QSAR TOOLBOX

The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

User manual

Toolbox 4.0 Release Notes

Document history

Version	Comment
Version 1.0	March 2017: Toolbox 4.0 Release Notes

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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

The Toolbox 4 installation is a major update of Toolbox. It can be installed as a separate product alongside previous major releases of Toolbox (3.4, 3.3, etc.)

2   System Requirements

Minimum system requirements

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OS: Windows 7

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

RAM: At least 3GB 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: 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

Microsoft .NET Framework 4.5.1

3   Change log

The QSAR Toolbox 4 is a complete rewrite of QSAR Toolbox using Microsoft's .NET framework.

Core modules features:

1. Expanded chemical identification
2. SMART language and 2D Editor (overview)
3. Grouping with metabolism
4. Structural similarity expanded with PubChem features
5. Expanded species taxonomy
6. New format of the Report
7. New database management server - PostgreSQL

New functionalities:

1. Added target endpoint concept for workflow streamlining
2. Reliability scores for Databases and data
3. Relevancy of profilers to the target endpoint
4. Alert performance calculation for:
    a. alert identified in the target
    b. alert identified after AU or SM activation
5. Automated/Standardized workflows for:
    a. Skin sensitization
    b. Ecotox endpoints
6. Quantitative metabolic information and related functionalities
7. Pilot predefined prioritisation schemes

User interface modifications:

1. Document tree manipulation
2. Filtering/Sorting/Coloring of resources (profilers and databases)
3. Helpers
4. Display active and background working actions status

OECD

2, rue André Pascal

75775 Paris Cedex 16

France

Tel.: +33 1 45 24 82 00