

[User manual](#)

[Toolbox 4.6 Release Notes](#)

Document history

Version	Comment
Version 1.0	May 2023: Toolbox 4.6 Release Notes

Issue date: May 2023

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

Table of Contents

1 Overview	1
2 System Requirements.....	1
3 Change log	2

1 Overview

The Toolbox 4.6 installation is a major update of Toolbox 4.5. It can be installed as a separate product alongside previous major releases of Toolbox (4.5, 4.4, 4.3, 4.2, 4.1, 4.0, 3.4, 3.3, etc.)

2 System Requirements

Minimum system requirements

=====

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: 18 GB free hard drive space

File system: NTFS

Microsoft .NET 6.0

Recommended system requirements

=====

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 6.0

3 Change log

Input

1. New functionalities.

- *Simple search* - allowing searching by chemical IDs including possibility to select specific endpoint tree path and other relevant information for searching; multiple selections are allowed
- *Advanced search* - allowing more advanced search to be defined including criteria of the endpoint data to be defined (by defining specific meta data fields and threshold for the experimental data).
- Explanation of where the searched fragment is found using the simple search
- Automated collection of experimental data after a IUCLID or query tool search

Profiling

Profiling schemes

1. Updated profilers - 17 profilers have been updated:

- Acute aquatic toxicity MOA by OASIS
- Acute Oral Toxicity
- Carcinogenicity (genotox and nongenotox) alerts by ISS
- DNA alerts for AMES, CA and MNT by OASIS
- DNA binding by OASIS
- Hydrolysis half-life (pH 6.5-7.4)
- in vitro mutagenicity (Ames test) alerts by ISS
- in vivo mutagenicity (Micronucleus) alerts by ISS
- Oncologic Primary Classification
- Organic functional groups
- Organic functional groups (nested)
- Protein binding alerts for Chromosomal aberration by OASIS
- Protein binding alerts for skin sensitization according to GHS
- Protein binding alerts for skin sensitization by OASIS
- Protein binding by OASIS
- Repeated dose (HESS)
- Toxic hazard classification by Cramer V1.0 Updated

Note: The Cramer classification scheme has been significantly modified (as part of currently on-going SC04), aiming to provide transparency of predicted results.

2. New profilers: None

Documented/simulated metabolism

1. Documented metabolism databases – No updates.

2. Updated metabolic simulators:

- AU simulator
- AU simulator (alkaline medium)
- Dissociation simulator
- Hydrolysis simulator (acidic)
- Hydrolysis simulator (neutral)
- In vivo metabolic simulator
- In vitro metabolic simulator
- Microbial simulator
- Skin metabolism

Databases & inventories:

1. Updated databases & inventories

Databases:

- Acute oral toxicity DB
- Aquatic Japan MoE
- ECHA REACH
- ECOTOX
- Genotoxicity & Carcinogenicity ECVAM
- Genotoxicity OASIS
- Human Half-Life
- Hydrolysis rate constant OASIS
- OpenFood Tox
- Repeated Dose Toxicity HESS
- Skin Sensitization

Note: Currently, ECHA REACH is represented by two subsets: dossiers and test materials

Inventories:

- AIIC

2. New databases & inventories

- ECHA REACH Test materials
- Half-Life Mammalian Toxicokinetic Database MamTKDB
- Toxicity data on pharmaceuticals (US FDA)
- Skin sensitization OASIS (normalized)

3. Improvements

- Improvement of the IUCLID database import: possibility to filter the endpoint study records based on key criteria (e.g. reliability, purpose flag, etc.) before import

Category definition:

1. Improvements

- More intuitive category definition

2. New functionalities

- ADME layer is added as part of Category elements

Data Gap Filling:

1. Improvements

- AWs execution
- QSARs optimization – possibility to filter the QSAR models and to execute more than one at once

2. New functionalities

- DASS AW implemented as a QSAR model

Report & Export

- New organization of the prediction reports:
 - Standard prediction report including clear prediction protocol
 - Data matrix report – includes the information from the previous Category report
- Justification reporting documents in case of regulatory interest:
 - Read-across justification templates (corresponding to the RAAF scenarios)
 - QSAR justification templates (corresponding to the OECD principles)
- Possibility to filter the data based on metadata when export data matrix

Web Client:

Improvements:

- Multiple improvements in the way structures and data are presented on the data matrix (fixed hiding/overlapping of chemical structures, number formatting, data multiplication, etc.)
- Better indication of communication errors and task progress (fixed endless progress bar)
- Logging debug information for identifying problems
- Better switching between the Toolbox and IUCLID sections with warnings for possible data loss

Other improvements:

- Simplification of the Toolbox installation procedure. Possibility to install the Toolbox database without PostgreSQL installation
- New profiling and metabolites caches.
- Harmonization of endpoints: Genetic toxicity and Biodegradation
- Possibility to export statistics of a list from the document tree
- Explanations on the colors
- Quality of the 2D depictions
- Importing chemical list with custom ID information
- Options to hide/show specific Toolbox modules
- New nodes in the library of the Workflow editor
- Possibility to copy the table with the Alert performance results

OECD

2, rue André Pascal

75775 Paris Cedex 16

France

Tel.: +33 1 45 24 82 00

Fax: +33 1 45 24 85 00

ECHA

Annankatu 18

00120 Helsinki

Finland

Tel.: +358-9-686180

Fax: +33 1 45 24 85 00

LMC

Yakimov St. #1 Prof. Assen Zlatarov" University

8010 Bourgas

Bulgaria

Tel.: +359 56 880230