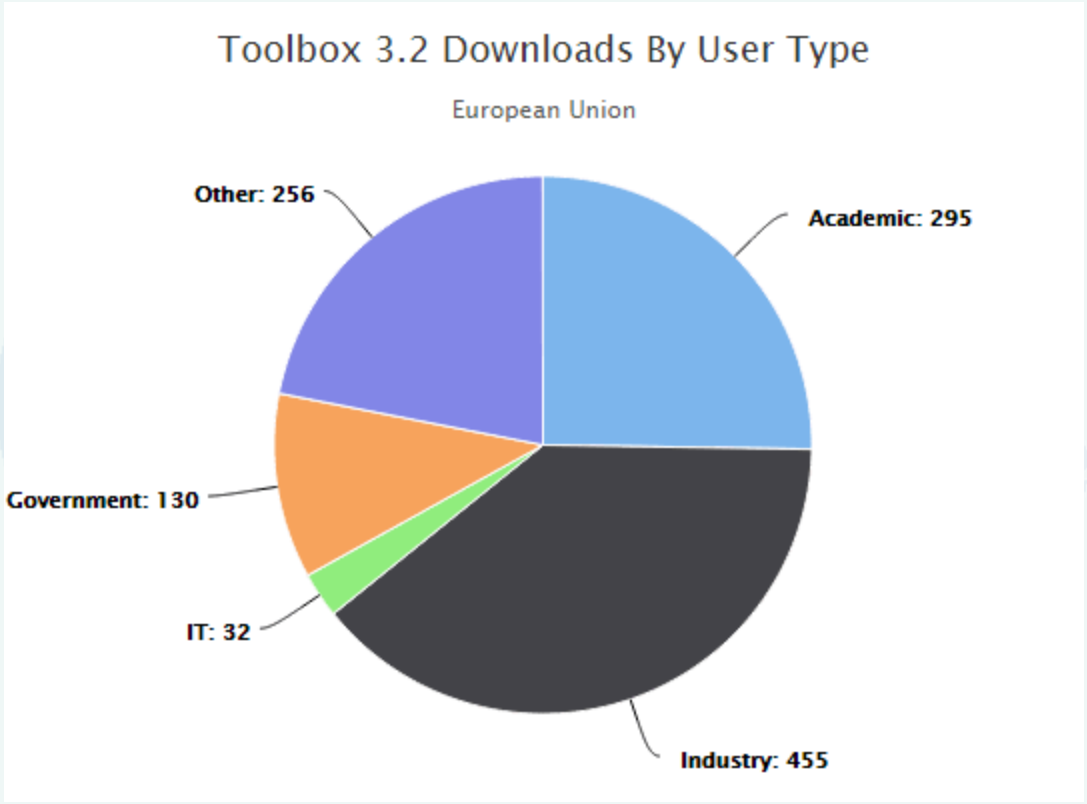

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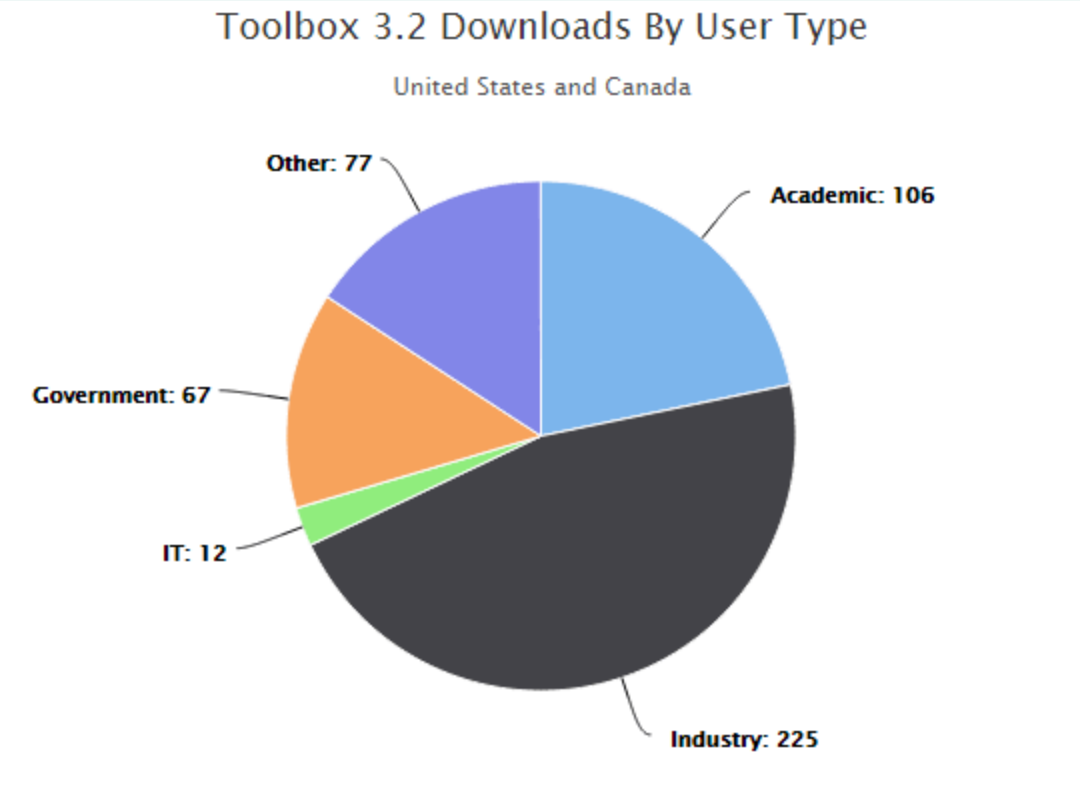

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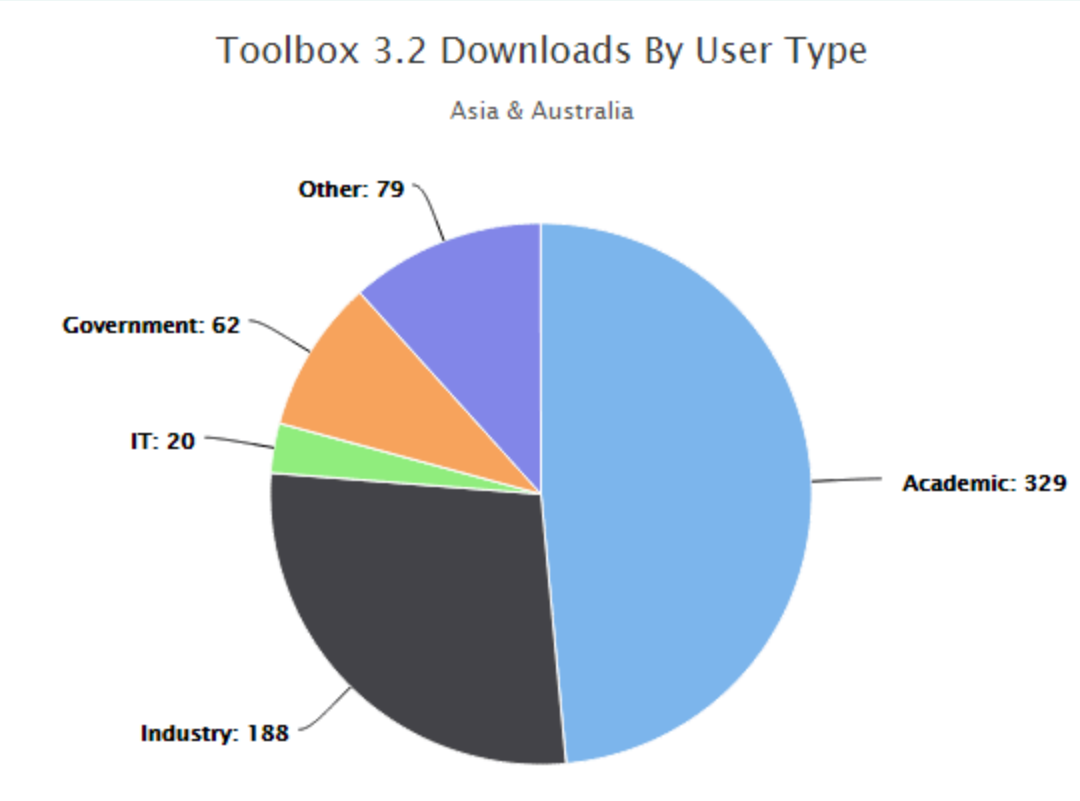
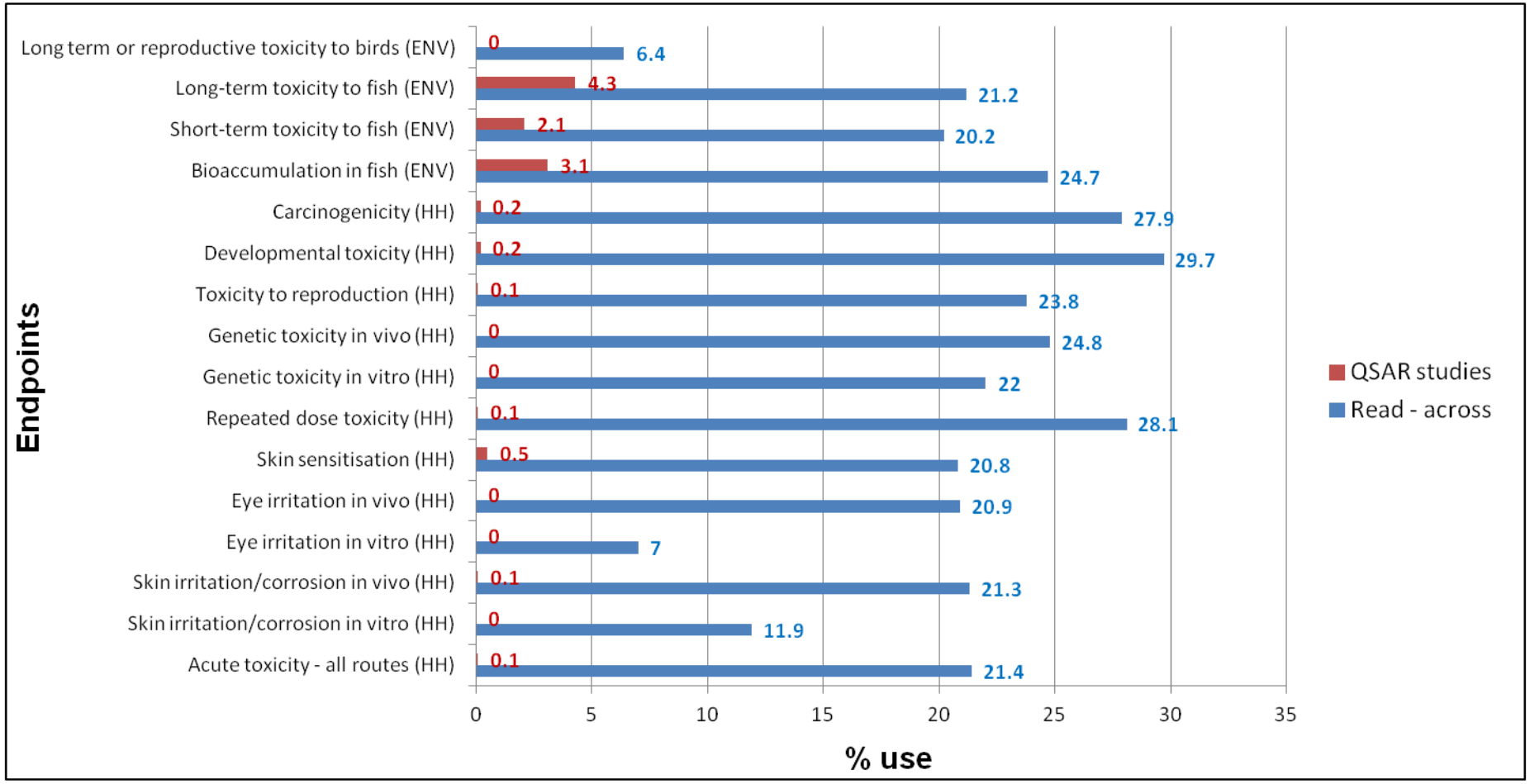


QSAR and read-across based submissions to the ECHA

For existing substances at or above 1000 tpa*
(2011 ECHA report)



ENV = environmental endpoint; HH = human health endpoint

*H. Spielmann et al. ATLA 39, 481–493, 2011

Outlook

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General scheme and workflow
Basic functionalities
Forming categories

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General Scheme

- Theoretical knowledge,
- Empiric knowledge,
- Computational methods,
- Information technologies.

⇓ Input

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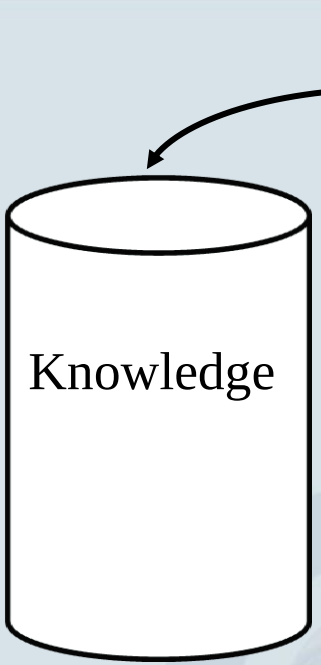

- Is the chemical included in regulatory or chemical categories?
- Could this chemical interact with DNA or specific proteins?
- Could this chemical cause adverse effects?
- Is the effect due to parent chemical or its metabolites?

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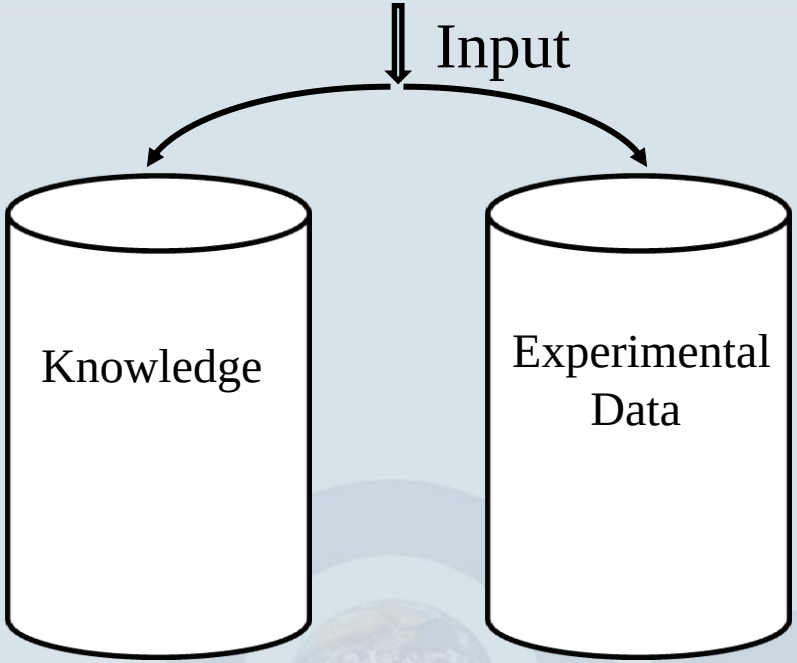

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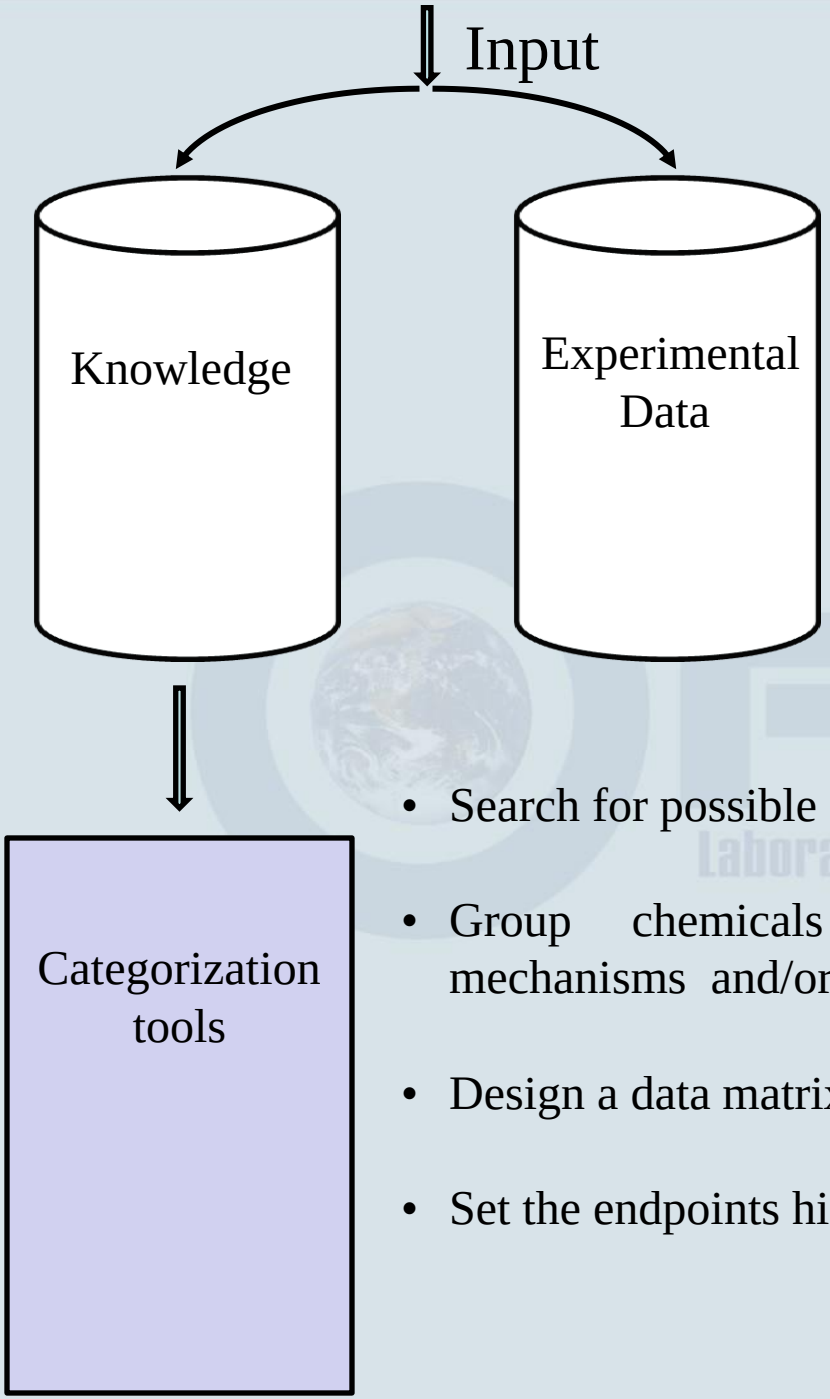
- Are data available for assessed endpoints of target chemical?
- Is information for the data sources available?



- Search for possible analogues using existing categorization schemes
- Group chemicals based on common chemical/toxicological mechanisms and/or metabolism
- Design a data matrix of a chemical category
- Set the endpoints hierarchy in the data matrix

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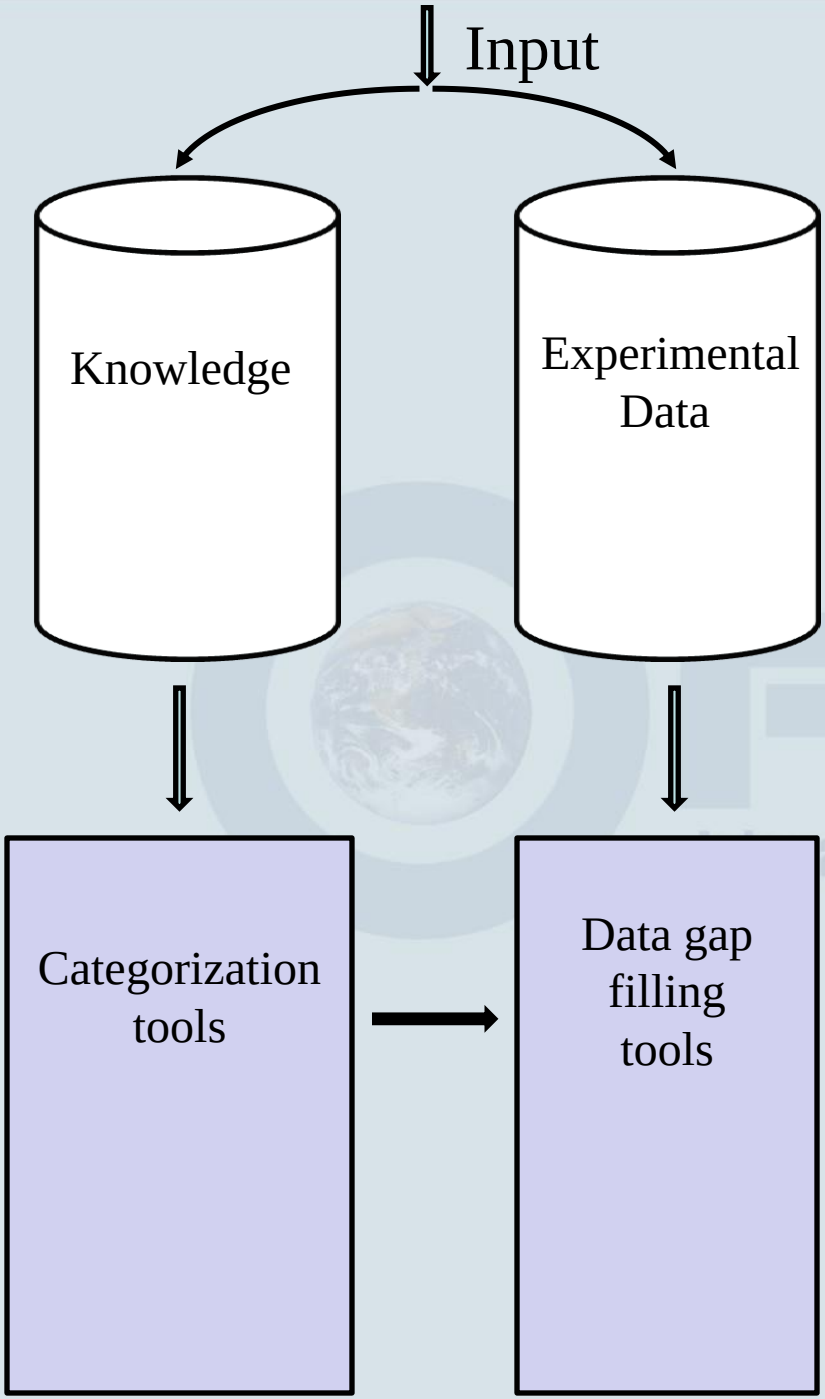
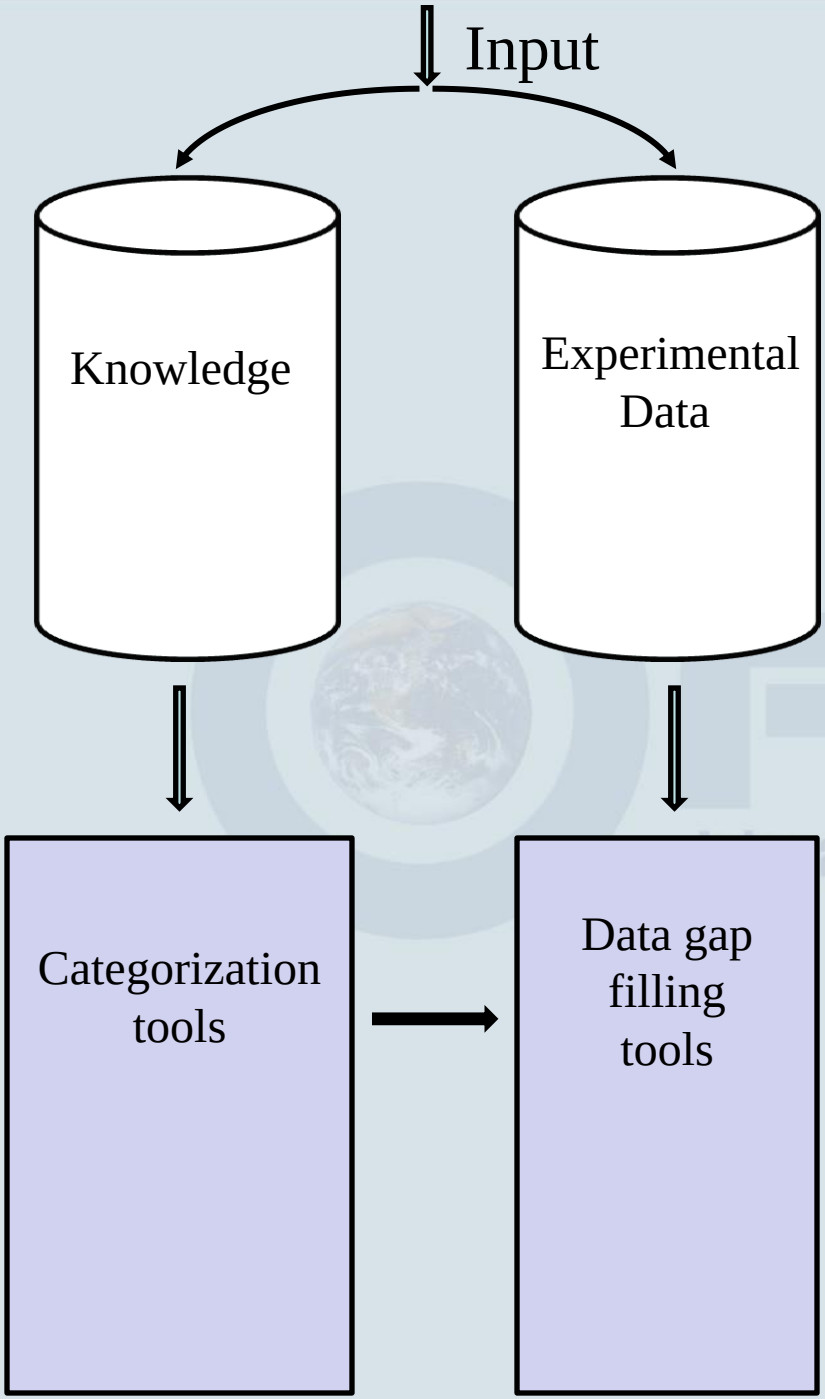
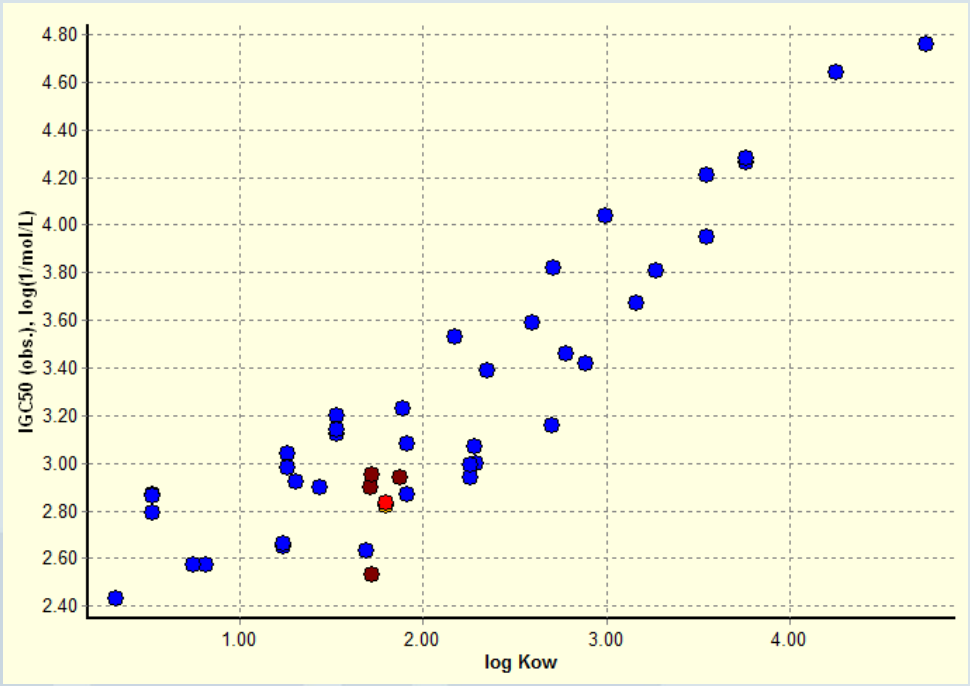
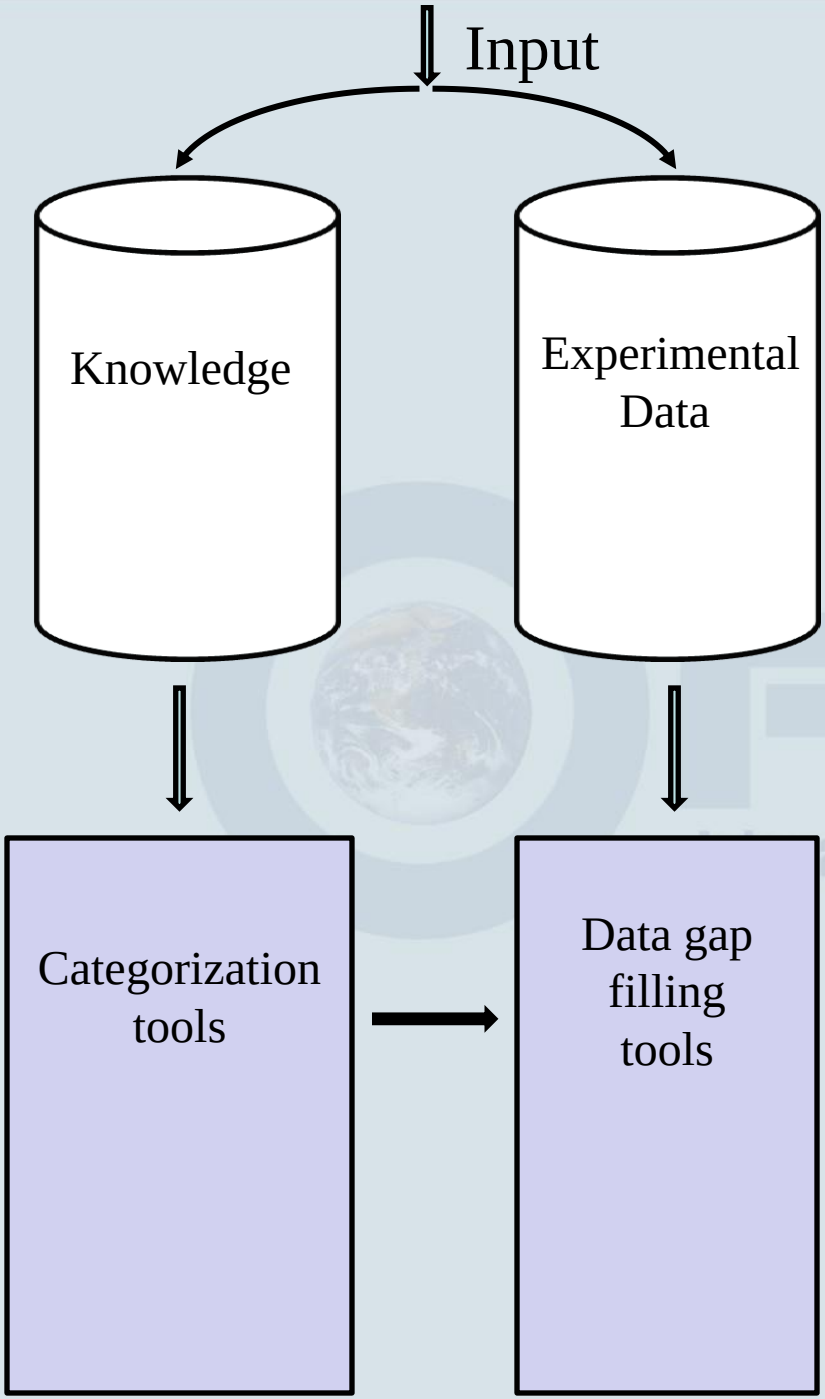


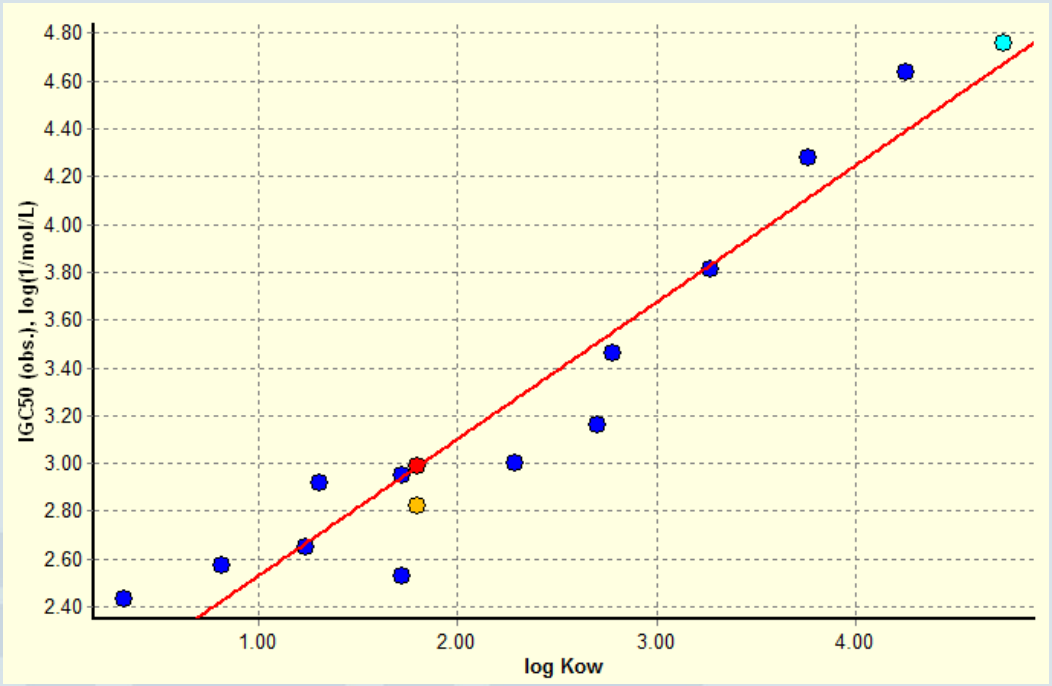
- Read-across
- Trend Analysis
- (Q)SAR



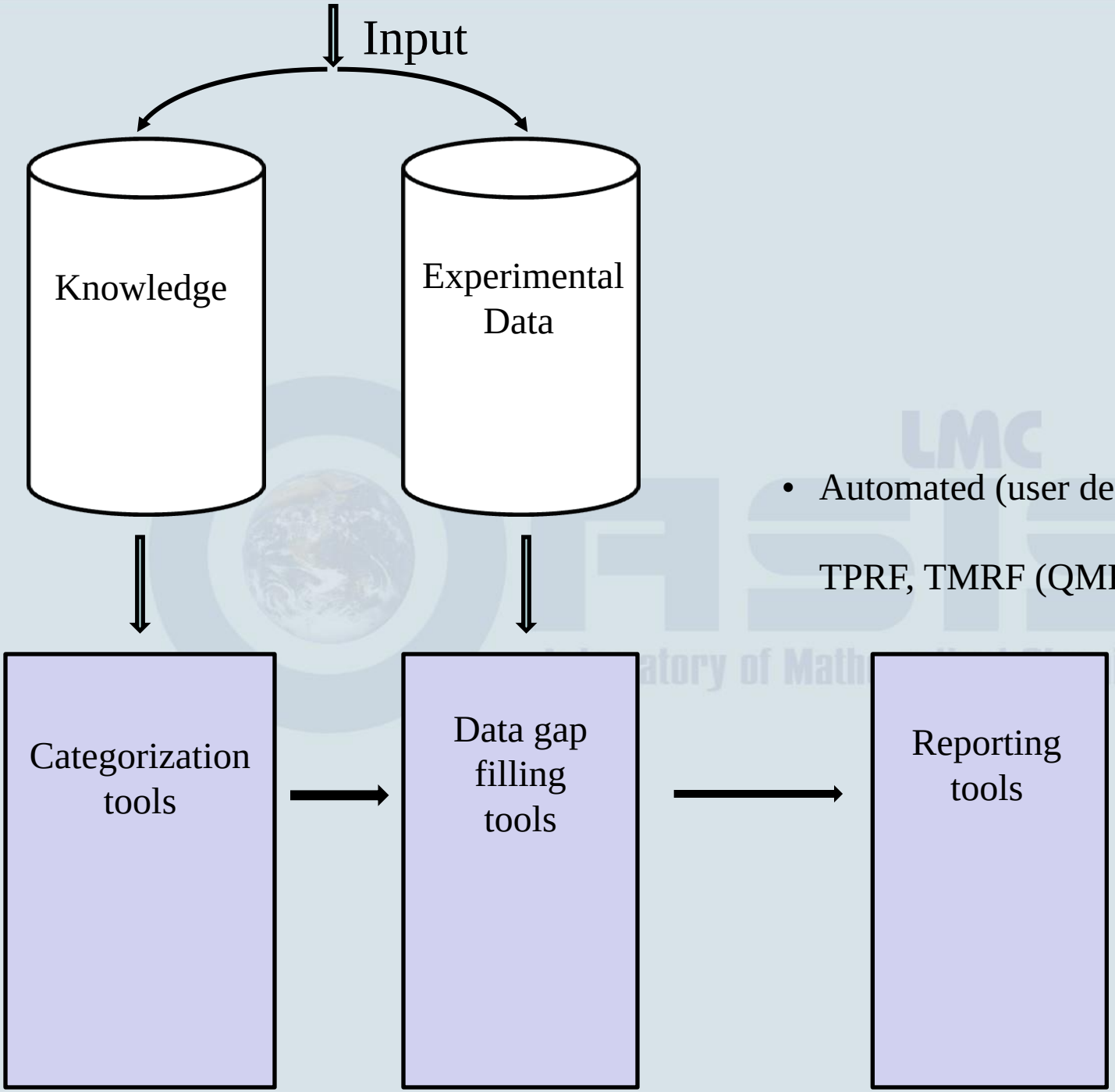


- **Read-across**
- Trend Analysis
- (Q)SAR



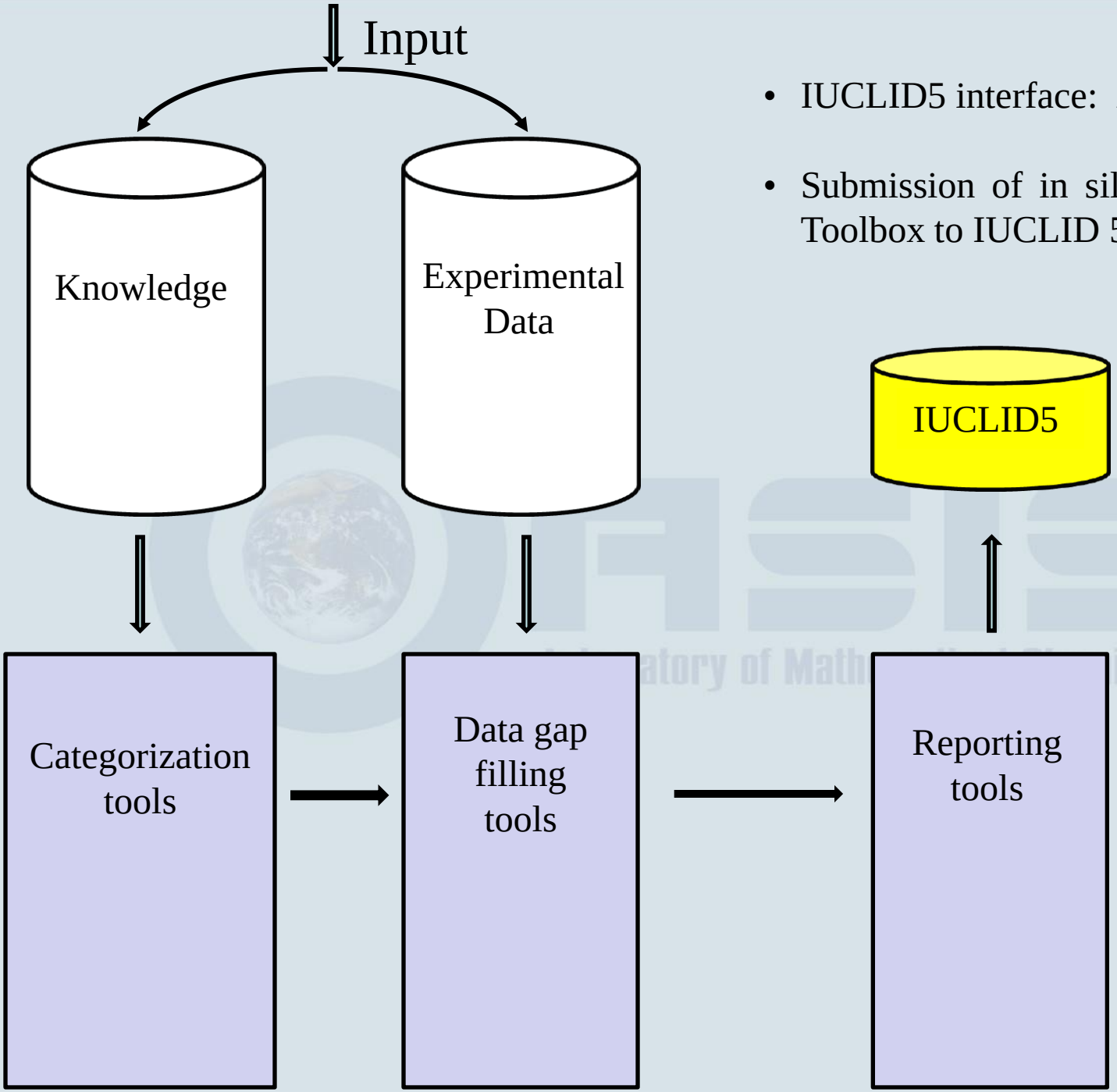


- Read-across
- **Trend Analysis**
- (Q)SAR

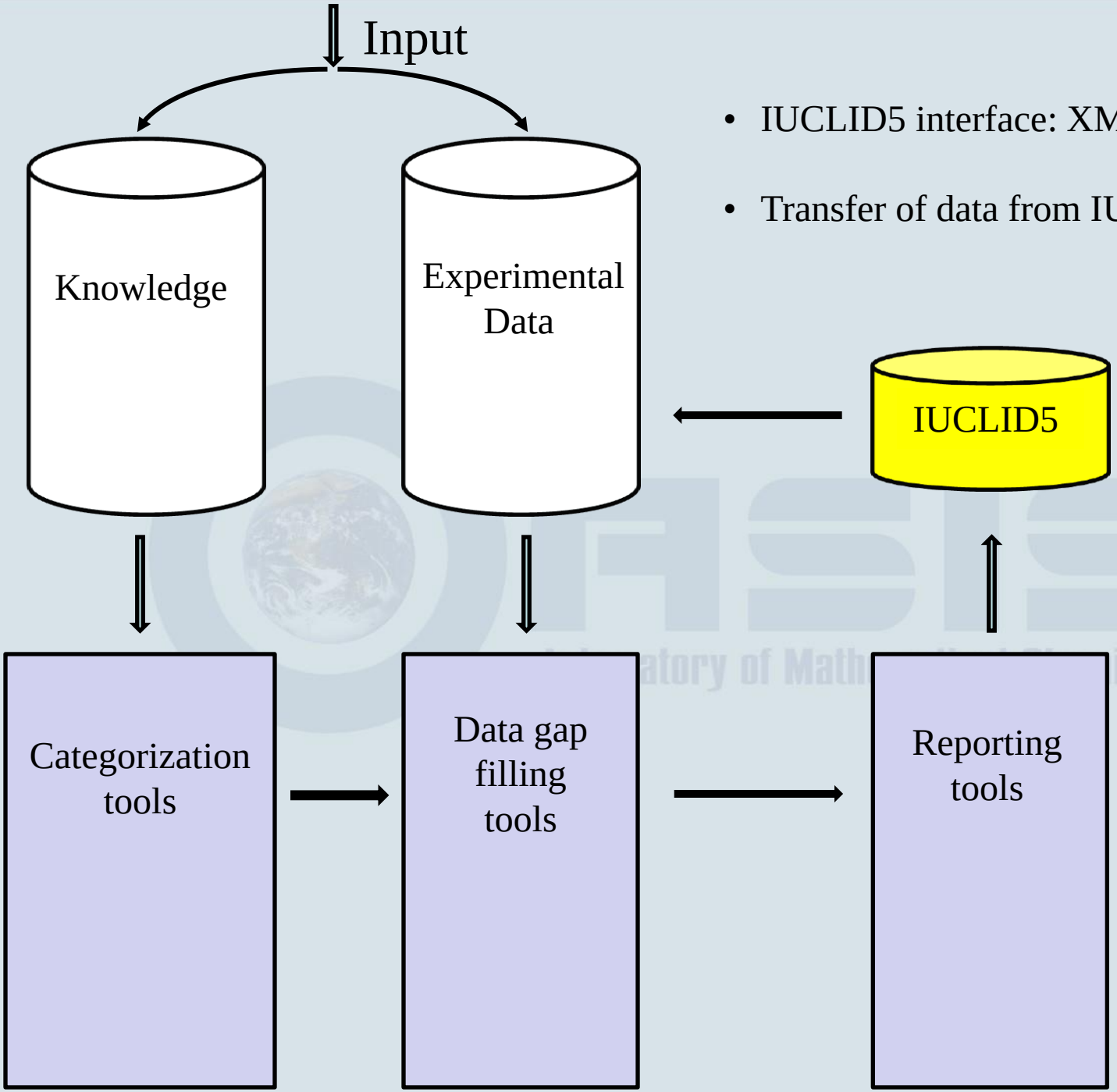


- Automated (user defined) reports:

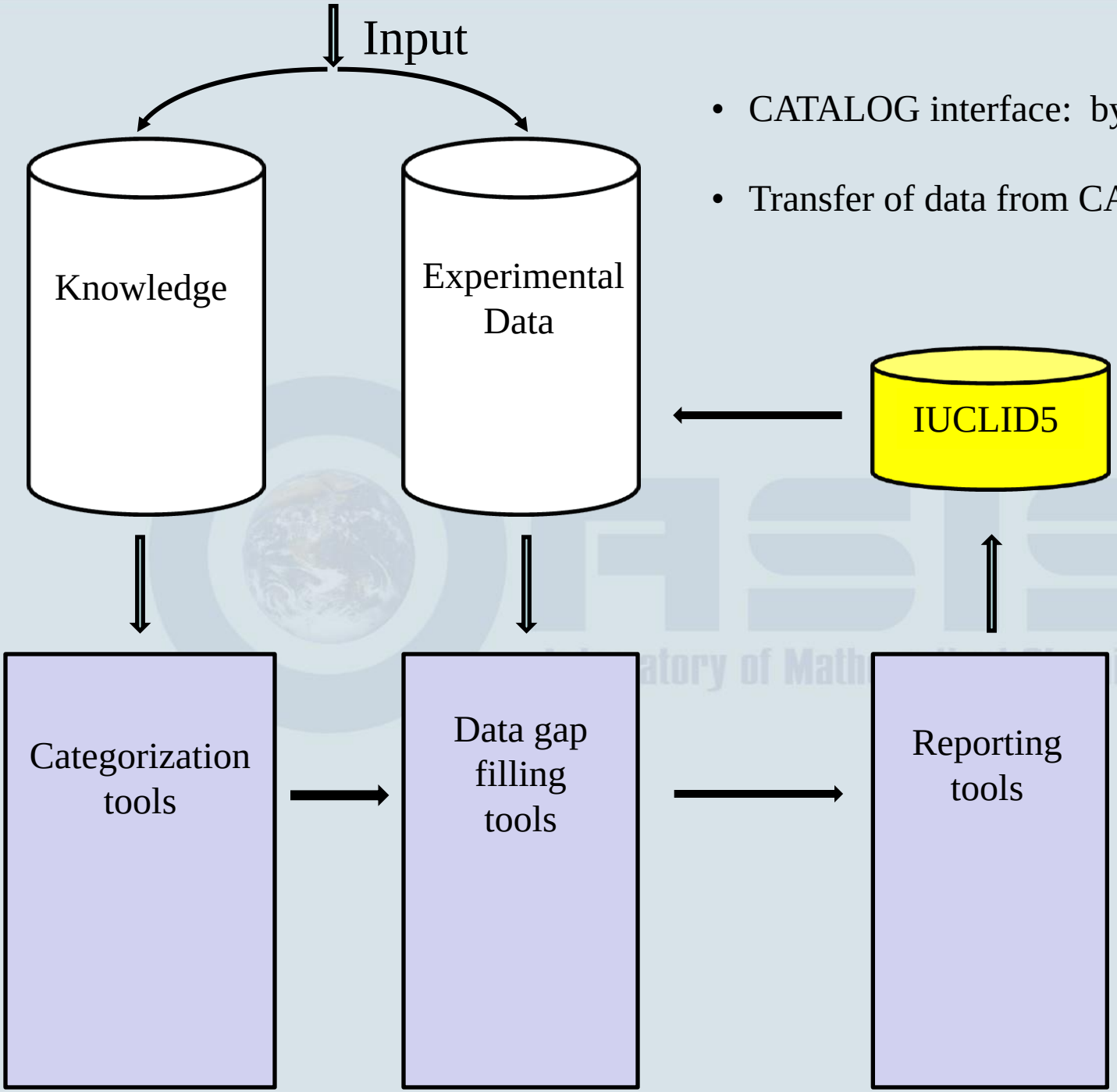
  TPRF, TMRF (QMRF), CCRF



- IUCLID5 interface: XML, Web Services
- Submission of in silico predictions from Toolbox to IUCLID 5

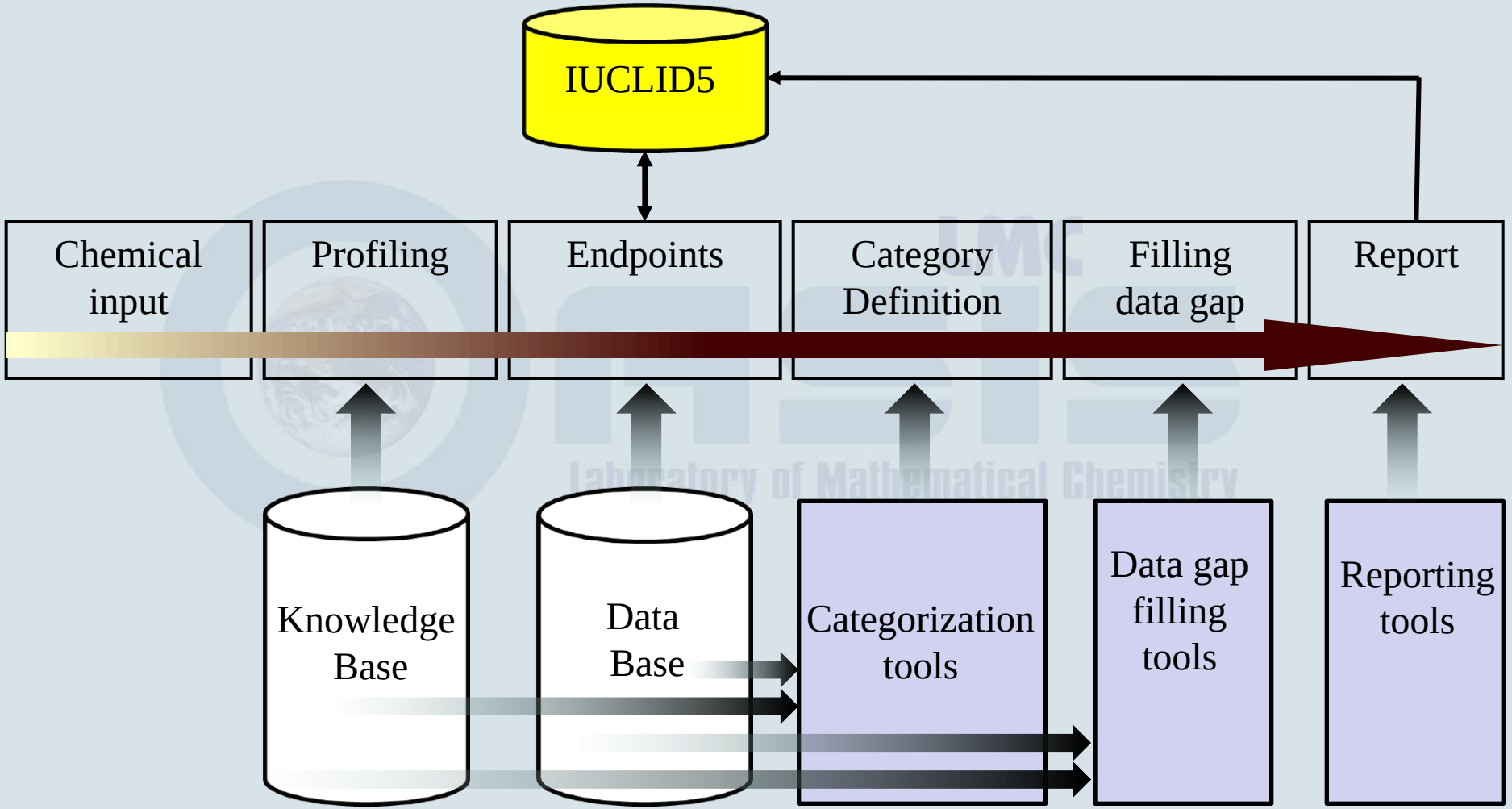


- IUCLID5 interface: XML, Web Services
- Transfer of data from IUCLID 5 to Toolbox



- CATALOG interface: by XML (*.i5z)
- Transfer of data from CATALOG to Toolbox

System Workflow



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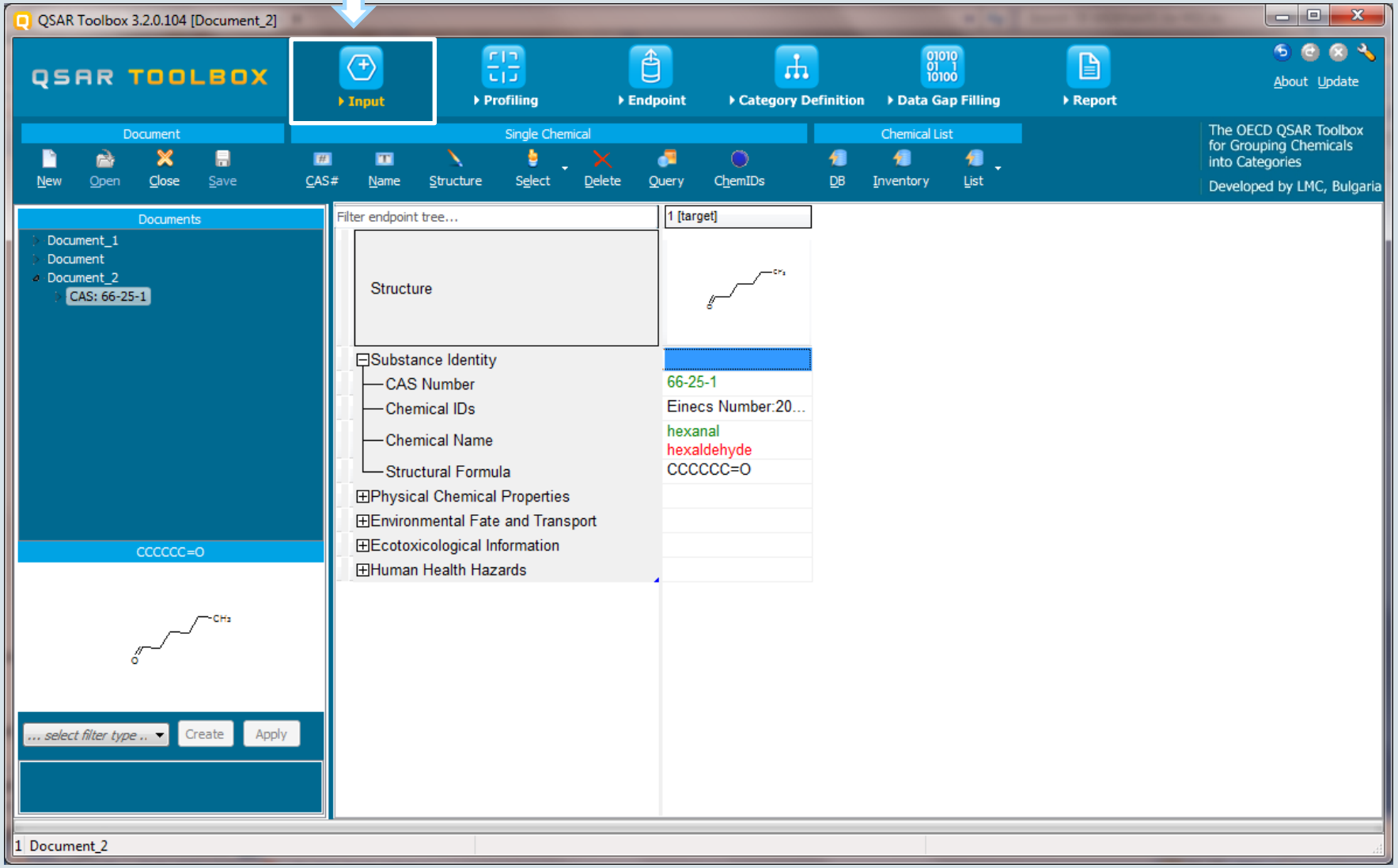
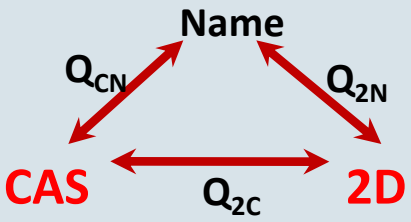

QSAR Toolbox 3.2.0.104 [Document_2]
QSAR TOOLBOX
Input
Profiling
Endpoint
Category Definition
Data Gap Filling
Report
About
Update
Document
Single Chemical
Chemical List
New
Open
Close
Save
CAS#
Name
Structure
Select
Delete
Query
ChemIDs
DB
Inventory
List
The OECD QSAR Toolbox for Grouping Chemicals into Categories
Developed by LMC, Bulgaria
Documents
Document_1
Document
Document_2
CAS: 66-25-1
CCCCCC=O
... select filter type ..
Create
Apply
Filter endpoint tree...
1 [target]
Structure
Substance Identity
CAS Number
66-25-1
Chemical IDs
Einecs Number:20...
Chemical Name
hexanal
hexaldehyde
Structural Formula
CCCCCC=O
Physical Chemical Properties
Environmental Fate and Transport
Ecotoxicological Information
Human Health Hazards
1 Document_2

Input

QA of chemical structures



QSAR Toolbox 2.1.2.865 [Document_2]

QSAR TOOLBOX

Input | Profiling | Endpoint | Category Definition | Data Gap Filling | Report | About | Update

New | Open... | Save | Close — Document

CAS # | Chemical Name | Structure | Select from Database | Select from Inventory | Select from File | Delete chemical — Single Chemical

Load Database | Load Inventory | Load Chemical List — Chemical List

The OECD QSAR Toolbox for Grouping Chemicals into Categories

Developed by LMC, Bulgaria

Documents: Document_1, Document_2

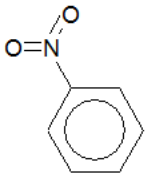
Filter endpoint tree... | 1

Structure

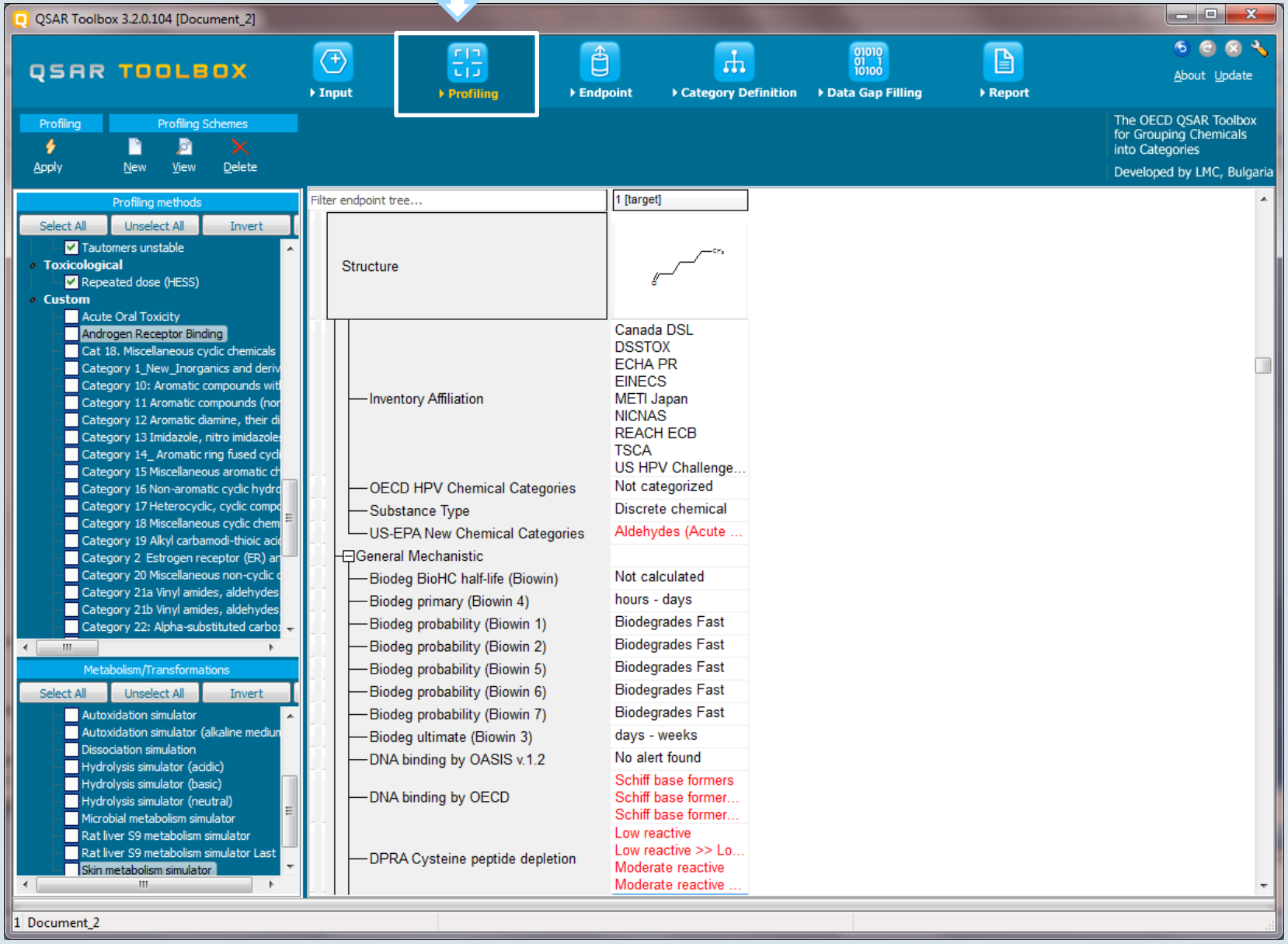
Substance Identity

CAS Number 98-95-3

Explain QA Form

Smiles	Depiction	Names	CAS/Name	2D/Name	CAS/2D
c1(N(=O)=O)ccccc1		1: nitrobenzene 2: benzene, nitro- 3: nitro-benzene	1: High Quality 1: Aquatic ECETOC 2: Aquatic OASIS 3: Aquatic US-EPA ECO 4: Bioaccumulation fish 5: Biodegradation OASI 6: COSING 7: Carcinogenic Potency 8: Carcinogenicity & Mu 9: DSSTox 10: ECHA PR 11: EINECS 12: Genotoxicity OASIS 13: HPVC OECD 14: MITI Japan 15: Phys-chem EPISUIT	1: High Quality 1: Aquatic ECETOC 2: Aquatic OASIS 3: Aquatic US-EPA EC 4: Bioaccumulation fis 5: Biodegradation OA 6: COSING 7: Carcinogenic Poten 8: Carcinogenicity & M 9: DSSTox 10: ECHA PR 11: EINECS 12: Genotoxicity OASI 13: HPVC OECD 14: MITI Japan 15: Phys-chem EPISUI	1: High Quality 1: AICS A 2: Aquatic ECETOC 3: Aquatic OASIS A 4: Aquatic US-EPA ECC 5: Bioaccumulation Car 6: Bioaccumulation fish 7: Biodegradation OAS A 8: COSING 9: Canada DSL 10: Carcinogenic Poten 11: Carcinogenicity & M 12: DSSTox A 13: ECHA PR

Profiling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Report
About
Update
Profiling
Profiling Schemes
Apply
New
View
Delete
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Developed by LMC, Bulgaria
Profiling methods
Select All
Unselect All
Invert
Tautomers unstable
Toxicological
Repeated dose (HESS)
Custom
Acute Oral Toxicity
Androgen Receptor Binding
Cat 18. Miscellaneous cyclic chemicals
Category 1_New_Inorganics and deriv
Category 10: Aromatic compounds wit
Category 11 Aromatic compounds (nor
Category 12 Aromatic diamine, their di
Category 13 Imidazole, nitro imidazole
Category 14_ Aromatic ring fused cycl
Category 15 Miscellaneous aromatic ch
Category 16 Non-aromatic cyclic hydro
Category 17 Heterocyclic, cyclic compo
Category 18 Miscellaneous cyclic chem
Category 19 Alkyl carbamodi-thioic acid
Category 2 Estrogen receptor (ER) an
Category 20 Miscellaneous non-cyclic c
Category 21a Vinyl amides, aldehydes
Category 21b Vinyl amides, aldehydes
Category 22: Alpha-substituted carbox
Metabolism/Transformations
Select All
Unselect All
Invert
Autoxidation simulator
Autoxidation simulator (alkaline mediun
Dissociation simulation
Hydrolysis simulator (acidic)
Hydrolysis simulator (basic)
Hydrolysis simulator (neutral)
Microbial metabolism simulator
Rat liver S9 metabolism simulator
Rat liver S9 metabolism simulator Last
Skin metabolism simulator
Filter endpoint tree...
1 [target]
Structure
Inventory Affiliation
Canada DSL
DSSTOX
ECHA PR
EINECS
METI Japan
NICNAS
REACH ECB
TSCA
US HPV Challenge...
OECD HPV Chemical Categories
Not categorized
Substance Type
Discrete chemical
US-EPA New Chemical Categories
Aldehydes (Acute ...
General Mechanistic
Biodeg BioHC half-life (Biowin)
Not calculated
Biodeg primary (Biowin 4)
hours - days
Biodeg probability (Biowin 1)
Biodegrades Fast
Biodeg probability (Biowin 2)
Biodegrades Fast
Biodeg probability (Biowin 5)
Biodegrades Fast
Biodeg probability (Biowin 6)
Biodegrades Fast
Biodeg probability (Biowin 7)
Biodegrades Fast
Biodeg ultimate (Biowin 3)
days - weeks
DNA binding by OASIS v.1.2
No alert found
DNA binding by OECD
Schiff base formers
Schiff base former...
Schiff base former...
DPRA Cysteine peptide depletion
Low reactive
Low reactive >> Lo...
Moderate reactive
Moderate reactive ...
1 Document_2

Profiling

- Predefined
- General Mechanistic
- Endpoint Specific
- Empiric
- Custom

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Profiling

- **Predefined**
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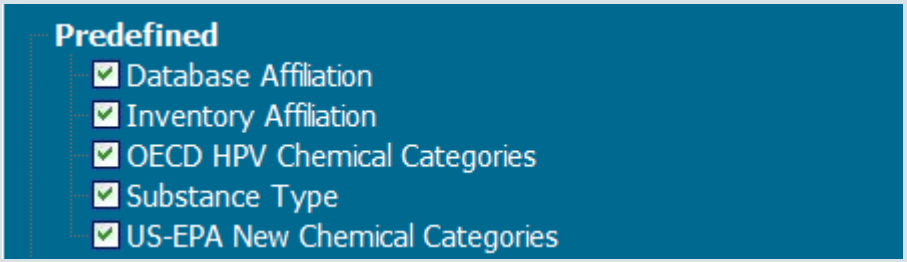
- Endpoint Specific
- Empiric
- Custom



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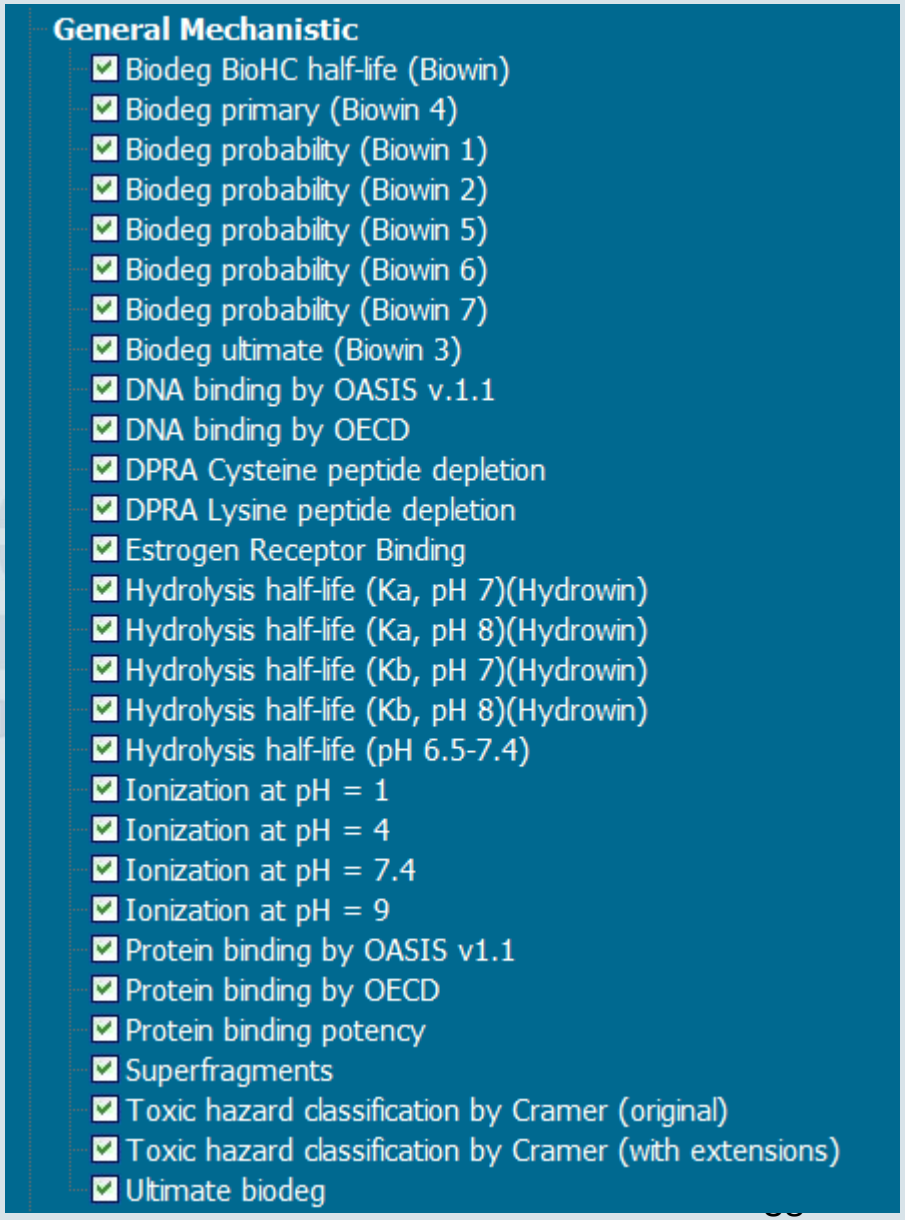

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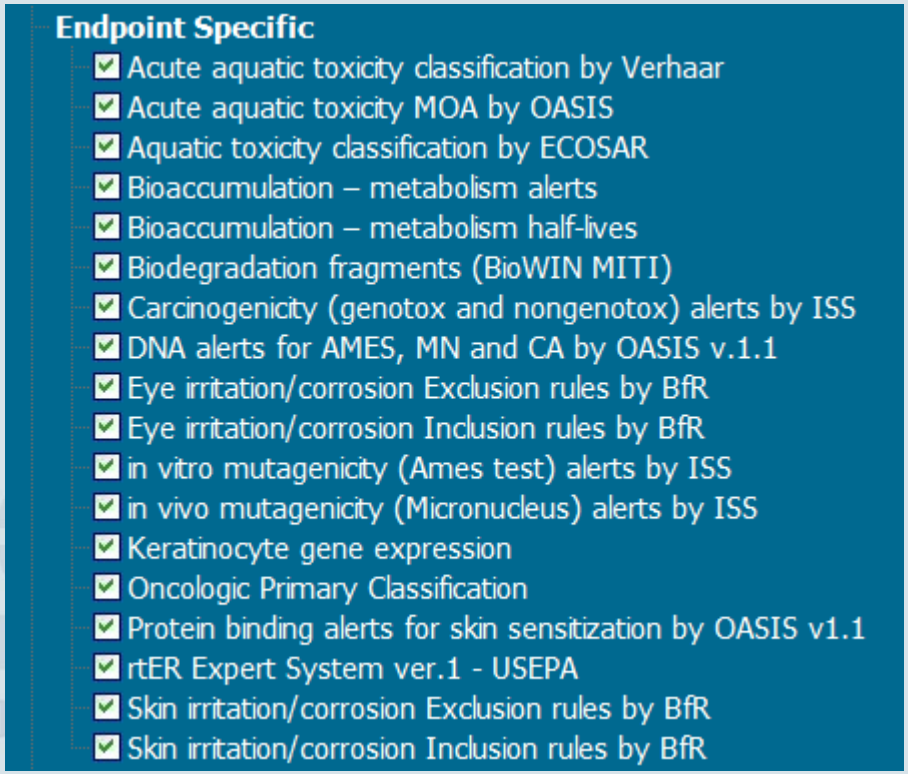
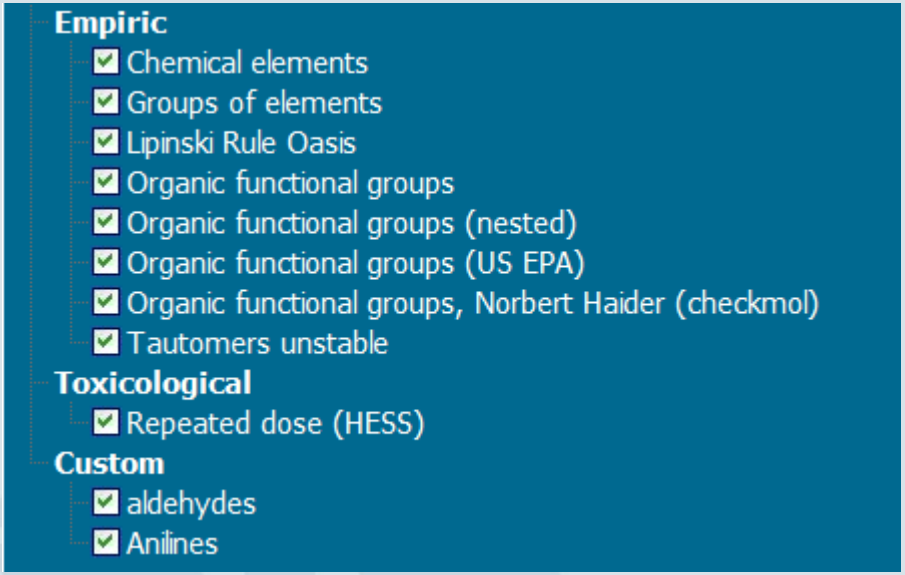


Profiling

- Predefined
- General Mechanistic
- Endpoint Specific
- **Empiric**
- **Custom**



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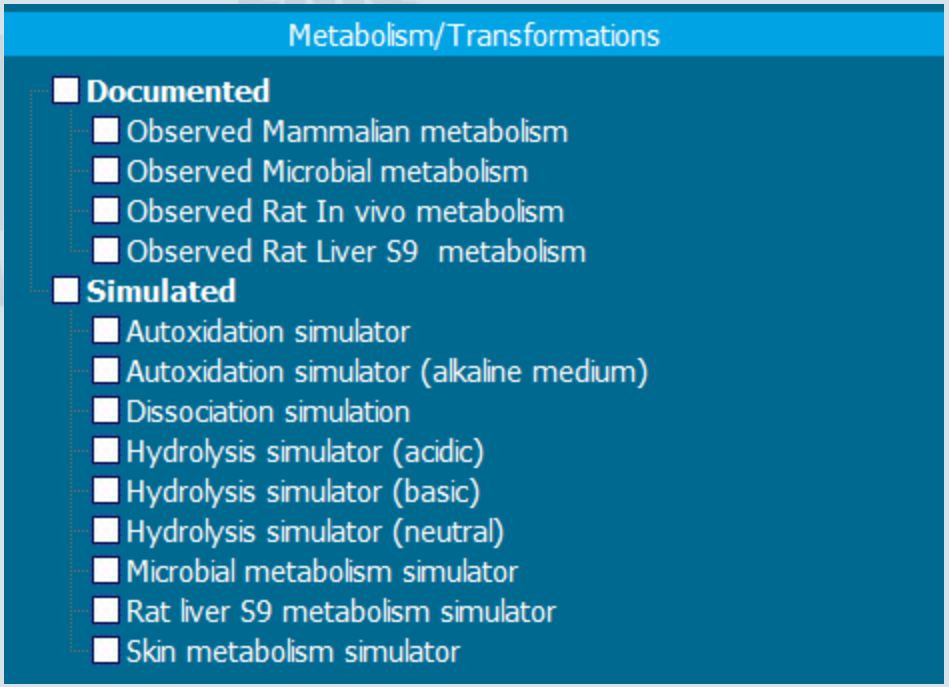
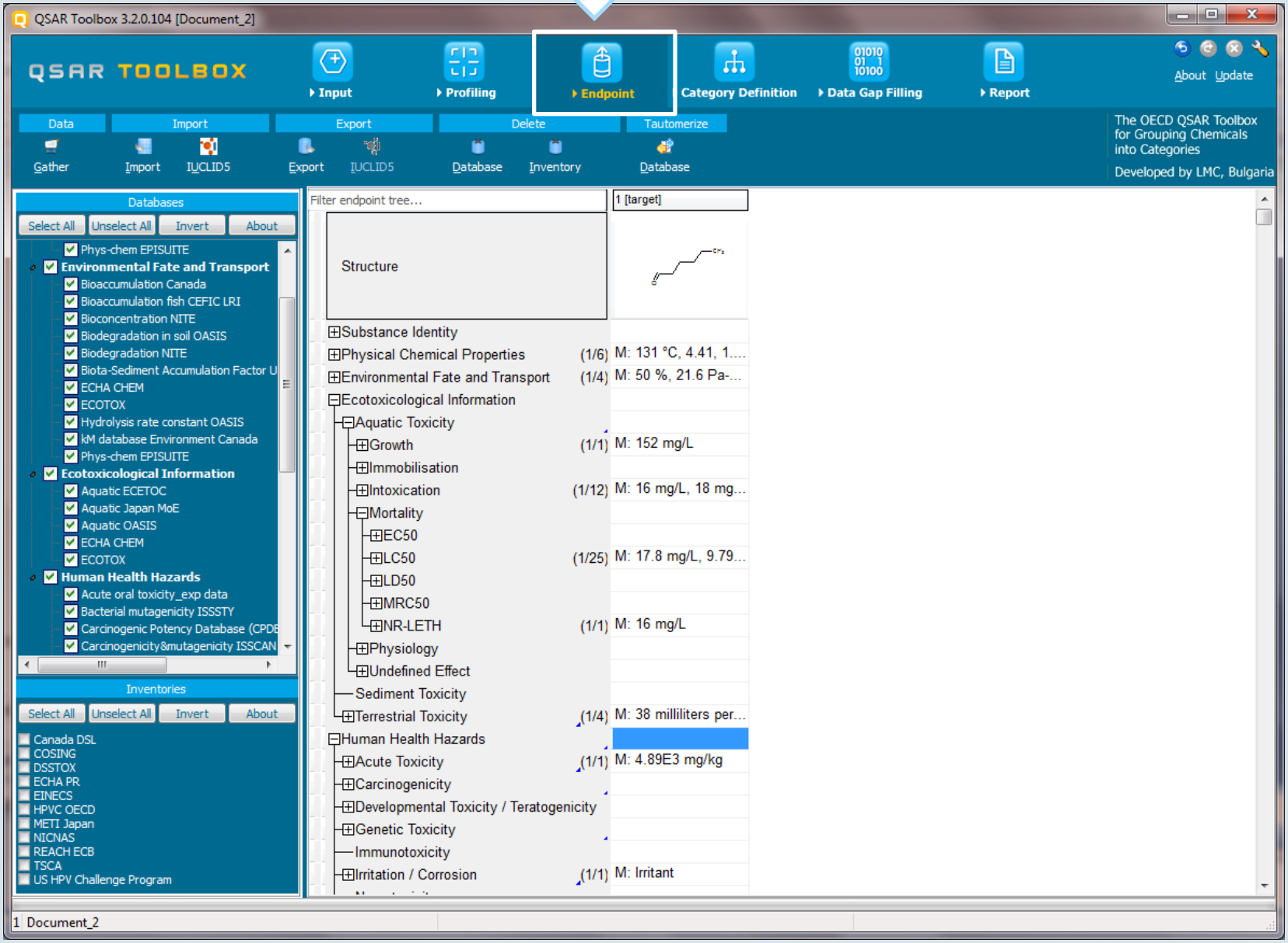
Profiling

- Predefined
- General Mechanistic
- Endpoint Specific
- Empiric
- Custom

- **Molecular transformations**



Endpoint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Data Gap Filling
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Delete
Tautomerize
Gather
Import
IUCLID5
Export
IUCLID5
Database
Inventory
Database
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Databases
Select All
Unselect All
Invert
About
Phys-chem EPISUITE
Environmental Fate and Transport
Bioaccumulation Canada
Bioaccumulation fish CEFIC LRI
Bioconcentration NITE
Biodegradation in soil OASIS
Biodegradation NITE
Biota-Sediment Accumulation Factor U
ECHA CHEM
ECOTOX
Hydrolysis rate constant OASIS
kM database Environment Canada
Phys-chem EPISUITE
Ecotoxicological Information
Aquatic ECETOC
Aquatic Japan MoE
Aquatic OASIS
ECHA CHEM
ECOTOX
Human Health Hazards
Acute oral toxicity_exp data
Bacterial mutagenicity ISSSTY
Carcinogenic Potency Database (CPDE
Carcinogenicity&mutagenicity ISSCAN
Inventories
Select All
Unselect All
Invert
About
Canada DSL
COSING
DSSTOX
ECHA PR
EINECS
HPVC OECD
METI Japan
NICNAS
REACH ECB
TSCA
US HPV Challenge Program
Filter endpoint tree...
1 [target]
Structure
Substance Identity
Physical Chemical Properties (1/6) M: 131 °C, 4.41, 1....
Environmental Fate and Transport (1/4) M: 50 %, 21.6 Pa-...
Ecotoxicological Information
Aquatic Toxicity
Growth (1/1) M: 152 mg/L
Immobilisation
Intoxication (1/12) M: 16 mg/L, 18 mg...
Mortality
EC50
LC50 (1/25) M: 17.8 mg/L, 9.79...
LD50
MRC50
NR-LETH (1/1) M: 16 mg/L
Physiology
Undefined Effect
Sediment Toxicity
Terrestrial Toxicity (1/4) M: 38 milliliters per...
Human Health Hazards
Acute Toxicity (1/1) M: 4.89E3 mg/kg
Carcinogenicity
Developmental Toxicity / Teratogenicity
Genetic Toxicity
Immunotoxicity
Irritation / Corrosion (1/1) M: Irritant
1 Document_2

Endpoint

- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazard

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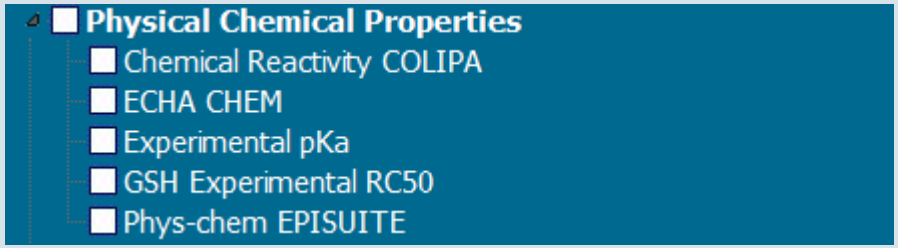
Endpoint

- **Physical Chemical Properties**
- Environmental Fate and Transport
- Ecotoxicological Information
- Human Health Hazard



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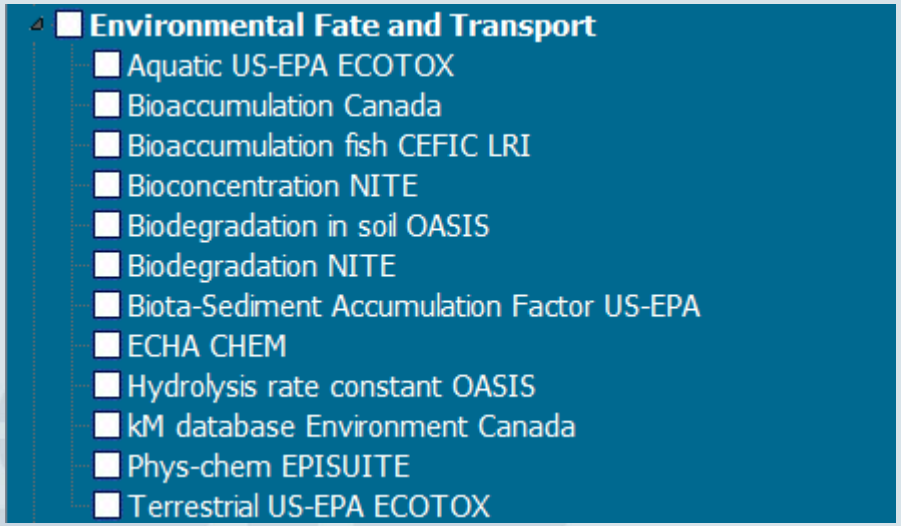
Endpoint

- Physical Chemical Properties
- **Environmental Fate and Transport**
- Ecotoxicological Information
- Human Health Hazard



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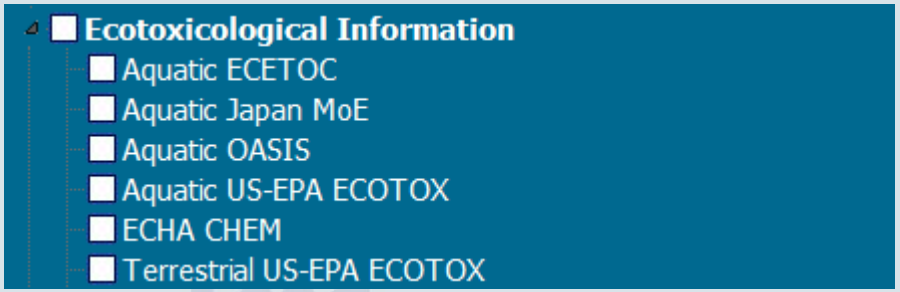
Endpoint

- Physical Chemical Properties
- Environmental Fate and Transport
- **Ecotoxicological Information**
- Human Health Hazard



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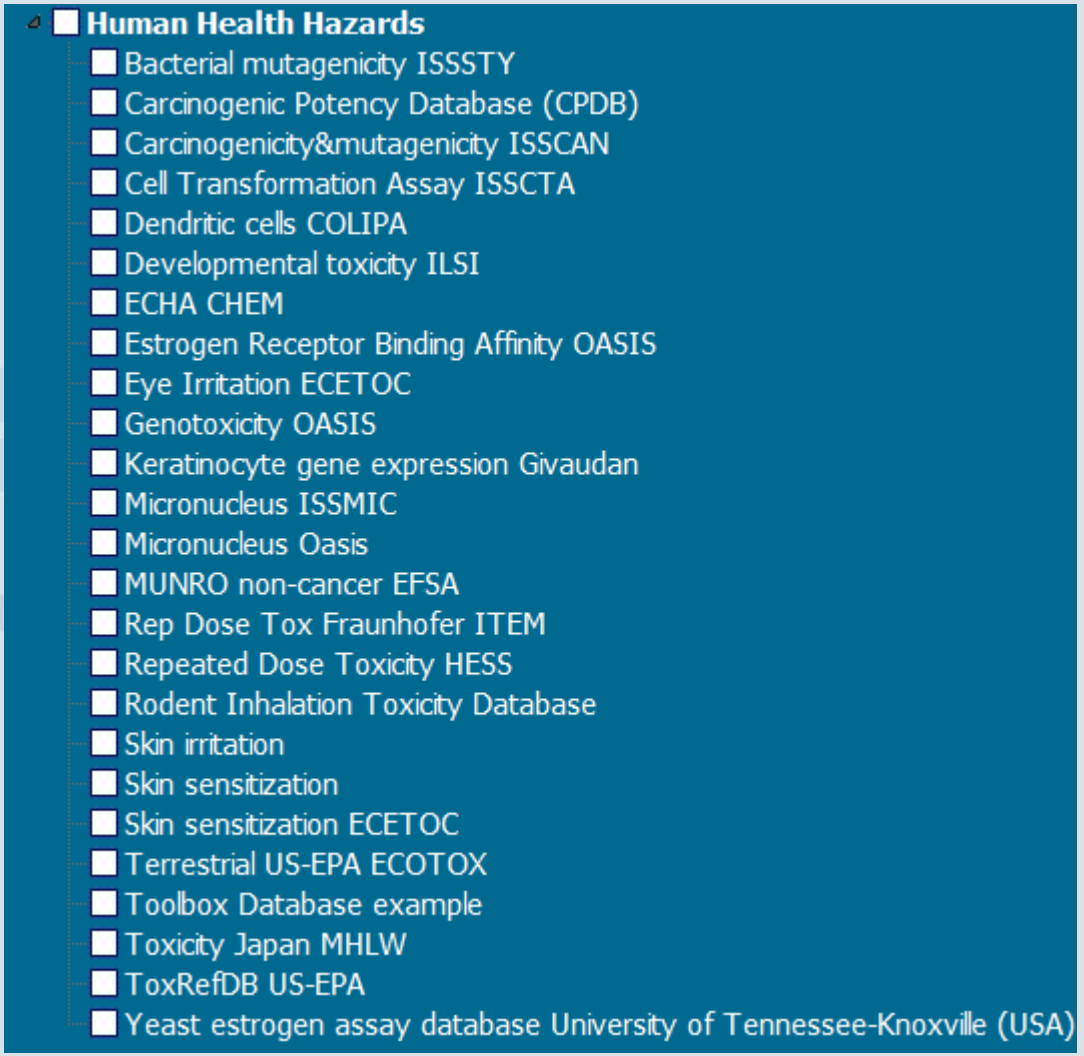
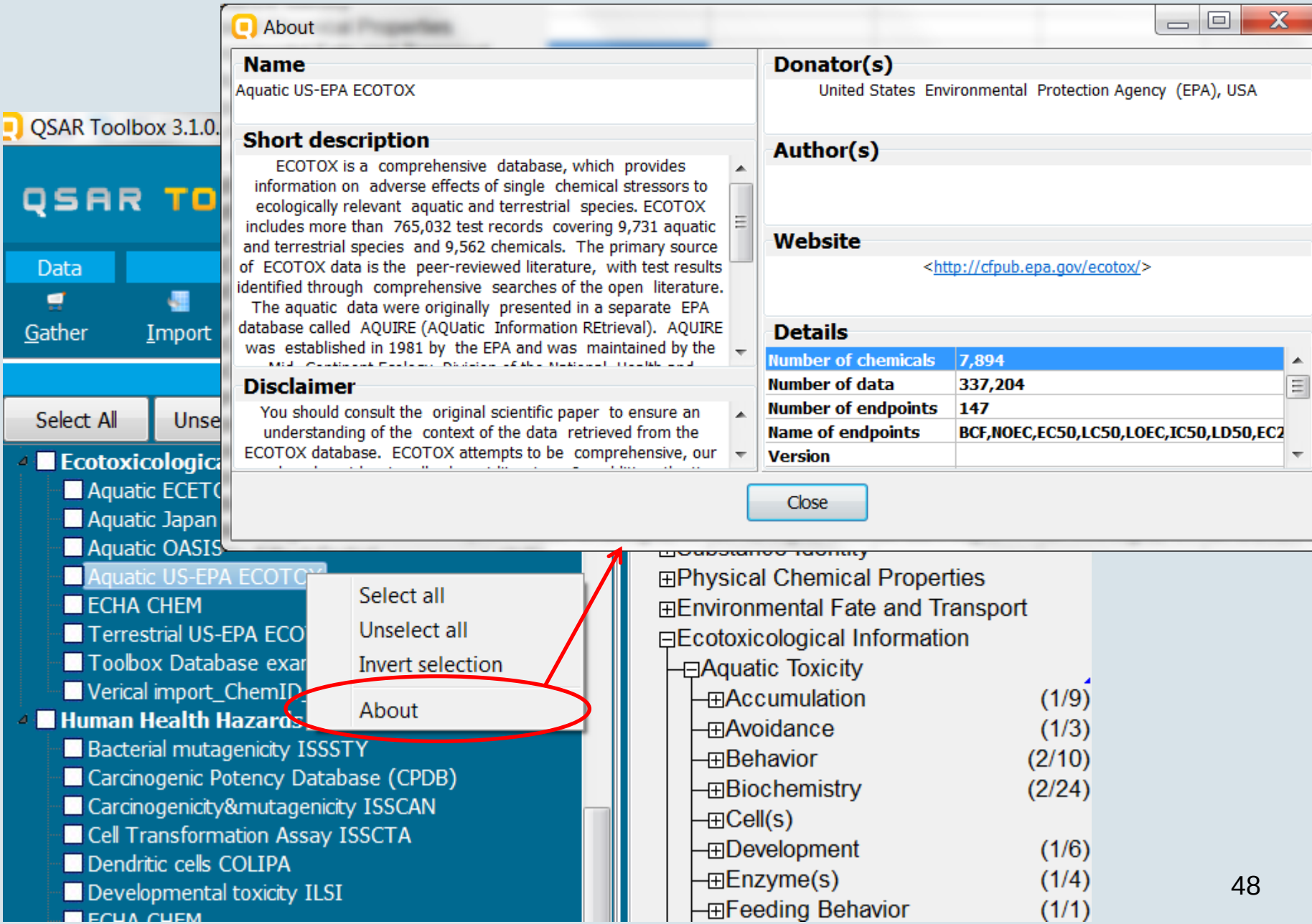
Endpoint

- Physical Chemical Properties
- Environmental Fate and Transport
- Ecotoxicological Information
- **Human Health Hazard**



Endpoint


About
Name
Aquatic US-EPA ECOTOX
Short description
ECOTOX is a comprehensive database, which provides information on adverse effects of single chemical stressors to ecologically relevant aquatic and terrestrial species. ECOTOX includes more than 765,032 test records covering 9,731 aquatic and terrestrial species and 9,562 chemicals. The primary source of ECOTOX data is the peer-reviewed literature, with test results identified through comprehensive searches of the open literature. The aquatic data were originally presented in a separate EPA database called AQUIRE (AQUatic Information REtrieval). AQUIRE was established in 1981 by the EPA and was maintained by the
Disclaimer
You should consult the original scientific paper to ensure an understanding of the context of the data retrieved from the ECOTOX database. ECOTOX attempts to be comprehensive, our
Donator(s)
United States Environmental Protection Agency (EPA), USA
Author(s)
Website
<http://cfpub.epa.gov/ecotox/>
Details
Number of chemicals 7,894
Number of data 337,204
Number of endpoints 147
Name of endpoints BCF,NOEC,EC50,LC50,LOEC,IC50,LD50,EC2
Version
Close
QSAR Toolbox 3.1.0.
Data
Gather
Import
Select All
Unse
Ecotoxicologic
Aquatic ECET
Aquatic Japan
Aquatic OASIS
Aquatic US-EPA ECOTOX
ECHA CHEM
Terrestrial US-EPA ECO
Toolbox Database exar
Verical import_ChemID
Human Health Hazard
Bacterial mutagenicity ISSSTY
Carcinogenic Potency Database (CPDB)
Carcinogenicity&mutagenicity ISSCAN
Cell Transformation Assay ISSCTA
Dendritic cells COLIPA
Developmental toxicity ILSI
Select all
Unselect all
Invert selection
About
Physical Chemical Properties
Environmental Fate and Transport
Ecotoxicological Information
Aquatic Toxicity
Accumulation (1/9)
Avoidance (1/3)
Behavior (2/10)
Biochemistry (2/24)
Cell(s)
Development (1/6)
Enzyme(s) (1/4)
Feeding Behavior (1/1)

Task C - ECHA CHEM database

C. Expansion of the repertoire of databases including data content normalization

Development of methodology to explore ECHA CHEM database

QSAR Toolbox data and ECHA CHEM contribution

Endpoint tree	QSAR Toolbox (without ECHA CHEM)		ECHA CHEM contribution	
	Substances	Data	Substances	Data
Phys-chem properties	38 000	71 000	5 700 (15%)	85 000 (120%)
Environmental	4 500	58 000	4 000 (88%)	28 000 (48%)
Ecotoxicological	8 500	510 000	4 600 (54%)	95 000 (18%)
Human health	15 000	550 000	5 400 (36%)	140 000 (25%)
Total	**55 000**	**1 200 000**	6 200 (9%)	350 000 (29%)

QSAR Toolbox databases

Contribution of REACH dissemination data
ECHA CHEM database

Endpoint tree	ECHA CHEM		Total	
	Substances	Data	Substances	Data
Substance Identity	**6188**	**301 868**	**92 854**	**1 538 014**
Physical Chemical Properties	5 738	86 453	41931	156 528
Environmental Fate and Transport	4 001	25 759	7581	85 585
Ecotoxicological Information	4 626	94 009	11 895	608 065
Human Health Hazards	5 426	95 647	18 813	687 836

Inventories

Inventories	Number of chemicals
AICS	38760
COSING	1314
DSSTOX	8606
ECHA PR	142619
EINECS	72561
HPVC EU	4843
METI Japan	16133
REACH ECB	74074
US HPV Challenge Program	9125
TSCA 2005	65709
Canada DSL	22017
Total number	**197015**

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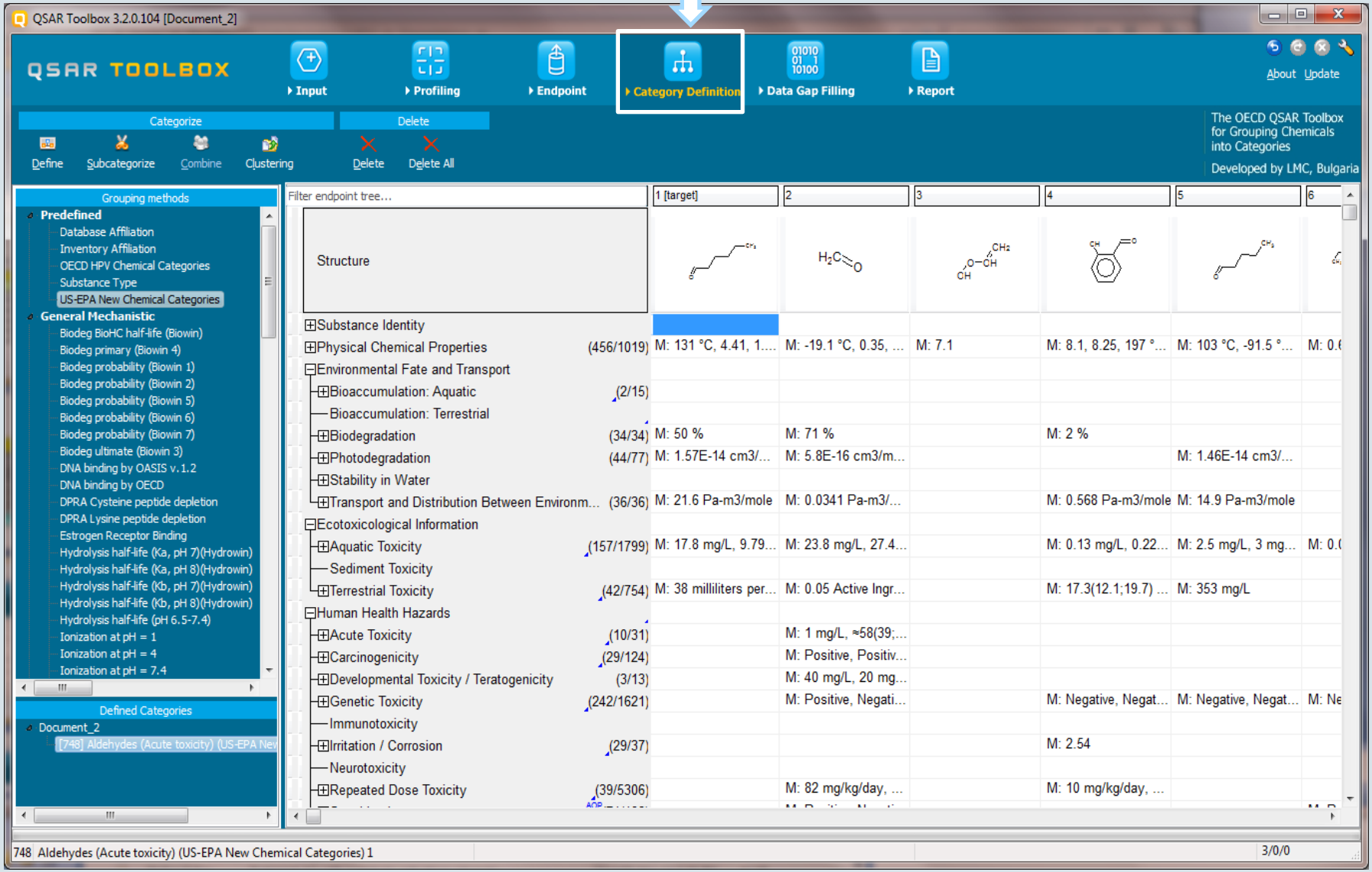
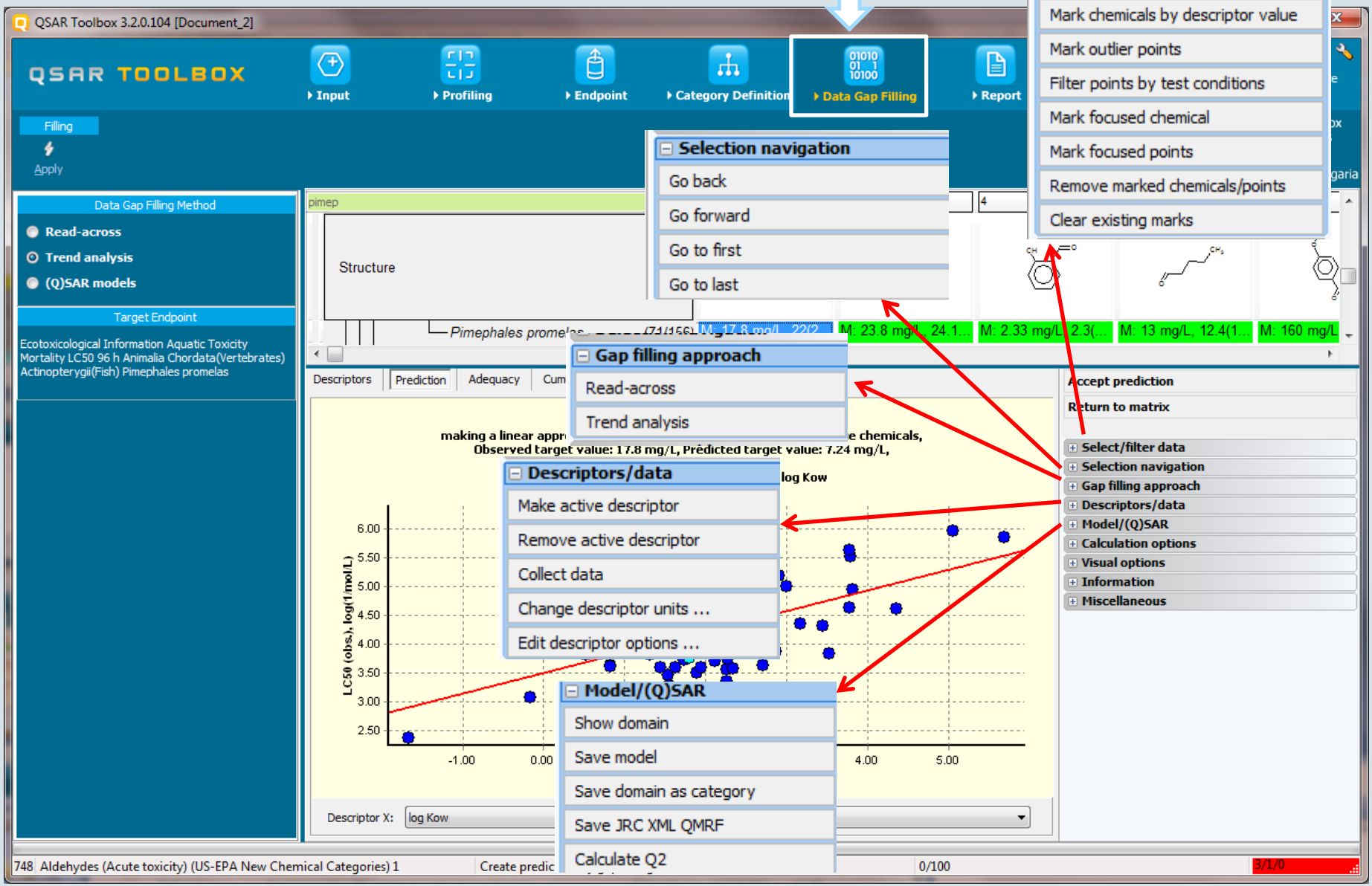
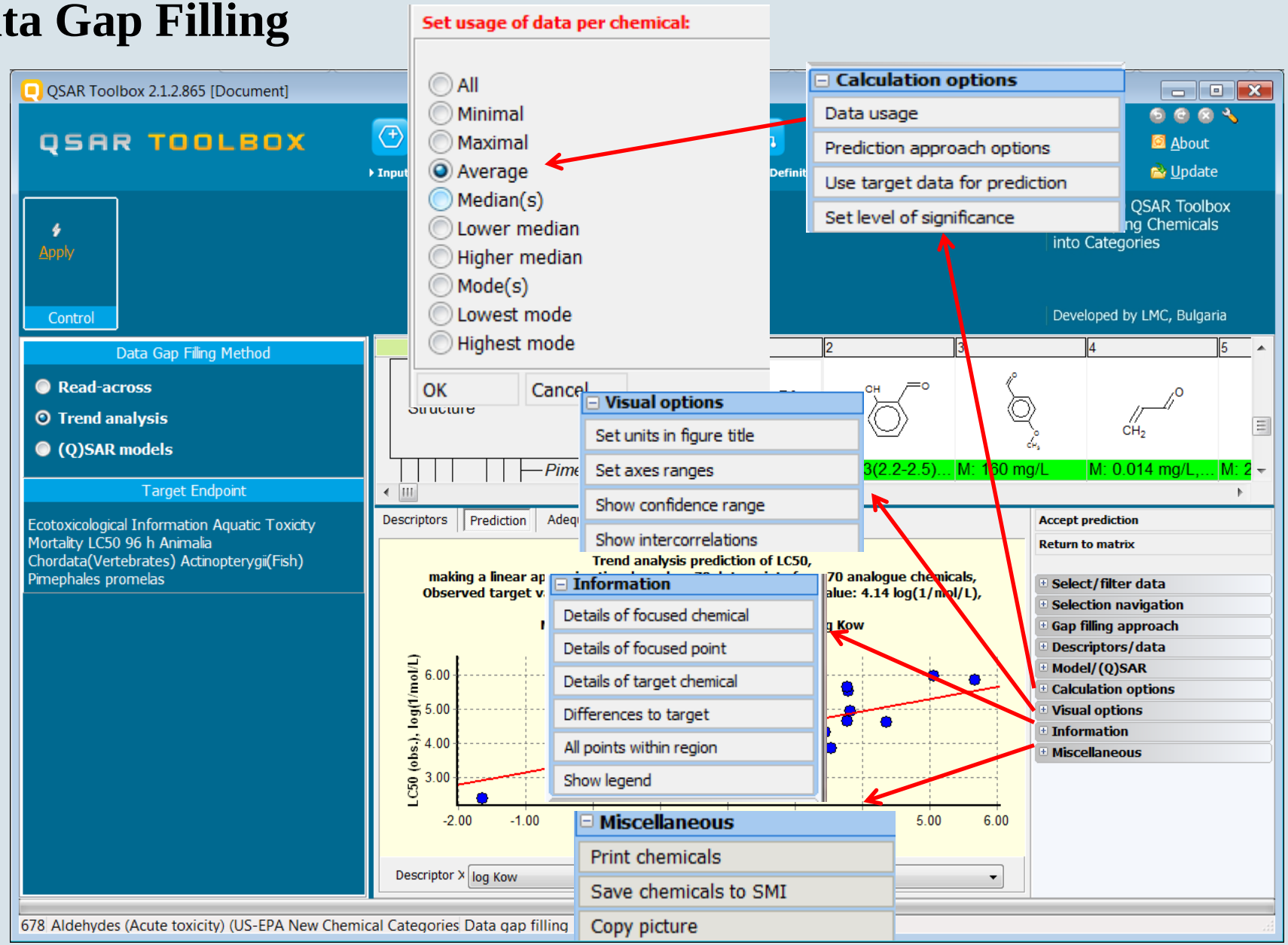
Category definition



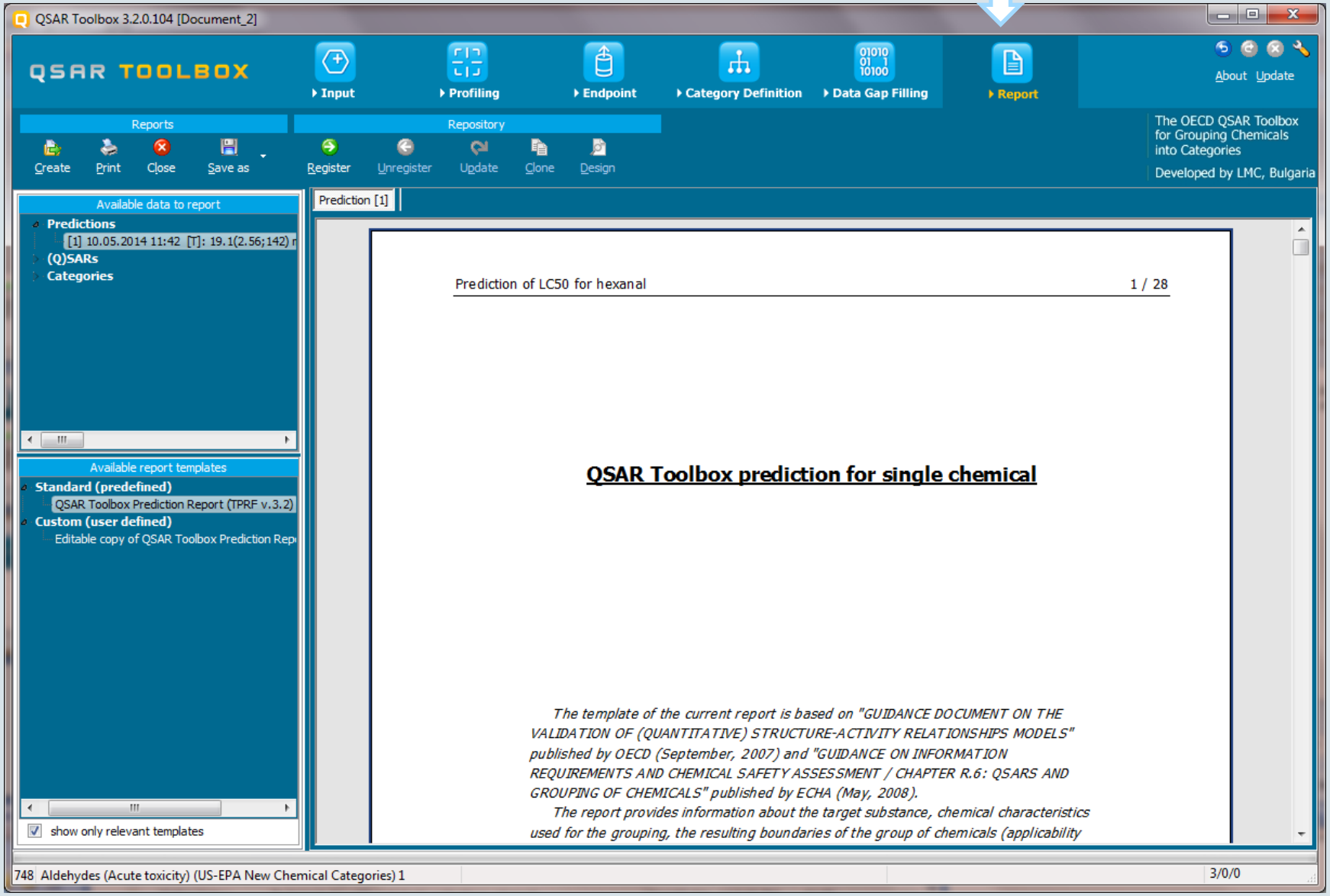
Data Gap Filling



Data Gap Filling



Report


QSAR Toolbox 3.2.0.104 [Document_2]
QSAR TOOLBOX
Input
Profiling
Endpoint
Category Definition
Data Gap Filling
Report
About
Update
Reports
Create
Print
Close
Save as
Repository
Register
Unregister
Update
Clone
Design
The OECD QSAR Toolbox for Grouping Chemicals into Categories
Developed by LMC, Bulgaria
Available data to report
Predictions
[1] 10.05.2014 11:42 [T]: 19.1(2.56;142) r
(Q)SARs
Categories
Available report templates
Standard (predefined)
QSAR Toolbox Prediction Report (TPRF v.3.2)
Custom (user defined)
Editable copy of QSAR Toolbox Prediction Rep
show only relevant templates
Prediction [1]
Prediction of LC50 for hexanal
1 / 28
QSAR Toolbox prediction for single chemical
The template of the current report is based on "GUIDANCE DOCUMENT ON THE VALIDATION OF (QUANTITATIVE) STRUCTURE-ACTIVITY RELATIONSHIPS MODELS" published by OECD (September, 2007) and "GUIDANCE ON INFORMATION REQUIREMENTS AND CHEMICAL SAFETY ASSESSMENT / CHAPTER R.6: QSARS AND GROUPING OF CHEMICALS" published by ECHA (May, 2008).
The report provides information about the target substance, chemical characteristics used for the grouping, the resulting boundaries of the group of chemicals (applicability
748 Aldehydes (Acute toxicity) (US-EPA New Chemical Categories) 1
3/0/0

Outlook

Description
General scheme and workflow
Basic functionalities
Forming categories

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How to build categories?

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Basic guidance for category formation

Recomended categorization phases:

1. Phase I. Endpoint non-specific - structure-related profilers (primary categorization)
2. Phase II. Endpoint specific profilers (for subcategorization) – based on endpoint driving interaction mechanisms
3. Phase II. Additional structure-related profilers, to further eliminate dissimilar chemicals (to increase the consistency of category)

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Recommended Categorization Phases

Phase I. Structure based

- US EPA Categorization
- OECD Categorization
- Organic functional group
- Structural similarity
- ECOSAR

Repeating Phase I due to Multifunctionality of chemicals

Broad grouping
Endpoint Non-specific

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Broad grouping
Endpoint Non-specific

Repeating Phase I due to Multifunctionality of chemicals

Phase II. Mechanism based

- DNA binding mechanism
- Protein binding mechanism
- Mode of action –acute aquatic toxicity
- Genotoxicity/carcinogenicity
- Cramer rules
- Verhaar rule
- Skin/eye irritation corrosion rules

Subcategorization
Endpoint Specific

Metabolism accounted for

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Recommended Categorization Phases

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Endpoint Non-specific

Repeating Phase I due to Multifunctionality of chemicals

Phase II. Mechanism based

- DNA binding mechanism
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- Mode of action –acute aquatic toxicity
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- Verhaar rule
- Skin/eye irritation corrosion rules

Subcategorization
Endpoint Specific

Metabolism accounted for

Phase III. Eliminating dissimilar chemicals

Apply Phase I categorization

Subcategorization
Endpoint Specific

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Basic guidance for category formation

Suitable categorization phases:

1. Phase I. Endpoint non-specific - structure-related profilers (primary categorization)
2. Phase II. Endpoint specific profilers (for subcategorization) – based on endpoint driving interaction mechanisms
3. Phase II. Additional structure-related profilers, to further eliminate dissimilar chemicals (to increase the consistency of category)

Performing categorization:

1. The categorization phases should be applied successively
2. The application order of the phases depend on the specificity of the data gap filling performed (data availability, endpoint specificity)
3. More categories of same phase could be used in forming categories
4. Some of the phases could be skipped if consistency of category members is reached
5. Subcategorization should be applied at Data gap filling stage

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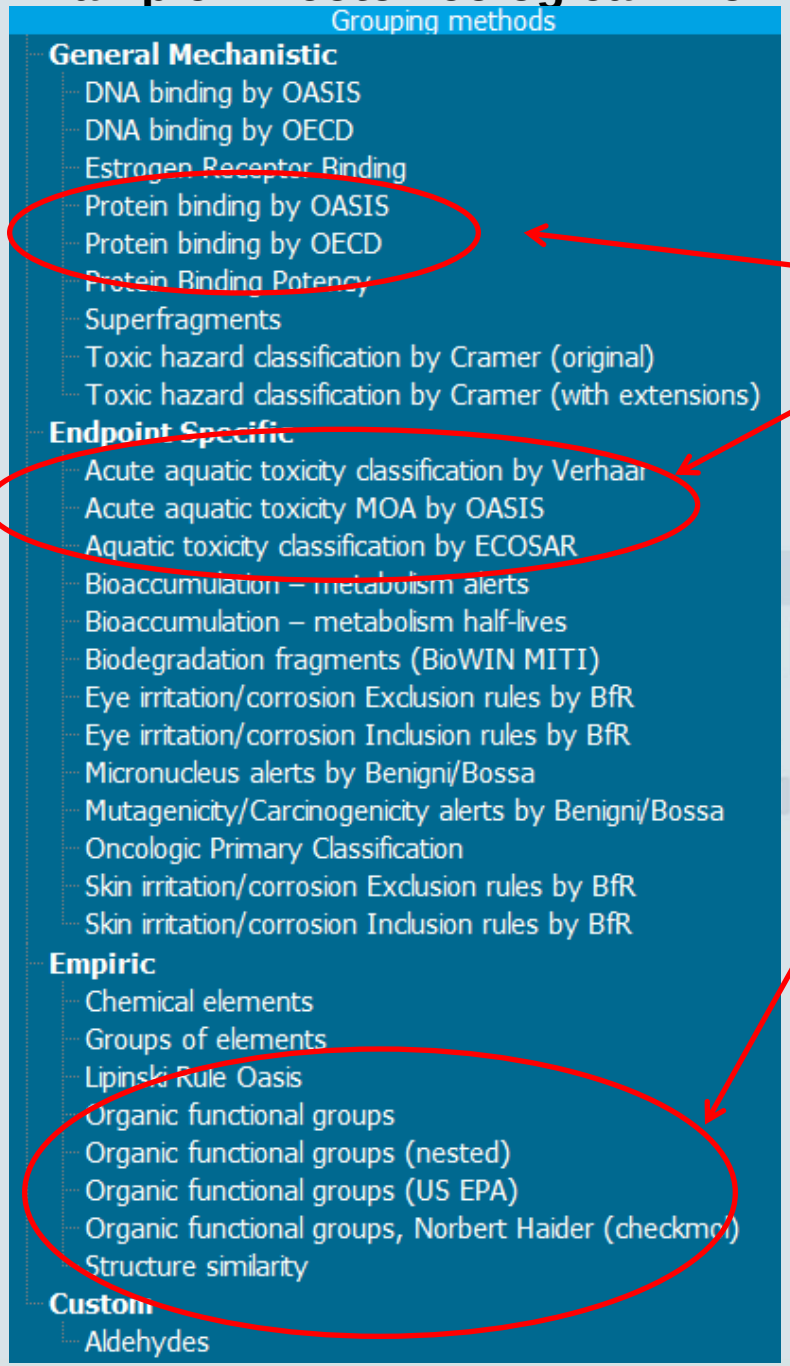
Example – Ecotoxicological Information



Acute Aquatic Toxicity

Mode of Action

Structural similarity (not for narcotics)

Data Gap Filling Approach

Trend analysis, External QSARs

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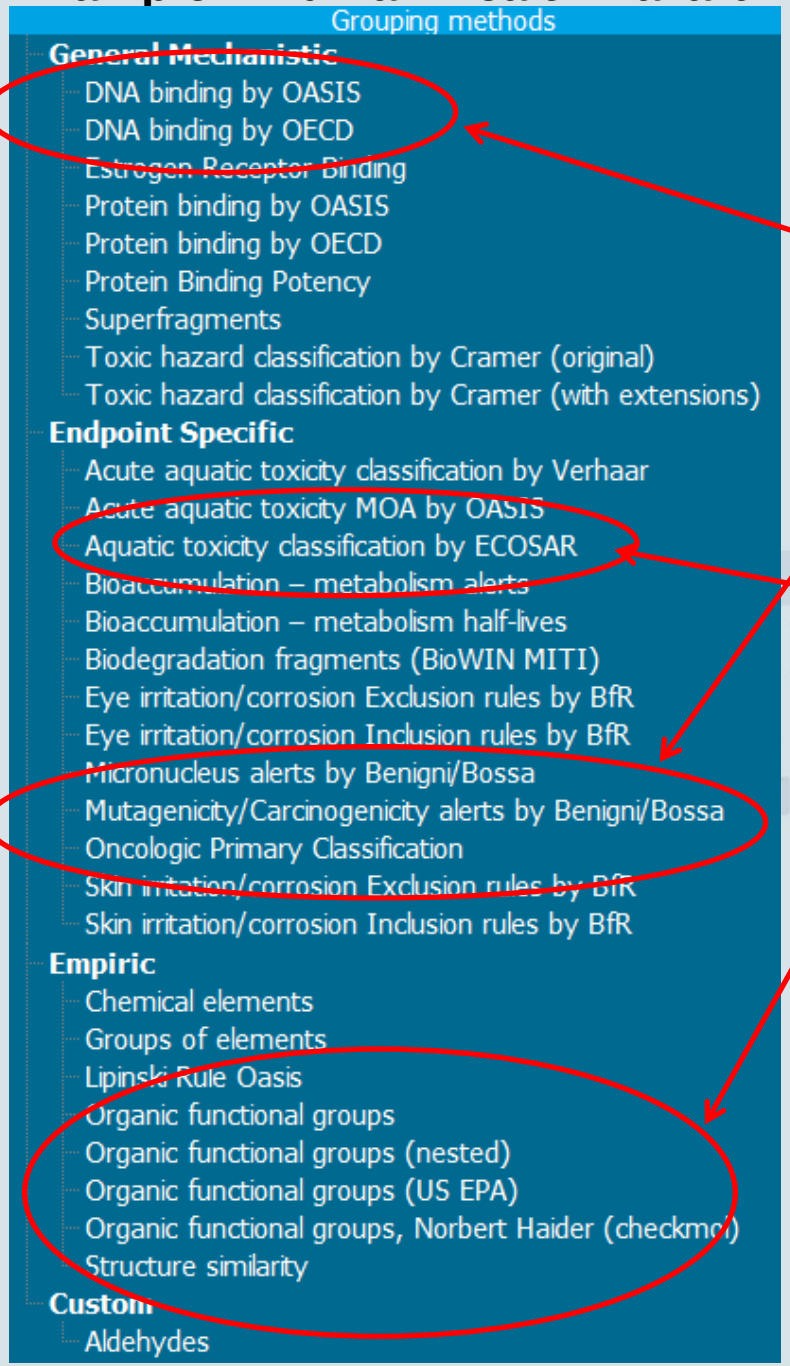
Example – Human Health Hazard



Mutagenicity/Carcinogenicity

Mechanism

Structural similarity

Data Gap Filling Approach

Trend analysis, External SARs

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