QSAR TOOLBOX

The OECD QSAR Toolbox for Grouping Chemicals into Categories

User manual

Toolbox 3.0 Release Notes

Document history

Version	Comment
Version 1.0	October 2012: Toolbox 3.0 Release Notes

Issue date: October 2012

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

The Toolbox 3 installation is designed as a separate product. It is designed to be separate (technically it is a completely different product) form earlier versions of the QSAR Toolbox and as such it can coexists on a single machine with previous versions of the Toolbox.

The new version has changes in its databases, profiling schemes, program modules and installation suite. It has a number of bug-fixes as well as some new features.

The Toolbox 3 deploys a new database repository which means that the user needs to re-import private databases or use the provided **Database Copy** tool. This tool can transfer all user databases from an existing Toolbox repository (ver. 2.3) format to a database in the Toolbox 3.0 format. For example it can transfer the data from an old Toolbox 2.3 database into the database deployed by the Toolbox 3.0 installation.

2 System Requirements

Minimum system requirements

==========

OS: Windows 98 SE, Windows ME, Windows NT 4.0,

Windows 2000, or Windows XP

CPU: Pentium 4 2GHz

RAM: At least 2GB of RAM

HDD: 10GB free hard drive space

File system: NTFS

Recommended system requirements

==========

OS: Windows 2000, XP or newer

CPU: Pentium 4 2.5GHz or faster processor

RAM: 4GB of RAM

HDD: 12 GB free hard drive space

File system: NTFS

3 Change log

1. Software/program workflow

- ✓ Implementation of Interactive help functionality – F1 help
- ✓ Advanced database query tool
- ✓ IUCLID 5.4 compatibility
- ✓ Capability to import an search by user defined chemical ID
- ✓ AOP for Skin sensitization
- ✓ Enhanced reporting engine to handle mixtures, tautomers and metabolites
- ✓ Inclusion of study results from the REACH dissemination website
- ✓ Quantitative mixtures toxicity prediction
- ✓ Tautomeric set prediction approach
- ✓ Prediction accounting for metabolism
- ✓ Development of capability to generate and use 3D-descriptors
- ✓ Export molecular formula of chemicals
- ✓ Hierarchical organizations of categories in profiling schemes
- ✓ New organization of databases under Endpoint section
- ✓ Export/Import of user databases in transportable format

2. New profilers

- ✓ General Mechanistic - 20 new profilers are added
  - o Biodegradation profilers - models from 1 to 7 (Biowin)
  - o Biodeg BioHC Half-Life (Biowin)
  - o Ulitimate Biodegradability
  - o Hydrolysis Half-Life (PH= 6.5 – 7.4)
  - o Ionization degrees at different pH - pH = 1, 4, 7.4 and 9

- Hydrolysis half-Life (Kb, pH 7) (Hydrowin)– base catalyzed hydrolysis half-life at PH 7(HYDROWIN)
- Hydrolysis half-Life (Kb, pH 8) (Hydrowin) - base catalyzed hydrolysis half-life at PH 8(HYDROWIN)
- Hydrolysis half-Life (Ka, pH 7) (Hydrowin) – acid catalyzed hydrolysis half-life at PH 7(HYDROWIN)
- Hydrolysis half-life (Ka, pH 8) (Hydrowin) – acid catalyzed hydrolysis half-life at PH 8(HYDROWIN)
- DPRA Cysteine peptide depletion
- DPRA Lysine peptide depletion

✓ Endpoint specific – 4 new profilers
- DNA alerts for AMES, MN and CA by OASIS v.1.1
- Protein binding alerts for skin sensitization by OASIS v1.1
- Keratinocyte gene expression
- rtER Expert System ver.1 - USEPA

✓ Empiric - one new profiler
- Tautomers unstable

✓ Toxicological – one new profiler
- Repeated dose (HESS) – NITE METI Japan/LMC

3. Updated profilers

✓ General Mechanistic – modifications in structural boundaries
- Protein binding by OASIS v.1.1
- DNA binding by OASIS v.1.1
- Protein binding potency
- Toxic hazard classification by Cramer (original)
- Toxic hazard classification by Cramer (with extensions)

✓ Endpoint specific - modifications in structural boundaries
- Acute aquatic toxicity MOA by OASIS
- Oncologic Primary Classification
- Skin irritation/corrosion Inclusion rules by BfR

✓ Empiric - modifications in structural boundaries
- Organic functional groups
- Organic functional groups (nested)

4. New simulators

✓ Autoxidation simulator
✓ Autoxidation simulator(alkaline medium)
✓ Hydrolysis (Acidic) simulator
✓ Hydrolysis (Basic) simulator
✓ Hydrolysis (Neutral) simulator

5. Updated simulators

✓ Skin metabolism simulator
✓ Rat liver S9 metabolism simulator

6. New observed databases

- ✓ Observed Mammalian metabolism database
- ✓ Observed Rat Liver S9 metabolism database

7. New QSAR models

- ✓ rtER Expert System ver.1 – USEPA

8. New databases

- ✓ Bioconcentration NITE
- ✓ Biodegradation NITE
- ✓ Cell Transformation Assay ISSCTA
- ✓ Chemical Reactivity COLIPA
- ✓ Dendritic cells COLIPA
- ✓ Keratinocyte gene expression Givaudan
- ✓ Developmental toxicity ILSI
- ✓ ECHA CHEM
- ✓ Yeast estrogen assay database University of Tennessee-Knoxville (USA)

9. Updated databases

- ✓ Biodegradation in soil OASIS
- ✓ Hydrolysis rate constant OASIS
- ✓ Micronucleus OASIS
- ✓ Genotoxicity OASIS
- ✓ Repeated Dose Toxicity HESS
- ✓ Rep Dose Tox Fraunhofer ITEM
- ✓ Skin sensitization

OECD
2, rue André Pascal
75775 Paris Cedex 16
France

Tel.: +33 1 45 24 82 00
Fax: +33 1 45 24 85 00

ehscont@oecd.org