User manual

Toolbox 4.4.1 Release Notes

Document history

Version	Comment
Version 1.0	April 2020: Toolbox 4.4.1 Release Notes

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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 4.4.1 installation is a replacement of version 4.4, it will replace it. It is also a major update of Toolbox 4.3. It can be installed as a separate product alongside previous major releases of Toolbox (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 8GB of RAM

HDD: 14 GB free hard drive space

File system: NTFS

Microsoft .NET Framework 4.5.1

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: 16 GB of RAM

HDD: 20 GB free hard drive space

File system: NTFS

Microsoft .NET Framework 4.5.1

3 Change log

1. Fixed a problem in metabolization module leading to random error which produces no metabolites for about 1% of chemicals.

2. Only the organic metabolites as a result of skin and in vitro rat liver metabolisms will be shown on data matrix.

3. Fixed bug where extracting data from WebServices doubles data in some cases.

4. Fixed bug when applying QSARs on multi constituent substances, which contains a constituent with an empty SMILES.

5. Fixed bug which causes TB Sever to shut down when unsuccessful copy of error log.

6. Fixed bug when exporting DataMatrix which contains results for Similarity of chemicals and Similarity related to category.

7. Fixed bug related to newly created 'data variation report item'.

8. Duplicated chemicals in SMI/SDF files are not loaded. This leads to different problems in TB workflow.

9. Fixed problems with clustering by structural similarity when 'overlapping' option is not taken into account.

10. Fixed bug related to correct execution of "data boundary" of profiling schemes.

11. After installing the ECHA REACH plug-in, additional metadata from ECHA REACH data are now included in Toolbox reports. The list of reported ECHA REACH metadata from the Toolbox is now aligned with the content of the updated REACH Study Results file available at the IUCLID website.

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