

User manual

Toolbox 3.3.2 Release Notes

Document history

Version	Comment
Version 1.0	October 2014: Toolbox 3.3 Release Notes
Version 2.0	February 2015: Toolbox 3.3.2 Release Notes

Issue date: February 2015

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 3.3.2 installation is a minor update of Toolbox 3.3. It is available as a patch to be installed over previous version 3.3 install as well as a full package for fresh installations.

Note: Version 3.3.2 refers to the Toolbox package. However the Toolbox main window will show version 3.3.0.152 which is the version of the executable file.

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. Significant improvement and modifications of both general mechanistic Cramer schemes:
 - Toxic hazard classification by Cramer (original)
 - Toxic hazard classification by Cramer (extension)
2. Associating section of F1 help explaining "Correlation" functionality with corresponding window.
3. Implementation of "Cancel" functionality during "Save model" procedure

II. Bug fixes

1. Fixed bug related to Save/Load documents
2. Fixed bug related to rebuilding existing QSAR models
3. Fixed bugs related to application of OASIS TIMES models docked to Toolbox
4. Fixed bug associated with import of data having same endpoint and predefined endpoint path (bug posted on OECD Toolbox forum)
5. Fixed bug in Database copy tool.
6. Fixed bugs in Query tool related to searches using Profile and logical operation with another query.
7. Fixed bug with execution of logically combined queries (bug posted on OECD Toolbox forum)
8. Fixed bug with searching for chemicals by using data ranges
9. Fixed bug with missing endpoint label within pop-up list of metadata field
10. Fixed bug related to explaining of profile of generated metabolites
11. Fixed bug in Gap filling module related to replacement of default X-descriptor with other endpoint tree descriptor by "Select endpoint tree descriptor" functionality.
12. Fixed bug associated with changing the location folder of storing XML files

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