QSAR TOOLBOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

User manual

Toolbox 3.3
What's new?

Document history

Version	Comment
Version 1.0	October 2012: Toolbox 3.0 What's new
Version 2.0	December 2013: Toolbox 3.2 What's new
Version 3.0	December 2014: Toolbox 3.3 What's new

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If you have questions or comments that relate to this document, please send them to ehscont@oecd.org or visit the QSAR Toolbox discussion forum at https://community.oecd.org/community/toolbox_forum

Table of Contents

1 What's new

A new functionalities and modifications are implemented in Toolbox v.3.3. Below you will find a list with basic additions and modifications implemented in TB v.3.3.

I. New scientific features

1. Databases

A. New databases

- Human Half-life (kM) – 1105 chemicals with 2045 half-life data points related to two endpoints:
  - Half Life (biotransformation)
  - Half-life (total Body)
- ToxCast DB – database is implemented as a plugin tool including 1813 chemicals with 54669 data points
- Developmental and Reproductive Toxicity (DART) database – 716 chemicals with 1430 data points separated as follows:
  - Developmental toxicity (716 data points)
  - Reproductive toxicity (714 data points)

B. Updated databases

- Genotoxicity database – QA of the database and addition of 514 new chemicals with 3753 new data points
- Skin sensitization database – addition of new skin sensitization data for two chemicals
- Hydrolysis rate constant – addition of 26 chemicals with 26 data points
- ECOTOX – new release from 12th of June 2014 with 489 new chemicals with 84256 data points
- Repeated dose toxicity HESS – addition of 77 chemicals with 43 667 new data points
- ECHA Chem – new release from July 2014 with 1189 chemicals with 91 340 data points

C. Modifications in databases

There are several "losses" (less number of chemicals) in the following list of databases with respect to Toolbox 3.2:

- Bioconcentration NITE "lost" four chemicals (from 771 to 767)
- Chemical Reactivity COLIPA "lost" 2 chemicals (from 113 to 111)
- Dendritic cells COLIPA "lost" also 2 chemicals (from 119 to 117)
- Experimental pKa "lost" 58 chemicals (from 14773 to 14715)

The losses are due to the duplicate number of chemicals. In TB 3.2 these duplicate number of chemicals are displayed as separate chemicals, while in TB 3.3 the unique number is displayed. This is the reason for the "losses" in database

2. Profilers

A. New profilers

- Respiratory sensitization
- DART scheme v1.0
- Protein binding alerts for Chromosomal aberration by OASIS v1.1
- Retinoic Acid Receptor Binding

B. Updated profilers based on expert analysis and consistency with private software (TIMES)

- DNA binding by OASIS v.1.3
- DNA alerts for AMES, MN and CA by OASIS v.1.3
- Protein binding by OASIS v1.3
- Protein binding alerts for skin sensitization by OASIS v1.3
- Organic functional group
- Organic functional group (nested)
- Repeated dose toxicity

3. Metabolism simulators

Updated metabolism simulators based on expert analysis and consistency with private software (TIMES and CATALOGIC)

- Autoxidation simulator

- Autoxidation simulator (alkaline medium)
- Microbial simulator
- Rat liver S9 metabolism simulator
- Skin metabolism simulator

4. **Templates for profile documentation**

   Pilot templates are prepared for the following types of profilers:

   - Donated Executable Profiler:
     - Aquatic toxicity classification by ECOSAR
   - Logical expression:
     - US-EPA New Chemical Categories
     - Protein binding alerts for skin sensitization by OASIS v1.3
     - Respiratory sensitization
   - Sequence of Logical Expressions
     - Acute aquatic toxicity classification by Verhaar (Modified)
   - Model (or (Q)SAR) Based Profiler
     - Biodegradation probability (Biowin 1)

5. **External SAR models**

   The following SAR models have been implemented:

   - Explosive properties (Impact sensitivity of nitroaliphatic compounds)
   - Phototoxicity models with different domains
     - Phototoxicity of PAH
     - Phototoxicity based on 3T3 NRU data
   - Developmental and Reproductive Toxicity DART (P&G)

II. New functionalities and usability improvements

1. Changed the way QSARs are displayed on the datamatrix
2. New template to document profilers
3. Possibility of saving predictions

4. Endpoint vs endpoint correlation
5. Maintain compatibility with the recent version of IUCLID (5.6)
6. Improving the Query Tool functionality
7. New categorization functionality applying metabolism
8. Implementation of ECOSAR models as individual QSARs
9. Possibility to filter chemicals in data gap filling by making use of measured data
10. Functionality to create correlations between data of different or equal endpoints. This functionality allows creating a correlation between data and categories from a selected profiling group.

III. General

1. Various usability improvements for Query Tool
2. Improvements of sections of F1 Help functionality related to the new functionalities
   - ✓ Fixing bugs

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