

[User manual](#)

[Toolbox 4.2.1 Release Notes](#)

Document history

Version	Comment
Version 1.0	September 2018: Toolbox 4.2.1 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 1
2 System Requirements..... 1
3 Change log 2

1 Overview

The Toolbox 4.2.1 installation is a minor update of Toolbox 4.2. It can be installed as a separate product alongside previous major releases of Toolbox (4.1, 4.0, 3.4, 3.3, etc.). Alternatively version 4.2 can be updated to version 4.2.1 using the provided patch.

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 6GB 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: 16 GB of RAM

HDD: 20 GB free hard drive space

File system: NTFS

Microsoft .NET Framework 4.5.1

3 Change log

Bugfixes

1. Fixed a bug when predicting in domain with certain QSAR models.
2. Fixed an issue when cancelling QSAR prediction for a chemical list.
3. Fixed an issue with chemical depiction missing from report.
4. Fixed an issue where a QSAR explain dialog deadlocks the Toolbox Desktop Client.
5. Updated "No domain" dialog.
6. Various WebAPI fixes.
7. Fixed a dynamic tree building issue when predicting consecutively with QSARs.
8. Extended IUCLID prediction's caption length.
9. Improved mechanistic similarity report item for hierarchical schemes.
10. Improved handling of slow (3D) parameters for certain QSAR models.
11. Removed some cases for automatic calculation with slow QSARs.
12. Fixed an issue where QSAR selection dialog would select the wrong model.
13. Fixed an issue with custom QSAR models producing an error.
14. Fixed an issue with mol weight calculation when predicting mixtures.
15. Fixed a localization issue in the Grouping with metabolism options.
16. Fixed an issue with DataMatrix report not exporting data values.
17. Improved file save/load versioning.
18. Fixed an issue where Close of QSAR models window produce AV.
19. Fixed captions when reporting predictions of mixtures.
20. Fixed an issue with Category elements when invoked from data gap filling.
21. Fixed an issue when opening malformed SDF, providing additional information.

OECD

2, rue André Pascal

75775 Paris Cedex 16

France

Tel.: +33 1 45 24 82 00

ECHA

Annankatu 18

00120 Helsinki

Finland

Tel.: +358-9-686180

LMC

Yakimov St. #1 Prof. Assen Zlatarov" University

8010 Bourgas

Bulgaria

Tel.: +359 56 880230