User manual

Toolbox 4.2 Release Notes (summary)

Document history

Version	Comment
Version 1.0	January 2018: Toolbox 4.2 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 4.2 installation is a major update of Toolbox 4.1. It can be installed as a separate product alongside previous major releases of Toolbox (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 4GB 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: 6 GB of RAM

HDD: 20 GB free hard drive space

File system: NTFS

Microsoft .NET Framework 4.5.1

3 Change log

1. Improved data matrix interface, accelerating of data collection in data matrix
2. Extended substance identification - *Additional Ids* are included (EC Number, InChi keys)
3. Loading *.txt files containing CAS or SMILES only is now possible
4. Extended Predefined substance type – UVCB substances and polymers are indicated by substance name
5. Simplified filtering of the data matrix is provided (selecting endpoint tree nodes to work with)
6. Manual rearrangement of the columns in the data matrix
7. Manual transferring of data to target in data matrix (outside data gap filling module)
8. Profiling accounting for metabolism - Displaying of the metabolite that satisfy the profiling criteria
9. Experimental data for the chemicals in the local training sets is now shown
10. Historical log for changes implemented in Toolbox metabolism simulators
11. Possibility to import databases containing dimensionless data (e.g. logKow)
12. Possibility to search chemicals by CAS or Name in IUCLID 6 during Export/Import instead of working with all substances
13. Grouping DBs by data availability
14. Category consistency check (using category elements):
    - for list of chemicals and defined target endpoint; no need of data gap filling;
    - for category building during read across (after data gap filling)
15. "Alert performance" (AP) functionality accounting for metabolism is improved providing results for each of the identified alerts
16. Clustering by any profile/structural similarity is possible, now
17. Historical log for changes implemented in the Toolbox databases
18. Profiling. Currently available profilers: 69 profilers:

a. 12 updated profilers

b. 5 updated metabolism simulators

19. Data. Currently available databases – 55 with ~70 000 chemicals and ~2 116 700 data points:

- 5 new databases (including normalized BCF data from REACH for 220 new chemicals)
- 7 updated databases (including 2851 normalized skin allergy data from REACH for 2070 chemicals)

20. AW/SW for skin sensitization – new skin sensitization data is included (REACH Skin sensitisation database (normalized)); documentation is included; the activity log is modified

21. Endpoint vs. endpoint – possibility to create bins for the numerical data

22. Extension of the report by providing category consistency items;

23. RAAF scenario and related assessment elements could be included in the report

24. Category report is modified including consistency check elements

25. For category reporting a "Report basket" could be used storing items triggered automatically by the actions during the workflow

26. Short descriptions for each 3D parameter are added

27. Simplified database deployment

28. Added a Microsoft Windows Service configuration option for the QSAR Toolbox Server.

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