

User manual

Toolbox 3.2 Release Notes

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Document history

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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 | Overview | 4 |
| 2 | System Requirements..... | 4 |
| 3 | Change log | 5 |

Toolbox 3.2 Release Notes

1 Overview

The Toolbox 3.2 installation is designed as a separate product. It is designed to be separate (technically it is a completely different product) from earlier versions of the QSAR Toolbox and as such it can coexist on a single machine with previous versions of the Toolbox.

The new version has changes in its databases, profiling schemes, program modules and installation suite. It has a number of bug-fixes as well as some new features.

The Toolbox 3.2 deploys a new database repository which means that the user needs to re-import private databases or use the provided **Database Copy** tool. This tool can transfer all user databases from an existing Toolbox repository (ver. 2.3, 3.0, 3.1) format to a database in the Toolbox 3.2 format. For example it can transfer the data from an old Toolbox 2.3 database into the database deployed by the Toolbox 3.2 installation.

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

Toolbox 3.2 Release Notes

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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. Profilers – modifications have been done in the following profilers:

- DNA binding by OASIS v.1.1
- DNA alerts for AMES, MN and CA by OASIS v.1.1
- Protein binding by OASIS v1.1
- Protein binding alerts for skin sensitization by OASIS v1.1
- Acute aquatic toxicity classification by Verhaar
- Toxic hazard classification by Cramer (original)
- Toxic hazard classification by Cramer (with extensions)
- Skin irritation/corrosion Inclusion rules by BfR
- Eye irritation/corrosion Inclusion rules by BfR
- Organic functional groups
- Organic functional groups (nested)
- Repeated dose (HESS)

II. Simulators – slight modifications have been done in the following metabolic simulators, based on expert analysis:

- Rat liver S9 metabolism simulator
- Autooxidation simulator
- Autooxidation simulator (alkaline medium)

III. Databases – list with databases which have been modified:

Toolbox 3.2 Release Notes

- ECOTOX – this database substitute the two ECOTOX databases: Aquatic US-ECOTOX and Terrestrial US-EPA ECOTOX
- ECHA CHEM – update version of database
- Cell transformation assay – update version of database
- Carcinogenicity&mutagenicity ISSCAN – changes in database fields
- Micronucleus OASIS – update of data sets
- Hydrolysis rate constant OASIS – add new chemicals

IV. General improvements:

- Implemented communication with IUCLID 5.5 over WebServices
- Implemented new (IUCLID 5.5) version of harmonized templates.
- Improved canonization of SMILES notation – this does not reflect the workflow
- Acceleration the process of selecting databases/inventories and work with them
- Improved statistic for the reliability of “read-across” prediction (p-value/variation of data)
- Editing of 2D structure of already entered chemical
- Additional information about statistics of data/chemicals within the existing DB/Inventories
- Additional field within “Data filter” window is added such as: endpoint, test organism species etc.
- Interface improvement such as: warning messages, hint windows, last open folder with example files, keep last edited options, tree-like form of list with profilers etc.
- Better memory utilization when running on 64bit Windows version
- Faster execution when checking database/inventory in use. Improved database transaction handling resulting in better performance of database operations.
- Multithread model for the Server eliminating the need to restart Server in Import Mode.

V. Bug fixes

- Fixed a bug related to caching of dendroid schemes.
- Fixed an “out of memory” bug in Client Server version.
- Fixed bug in gathering data from tautomers.
- Fixed bug in depicting of 2D structures in Query Tool.
- Fixed bug when import new metadata fields.
- Fixed bug when import duration values in range.

Toolbox 3.2 Release Notes

- Set default scales for databases.
- Fixed bug related refreshing the list of QSARs after importing new model.
- In Scales editor the “Default” check box was enabled even if no scale was selected. Now it is fixed.
- Fixed bug during copying of a large custom database using the “Database copy” tool.
- Fixed PDF printing form of chemical structures.
- Removed unneeded "Profile statistics" menu item when the current selection is a discrete chemical
- Removed deprecated "Search" menu item from the data matrix context menu
- Enabled collapsing of profiling schemes into categories based on their type in the list on the Profiling screen
- Fixed a bug that caused an error message to be shown when entering a minus sign in the value field of a parametric boundary
- Fixed a bug that caused an error message to be shown when checking a profiling scheme that has just been exported via "Save as"
- Fixed a bug related to referential boundaries that refer to hierarchical schemes
- Fixed splitter in the bottom of the profiling scheme editor
- Added warning messages before deleting a profiling scheme category or clearing the entire scheme within the profiling scheme editor
- Updated the profiling scheme editor to focus a newly created category
- Updated the profiling scheme editor to show an 'M' next to queries which have metabolism options assigned
- “Save picture” functionality from 2D depiction window raised an error message when save in WMF
- Background of 2D depiction window is fixed to be white instead gray
- Fixed visualization of “smi” file loaded in 2D editor work panel. Column names CAS, Names and SMILES appears in duplicate form
- Fixed bug with defining of explicit hydrogen atoms within 2D editor panel, when valence of atoms is already defined. The explicit hydrogen atoms disappears
- Fixed bug with editing of definitions in exhaust fragment part of category Nitrosamine Type Compounds included in Oncologic profiler
- Fixed bug with entering chemical into 2D mode. The stereo information is not removed when is entered into this 2D mode
- Fixed bug: Polymers structures are considered as mixtures
- Fixed bug with form for searching of different chemicals ID numbers. The sequence of actions do not finished into same results
- Fixed bug with tautomerization of custom database, when structures contains stereo information
- Fixed bug with entering structures by CAS numbers. This happens when paste CAS numbers into CAS field
- Fixed bug in Query tool, when search for biodegradation data.

Toolbox 3.2 Release Notes

- Fixed bug with "Assign data by SMILES" functionality. In this case the data was moved from one structure to another, it is not multiplied
- Fixed various issues involving cancelation of gather data action.
- Fixed a bug when exporting profiling results with metabolism.
- Fixed a bug that produced an AV when canceling an initialization of a list of mixtures.
- Added unit "%" for "% Degr" field for harmonized templates 28, 29 and 30
- Removed predictions from going into data gap filling.
- Fixed a crash when changing dynamic tree hierarchy.
- Improved handling of stopping of an export procedure.
- Added popup menu-item to the "Possible data inconsistency" dialog that shows scale definitions.
- Fixed a bug when reordering the scale members in the scale definitions window.
- Fixed a bug with "Export molecular formula" feature.
- Fixed the counter for chemicals when importing from Excel (or tab delimited file).
- Fixed an AV when calling "About" button for newly created database.
- Improved progress reporting when using Bulk import.
- Fixed range check error which appeared on loading search FSQ for metabolic database
- When using Gap Filling, pressing of "STOP" button returns to data matrix
- Added is the possibility for selection when a chemical has more than one observed map within a selected database
- Added is the counter action for "show all points within region" in Gap Filling window
- Some wrong characters were removed from Appendix 3 of TPRF
- A wrong sentence was fixed in Appendix 7 of TPRF
- A sentence was improved in Summary page of TPRF
- A bug that combined different physico-chemical values in one table cell was fixed
- A missing table in Appendix 1 of TPRF was restored (appeared if count of chemicals with detailed info was set to 0)
- A catastrophic failure was fixed (after trying to display prediction domain using Toolbox QSAR)
- A bug was fixed related to selected databases listed in summary page of TPRF
- A bug was fixed in Gap Filling related to disappearing of target after eliminating data values by WS

OECD

2, rue André Pascal
75775 Paris Cedex 16
France

Tel.: +33 1 45 24 82 00

Fax: +33 1 45 24 85 00

ehscont@oecd.org