

User manual

Toolbox 4.5 SP1 Release Notes

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

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1 Overview

The QSAR Toolbox 4.5 SP1 installation is a service update for QSAR Toolbox 4.5. It is provided as a patch, to be applied on the October 2021 QSAR Toolbox 4.5 version, as well as a full installation package for first time installers. 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

A. Web Client improvements:

1. Link to the IUCLID entity and to the specific component (e.g. constituent, impurity, etc.) is added
2. 2D Editor is implemented in the Input section
3. Possibility to apply (Q)SAR models
4. Improvements of web matrix:
 - a. added possibility to delete chemical
 - b. possibility to enter more than one chemical when search by SMILES, CAS, etc.
 - c. indication for the number of chemicals/data points
 - d. filter information on data matrix
 - e. duplicated the organization of sections of the endpoint tree similarly to desktop version
5. Inclusion of additional information:
 - a. detailed information is added for different Toolbox objects (parameters, profilers, models)
 - b. showing metadata information for the available experimental data
 - c. explain of the profiling results – showing literature information
 - d. explain of the results of the automated workflow for defined approaches – showing information for the domain affiliation
6. Other small improvements (inclusion of filters, information messages, formatting, grouping of Toolbox objects, etc.)

B. Improvements in the Toolbox desktop version:

1. Simplification of the IUCLID import wizard.
 - a. Predefined list with picklists of “Study results type”, “Purpose flag” and “Reliability” fields are added
2. Resolved problems, reported via the Toolbox Helpdesk:
 - a. Fixed an issue when entering big CAS registry number into the system

- b. Clustering by structural similarity does not require target chemical
 - c. A fix is added when generate report using "iSafeRat Mechanisms of toxic action profiler" in combination with metabolic simulator
 - d. Resolved problem with the multi-user installation
 - e. Resolved an issue with IUCLID export
3. A fix is added when enter SMILES including quantities
4. Fixes in define target endpoint dialog:
- a. Validation of duration units
 - b. Fix a bug when modify fields hierarchy related to species taxonomy
5. Fixed bug when import inventories with defined additional chemical IDs
6. Several fixes are added related to docking of external software

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