QSAR TOOLBOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

User manual

Toolbox 3.3 Release Notes

Document history

Version	Comment
Version 1.0	October 2014: Toolbox 3.3 Release Notes

Issue date: October 2014

Language: English

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

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1 Overview

The Toolbox 3.3 installation is a major release of Toolbox and can function as a separate product from the previous QSAR Toolbox version. Thus it can be installed along-side older versions and will coexist peacefully.

A new Firebird version was used, version 2.5, that requires an upgrade of already existing Firebird installations.

2 System Requirements

Minimum system requirements

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OS: Windows XP

CPU: Core 2 duo at 1.8 GHz or equivalent AMD CPU

RAM: At least 3GB of RAM

HDD: 14 GB free hard drive space

File system: NTFS

Recommended system requirements

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OS: Windows 7 64 bit or newer

CPU: I5 at 2.4GHz or faster processor or equivalent AMD CPU

RAM: 6 GB of RAM

HDD: 20 GB free hard drive space

File system: NTFS

3 Change log

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)
- Photoinduced toxicity models with different domains

- Photoinduced toxicity of PAH
- Photoinduced toxicity 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 (not included in the contract)
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 QueryTool.
2. Improvements of sections of F1 Help functionality related to the new functionalities
3. BUGFIX: Missing information for the features used to define category
4. BUGFIX: information for the number of chemicals with data on the data matrix is not updated after removing chemicals by subcategorization
5. BUGFIX: Vertical import sets data value in MinValue field of data.
6. BUGFIX: profiling of a set of AU products with generated oligomer results in not responding system
7. BUGFIX: Selected chemicals in the GF are not green in the data matrix
8. BUGFIX: QT searching in checked DBs - not working when a chemical is loaded on the data matrix
9. BUGFIX: Importing I5Z files with long filenames.
10. BUGFIX: AV when clicking on view dendro scheme.

11. BUGFIX: AV when clicking on "View metabolism" for dendro schemes.
12. BUGFIX: QT does not find structures by molecular formula as copied from the data matrix
13. BUGFIX: "Invalid profile" when using categorization with Eye irritation/corrosion exclusion rules using of strict
14. BUGFIX: In any profiler could not see in 2D editor the charge of ionnic fragment and explicit {H}, which is available in the smiles?
15. BUGFIX: Not working alkyl chain fragment
16. BUGFIX: Changes in Similarity options by right click are not reflected to the investigated chemicals
17. BUGFIX: AV appears when try to filter data by test condition.
18. BUGFIX: R-fragment does not work
19. BUGFIX: List index out of bond when filter data
20. BUGFIX: Domain textual explanation
21. BUGFIX: 3D calculation problems
22. BUGFIX: Search by names is not working in QT
23. BUGFIX: After resizing category window it is not possible to return it back
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34. BUGFIX: Invalid profile when subcategorize by using All categories
35. BUGFIX: The system profiles after click on "Remove" in Subcategorization panel
36. BUGFIX: List index out of bonds when open 2D parameters from endpoint tree while in Gap filling

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