User manual

Toolbox 4.5 Release Notes

Document history

Version	Comment
Version 1.0	September 2021: Toolbox 4.5 Release Notes

Issue date: September 2021

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 4.5 installation is a major update of Toolbox 4.4. It can be installed as a separate product alongside previous major releases of Toolbox (4.4, 4.3, 4.2, 4.1, 4.0, 3.4, 3.3, etc.)

2 System Requirements

Minimum system requirements

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OS: 64 bit, Windows 7 or newer

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

RAM: At least 4GB of RAM

HDD: 14 GB free hard drive space

File system: NTFS

Microsoft .NET 5.0

Recommended system requirements

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OS: 64 bit, Windows 7 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

Microsoft .NET 5.0

3 Change log

I. General

- Web client - A pilot version of a web client will be available as part of the standard installation. It will provide basic features known from the Simplified UI along with a dedicated module for searching in imported IUCLID databases.

II. Input

New functionalities/improvements:

- Define target endpoint:
  - New form for easier definition of the target endpoint – following the endpoint tree organization;
  - Possibility to define supporting endpoints to the target endpoint
  - Possibility to save the definitions, import and export
- Possibility to enter target chemical by IUCLID ID (UUID of dossiers or substances)
- Possibility to explore in details the identity (i.e. composition) of a substance in the original source;
- Button (new functionality) allowing composition search in IUCLID databases

III. Profiling

70 profilers (Predefined: 5; General Mechanistic: 29; Endpoint Specific: 25; Empiric: 9; Toxicological: 1; Custom: 1) and 16 metabolisms (5 observed and 11 simulated) are available.

A. Updated profilers

1. *Acute Oral Toxicity*
2. *Biodeg Primary (Biowin 4)*
3. *Biodeg Ultimate (Biowin 3)*
4. *Carcinogenicity (genotox and nongenotox) alerts by ISS*
5. *DART scheme*
6. *DNA alerts for Ames, CA and MNT by OASIS*

7. *DNA binding by OASIS*
8. *Hydrolysis Half-life (pH 6.5 - 7.4)*
9. *in vitro mutagenicity (Ames test) alerts by ISS*
10. *in vivo mutagenicity (Micronucleus) alerts by ISS*
11. *Ionization pH 1*
12. *Ionization pH 4*
13. *Ionization pH 7.4*
14. *Ionization pH 9*
15. *OncoLogic Primary Classification*
16. *Organic Functional groups*
17. *Organic Functional groups (nested)*
18. *Organic functional groups (US EPA)*
19. *Organic functional groups, Norbert Haider (checkmol)*
20. *Protein binding alerts for Chromosomal aberration by OASIS v1.2*
21. *Protein binding alerts for skin sensitization according to GHS*
22. *Protein binding by OASIS*
23. *Repeated dose (HESS)*
24. *Substance type*
25. *Tautomers unstable*
26. *Toxic hazard classification by Cramer*
27. *Toxic hazard classification by Cramer (extension)*
28. *Uncouplers (MITOTOX)*

B. Updated simulators

1. *Autoxidation simulator*
2. *Autoxidation simulator (alkaline medium)*
3. *Dissociation simulator*
4. *Hydrolysis simulator (acidic)*
5. *Hydrolysis simulator (basic)*
6. *Hydrolysis simulator (neutral)*
7. *in vivo Rat metabolism*
8. *Microbial metabolism simulator*
9. *Rat liver S9 metabolism simulator*
10. *Skin metabolism simulator*
11. *Tautomerism*
12. *Observed Microbial metabolism*

IV. Data

59 databases are available in QSAR Toolbox v.4.5 (as compared to 57 databases in QSAR Toolbox v.4.4.1

New functionalities/improvements:

- Information for the composition of the test material provided as metadata
- Color-highlighting the data obtained for test material different than the substance
- Import from IUCLID
  - new options when import data from IUCLID
  - possibility to select specific data for importing (i.e. filtering data)

A. New databases

1. *Human skin sensitisation NICEATM/BfR*
   - New: 1 377 substances and 2 277 data points
2. *Photosensitivity database*
   - New: 73 substances and 563 data points

B. Updated databases

a. Databases with additional substances/data

1. *Bioconcentration&logKow NITE*
   - Available: 2 100 substances and 2 902 data points
   - New: 1 375 substances and 1 344 data points
2. *ECHA REACH*
   - Available: 24 124 substances and 1 070 616 data points
   - New: 10 818 substances and 268 386 data points
3. *ECOTOX*
   - Available: 12 326 substances and 1 068 143 data points
   - New: 504 substances and 98 791 data points
4. *Food Tox Hazard EFSA*
   - Available: 1 698 substances and 12 850 data points
   - New: 400 substances and 2 309 data points
5. *Genotoxicity & Carcinogenicity ECVAM*
   - Available: 970 substances and 10 903 data points
   - New: 226 substances and 1 717 data points
6. *Genotoxicity OASIS*
   - Available: 8587 substances and 39 929 data points
   - New: 556 substances and 8 986 data points
7. *Genotoxicity pesticides EFSA*
   - Available: 8587 substances and 39 929 data points
   - New: 556 substances and 8 986 data points

8. *Hydrolysis rate constant OASIS*
   - Available: 411 substances and 445 data points
   - New: 62 substances and 96 data points
9. *Repeated Dose Toxicity HESS*
   - Available: 777 substances and 487 201 data points
   - New: 32 substances and 1 359 data points
10. *Toxicity Japan MHLW*
   - Available: 450 substances and 4 406 data points
   - New: 60 substances and 435 data points

b. Databases with corrected substances/data

1. *Acute oral toxicity DB*
   - Available: 10 126 substances and 10 126 data points
   - New: missing ID information is added for some substances
2. *Micronucleus OASIS*
   - Available: 557 substances and 557 data points
   - New: One data point is changed
3. *Skin Sensitization*
   - Available: 1280 substances and 2 666 data points
   - New: One substance is removed
4. *Biocides and plant protection ISSBIOC*
   - Available: 299 substances and 1196 data points
   - New: some SMILES are corrected
5. *Carcinogenic Potency Database (CPDB)*
   - Available: 1 530 substances and 3 501 data points
   - New: some SMILES are corrected
6. *Carcinogenicity&mutagenicity ISSCAN*
   - Available: 1 148 substances and 4 518 data points
   - New: some SMILES are corrected
7. *Dendritic cells COLIPA*
   - Available: 257 substances and 933 data points
   - New: some SMILES are corrected
8. *Developmental & Reproductive Toxicity (DART)*
   - Available: 716 substances and 1 430 data points
   - New: some SMILES are corrected
9. *Human Half-Life*
   - Available: 1105 substances and 2045 data points
   - New: Changed endpoint paths
10. *Micronucleus ISSMIC*
   - Available: 563 substances and 1022 data points
   - New: some SMILES are corrected
11. *Experimental pKa*

- Available: 14 820 substances and 25 502 data points
- New: some SMILES are corrected

12. *Rep Dose Tox Fraunhofer ITEM*
    - Available: 949 substances and 5 321 data points
    - New: some SMILES are corrected

C. Updated inventories

1. *Australian Inventory of Industrial Chemicals (AIIC)*
    - Available: 38 918 substances

V. Data Gap Filling

New functionalities/improvements:

- Workflow editor – allowing automated and standardized workflows for predicting or grouping of chemicals to be developed by the users
- Possibility to export/import and delete custom workflows
- AW for Skin sensitization for Defined approaches (DASSAW) purposes – included automated check for domain affiliation
- New helper indicating presence of data with different test material

VI. Reporting/Exporting

New functionalities/improvements:

- Providing information in the report for the supporting endpoints in addition to the target endpoint
- Possibility to generate report for a prediction of the DASS AW obtained as a result of profiling

VII. IT improvements

- Completely reworked IUCLID Import
    - Use TEDRA IUCLID plugin
    - Added incremental update of IUCLID databases
- Profiling optimization
- Migration from .NET Framework to .NET 5
- Migrated from PostgreSQL version 9.6 to 13

VIII. Additional new features

- Caching of generated metabolites in Toolbox database (new combination of metabolic simulators and databases are cached);
- Preparing of additional user manual for the Workflow editor
- Calculation list of selected parameters
- Possibility to use combination of calculators, including custom defined
- Number of analogues and (sub)categorization steps in the export files
- Possibility to search by CAS by the combination of Ctrl+F buttons
- Hints for the number of data points in each cell of the data matrix
- Possibility to “freeze” the *Structure Info* part of the data matrix
- Possibility to auto expand the rows on the data matrix
- Possibility to adjust the columns/cells width
- Other small improvements (e.g. scrollers, expanders, highlights, corrected typos, etc.)

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