QSAR TOOLBOX

The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

User manual

Toolbox 3.3 Standalone Installation

Document history

Version	Comment
Version 1.0	October 2010: Installation notes for Toolbox version 2.0
Version 1.1	February 2011: Change of name to Toolbox 2.1 Standalone Installation
Version 1.2	July 2011: Changed name to Toolbox 2.2 and added Database migration manual
Version 1.3	March 2012: Changed the name to Toolbox 2.3. Minor changes reflecting the version change.
Version 1.4	October 2012: Changed the name to Toolbox 3.0. Minor changes reflecting the version change.
Version 1.5	December 2013: Changed the version to Toolbox 3.2. Minor changes reflecting the version change.
Version 1.6	November 2014: Changed the version to Toolbox 3.3. Added changes reflecting the version change.

Issue date: November 2014

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

November 2014

1   Introduction

This document provides a summary description of the installation procedure of the QSAR Toolbox (version 3.3) set-up kit on a local PC operating Microsoft® Windows®.

2   Requirements

It is recommended to use an up-to-date PC with a processor running at 2GHz or faster, 15 Gigabyte of hard disc space for storage and 4 Gigabyte of RAM to operate.

In order to run this installation you will need administrator rights on your local PC. However, once installed, normal user rights will be sufficient for running the application.

3   Installed components

The following components will be installed on your PC if they are not already available:

- The database manager Firebird 2.5.

- Microsoft Jet Database Engine 3.51

4   Automatic installation

Navigate to the CD on which you have received the application or to the folder into which you have downloaded the package. If you received the package as a ZIP archive, extract the content to a new directory.

> **Note:** The installation package was compressed using the WinZip software, version 17. Other applications might not be able do decompress the package as different applications implement the ZIP format differently. A free alternative that was tested with the installer package is the **7-Zip** application. **7-Zip** can be downloaded from http://www.7-zip.org/.

Execute the "StartInstall.exe" file in the root directory. This is executable is going to provide a dialog from which the user can install Firebird RDBMS and the QSAR Toolbox.

Microsoft Jet Database Engine 3.51 installations are included in the QSAR Toolbox installation package.

5   Manual installation

A manual installation needs to be performed when the automatic installation fails (for example, due to insufficient privileges of the current Windows account). In this case the following sequence of actions should be executed:

1.   Uninstall any existing older version of the QSAR Toolbox – go to "Control Panel", "Add or Remove Programs", select the older version of the program and click on the "Remove" button.

2.   If the Firebird server is not installed on the computer, go to the folder "FireBirdServer" on the installation package and run "Firebird-2.5.3.26778_0_Win32.exe" (Firebird-2.5.3.26778_0_x64.exe for 64bit OS).

3.   Go to the folder "TB" in the installation package and run "setup.exe". It should install the QSAR Toolbox files (executable, databases, libraries, help files, etc.).

6   Databases migration

6.1 Overview

The Toolbox application uses a Firebird powered database file that serves as a repository for numerous Toolbox sub-systems. This includes the QA subsystem, the profiling cache, the calculations cache etc. The QSAR Toolbox 3.3 release has a new database repository with new and updated databases. However users have been importing custom datasets into the Toolbox repository. The import procedure, with the preparation of the import files takes a significant effort. These datasets also build on the profiling and calculations

cache. This means that a simple, straightforward way of transferring these datasets to the new database repository needs to be provided.

6.2 DatabaseCopy Tool

This is an application with a very basic, easy to use user interface that is built to do two tasks – transfer user databases and inventories, transfer profiling cache and transfer calculations cache.
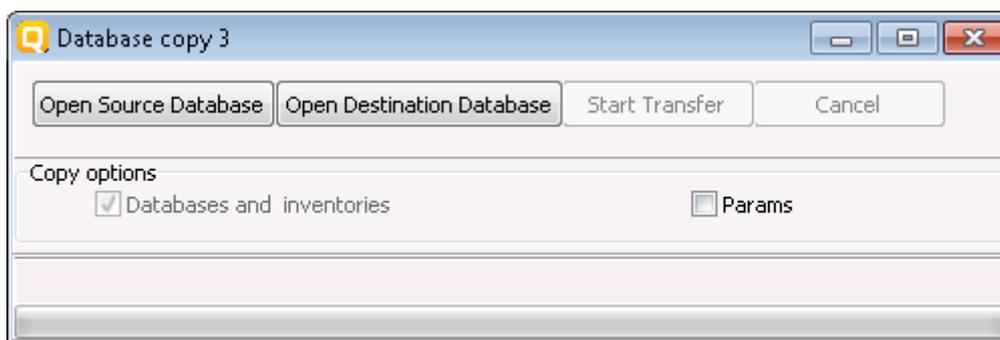

Figure 1

Usage of the program is pretty straightforward. The user interface (figure 1) provides for selection of source database file ("Open Source Database" button) and destination database file ("Open Destination Database" button). The user specifies his source (ver. 2.3, 3.0, 3.1, 3.2) database file, and the destination ver. 3.3 database file which comes with the QSAR Toolbox 3.3 installation. Then start the migration by clicking the "Start Transfer" button.

There are two check boxes presented to the user. One is always checked and serves only as a mark that the user databases and inventories will be transferred. The other is for transferring of the parameter calculations cache.

6.3 Technicalities

The first checkbox "Databases and inventories" is always checked. This is by implementation as a marker.

7 Known issues

7.1 Running the QSAR Toolbox on limited user accounts

The QSAR Toolbox is only installed per machine. That means that every user can run the program with or without elevated privileges. However the installation itself requires administrative privileges. To install the QSAR Toolbox on Windows Vista or Windows 7 the installer should be started using the "Run as administrator" option.

When uninstalling or updating no database files will be removed. This is an intended behaviour. The user has to manually delete the database file.

The QSAR Toolbox writes some files to the User folder. These files would also remain intact after uninstall.

7.2 Other possible problems

If the main installation fails ("setup.exe" from "TB" folder), the system cannot be installed on this computer via the current user account.

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