QSAR TOOLBOX

The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

User manual

Toolbox 3.0 Database migration

Document history

Version	Comment
Version 1.0	21.01.2011, first version
Version 1.1	15.02.2011, minor changes
Version 1.2	13.07.2011, updated for Toolbox version 2.2
Version 1.3	05.03.2012, updated for Toolbox version 2.3
Version 1.4	05.03.2012, updated for Toolbox version 3.0
Version 1.5	25.10.2012, updated for Transportable files

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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

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 3.0 release has a new database repository with new and updated databases. However, since the release of Toolbox 2.3, users have been importing custom datasets into the Toolbox repository. The import procedure, with the preparation of the import files takes a significant amount of 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.

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 to existing database or new database.
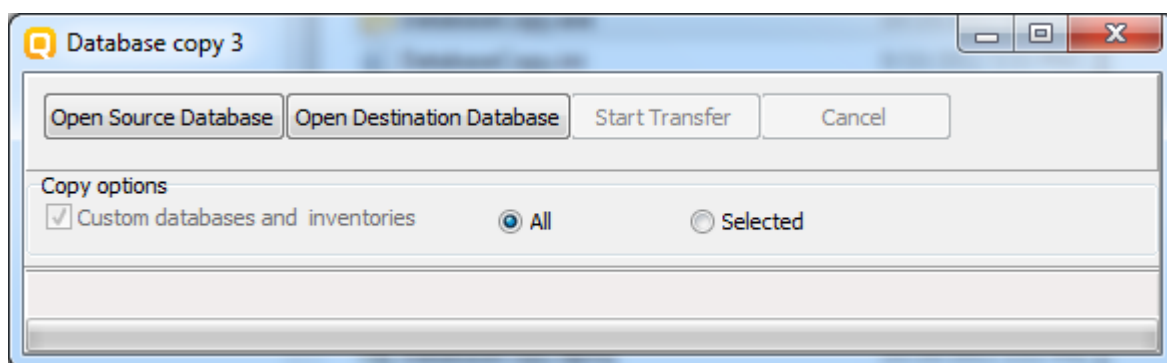

Figure 1

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 or transportable) database file, and the destination ver. 3.0 database file which comes with the QSAR Toolbox 3.0 installation. It is also possible to export custom databases/inventories to a new, transportable, file by specifying non-existing destination file in the "Open Destination Database" procedure. Created file contains only custom Databases and Inventories and may be used as a transport file to other Toolbox user who can import contained database and inventories again with DatabaseCopy tool by choosing the file as a "Source" database. To start the migration (file-save), click 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.

3 Technicalities

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

There two radio buttons "All" and "Selected" they are related with selection of custom database and inventories. By selecting "All" the tool will export /import all custom databases if "Selected" is checked then a dialog with all custom databases will appear and user should specify which of them will be exported.