

User manual

QSAR TOOLBOX

The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

Document history

Version	Comment
Version 1.0	March 2017: Installation notes for Toolbox version 4.0
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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

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I. Introduction & Requirements for QSAR Toolbox installation

1. Introduction

This document provides a step by step description of the installation procedure of the QSAR Toolbox (version 4.3) set-up kit on a local PC operating Microsoft® Windows®.

The new QSAR Toolbox 4.3 is not a continuation of the Toolbox 3.4 codebase. It is a new system, designed from the bottom up and rewritten using new underlying technologies and database management sub-system. This in turn means a completely different deployment experience. QSAR Toolbox 4.3 is a major update to Toolbox and can be installed alongside previous versions of 4.x.

2. Requirements

It is recommended to use an up-to-date PC with **64 bit operating system** (required) and a processor running at 2.4GHz or faster, 15 Gigabyte of hard disc space for storage and 6 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.

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

- The database manager PostgreSQL 9.6
- Microsoft .NET Framework 4.5.2

II. QSAR Toolbox installation

Before starting to install the Toolbox, make sure that all files are extracted from the downloaded package. Navigate to the CD on which you have received the application or to the folder into which you have downloaded the package. Right click over the package and select to extract the content to a new directory.

Do not start to install Toolbox directly from the downloaded package.

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Note: The installation package was compressed using the WinZip software, version 17. Other applications might not be able to 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/>.

QSAR Toolbox 4.3 is a major update to Toolbox and can be installed alongside previous versions of 4.x.

If you have not installed any of the previous versions of Toolbox 4. (i.e. versions 4.0, 4.1 and/or 4.2), you need to install the three basic components of QSAR Toolbox – 1) PostgreSQL, 2) Database and 3) QSAR Toolbox application.

If you have some of the previous Toolbox versions, skip Step 1 and start directly from [Step 2. Database](#).

Double click on the “**StartInstall.exe**” file (Figure 1) (located in the directory where the extracted content from the package is) and follow the steps described below.

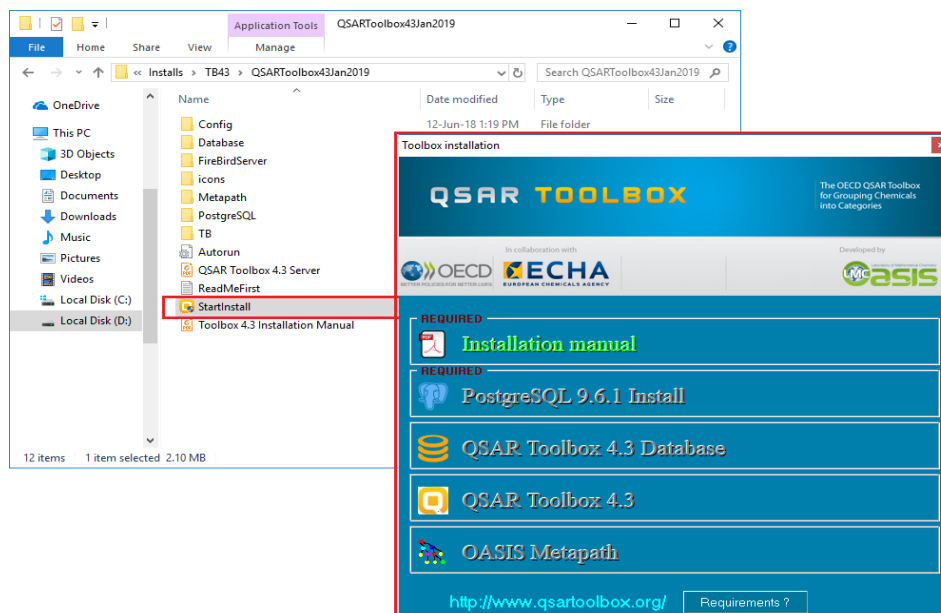


Figure 1. Installation Startup screen

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Step 1. PostgreSQL**Step 1.1. Click on PostgreSQL 9.6.1. Install (Figure 2)**

Figure 2. Start installation of PostgreSQL

Step 1.2. You will be asked to select where the PostgreSQL should be installed and data stored. Leave the default setting - click **Next** twice (Figure 3).

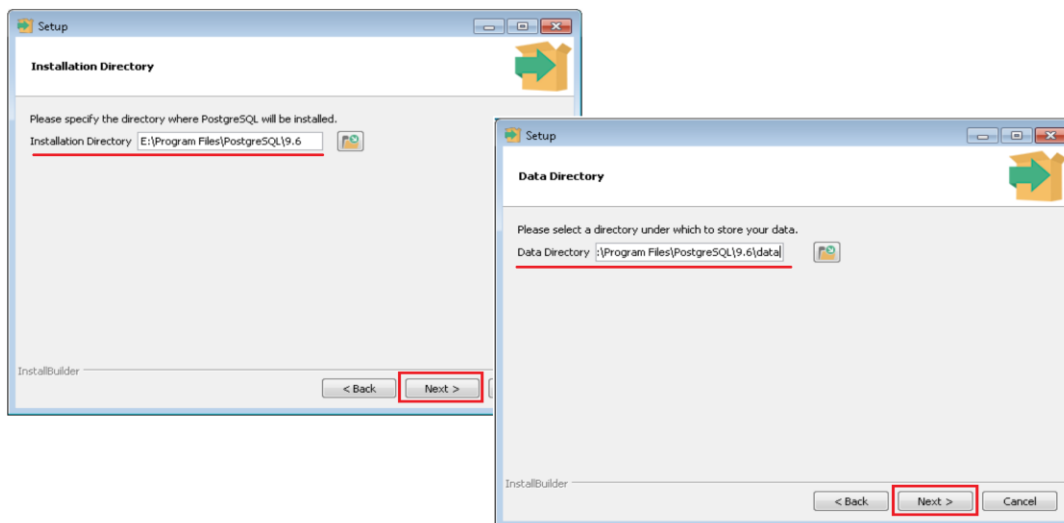


Figure 3. Selection of folders where the PostgreSQL should be installed and data stored

Note: Make sure the Data folder is on a drive that has at least 5GB of free space.

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Step 1.3. Next you will be asked to enter the password and port (Figure 4).

password: **postgres** (recommended)

port: **5432** (by default)

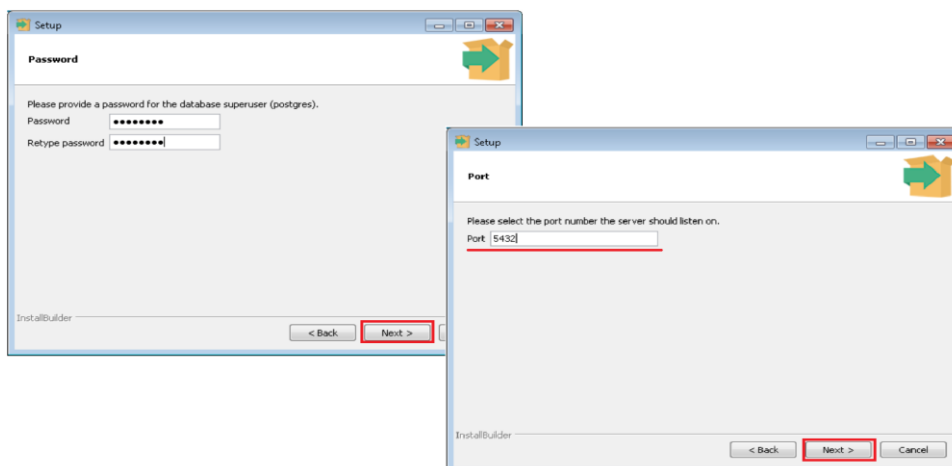


Figure 4 Specifying password and port for the PostgreSQL

Note: Whatever you decide to put as a password/port make sure you write it down or memorize it as it will be needed later in the installation procedure and generally throughout the PostgreSQL installation's lifetime.

Step 1.4. Finally uncheck *Launch Stack Builder* and click **Finish** (Figure 5)

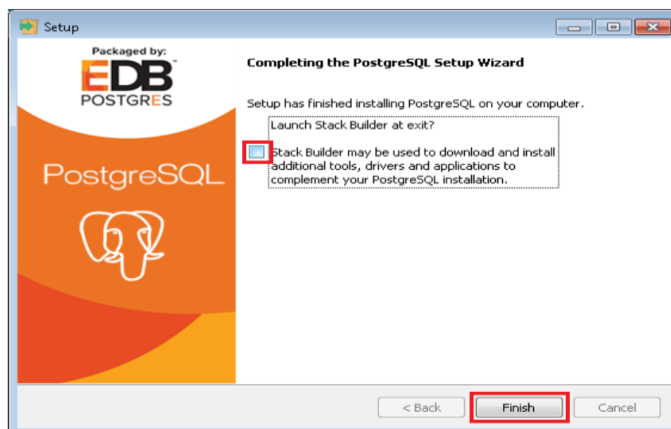


Figure 5. Uncheck launching of the Stack Builder and finish the PostgreSQL installation

Now PostgreSQL is installed and you can continue with the installation of the Toolbox database.

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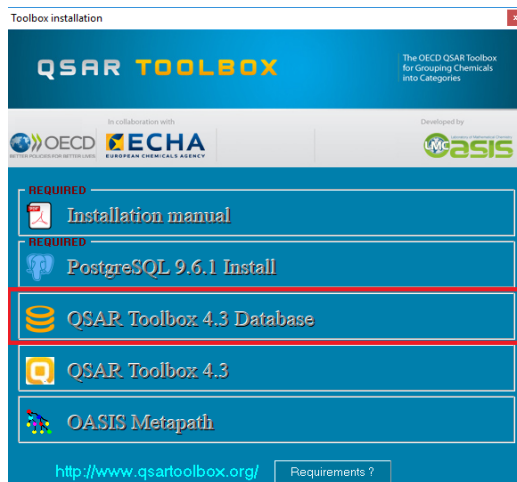
Step 2. Database**Step 2.1.** Select *QSAR Toolbox 4.3. Database* (Figure 6)

Figure 6. Start installation of the Toolbox database

Step 2.2. You will be asked (Figure 7) to provide the PostgreSQL superuser password and listen port. (see 1.3.):

- For password type **postgres** (recommended)
- For the port type **5432** (by default) and click *Start database deployment* button

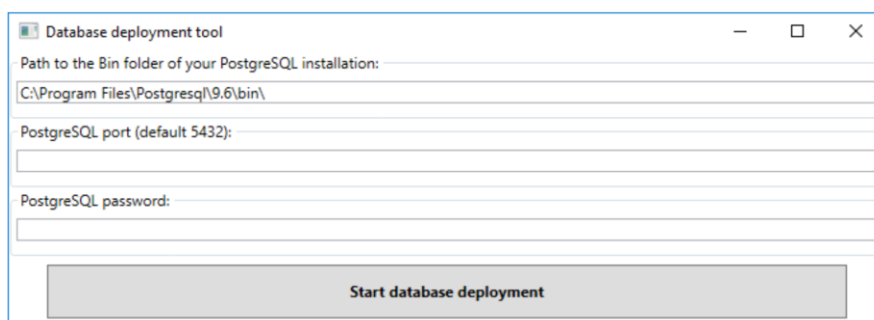


Figure 7 Start database deployment

Note: If you have changed the password and you do not remember it, please follow the steps you will find at the following link in order to reset your PostgreSQL password:

<http://toolbox.oasis-lmc.org/content/documents/ResettingPostgreSQLPassword.pdf>

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Step 2.3. On the next confirmation message click on “Yes” (Figure 8). This warning message is related only to the same version of Toolbox. Deployment of the Toolbox 4.3 database will not affect the previous databases.

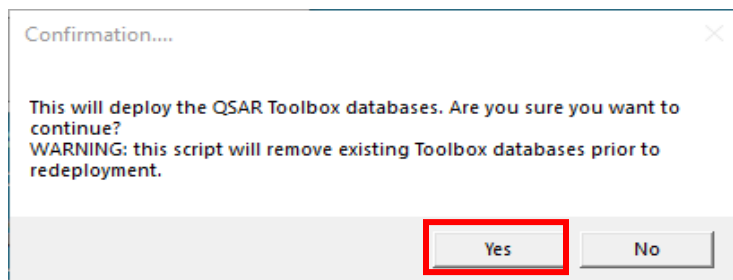


Figure 8. Confirmation message for starting database deployment

The full database deployment takes around 10-15 min depending on computer configuration and it should not be interrupted.

Note: A prerequisite for the database deployment step is that there is a functional PostgreSQL server listening. You could check that by going to Services tab of your Task manager (you can bring it up by holding Ctrl+Shift+Esc buttons). Look for a service with postgresql in its name (e.g. “postgresql-x64-9.4”), it should have “Running” in the Status column.

Continue with the last step of the Toolbox installation.

Step 3. Toolbox

Step 3.1. Select *QSAR Toolbox 4.3*. (Figure 9)

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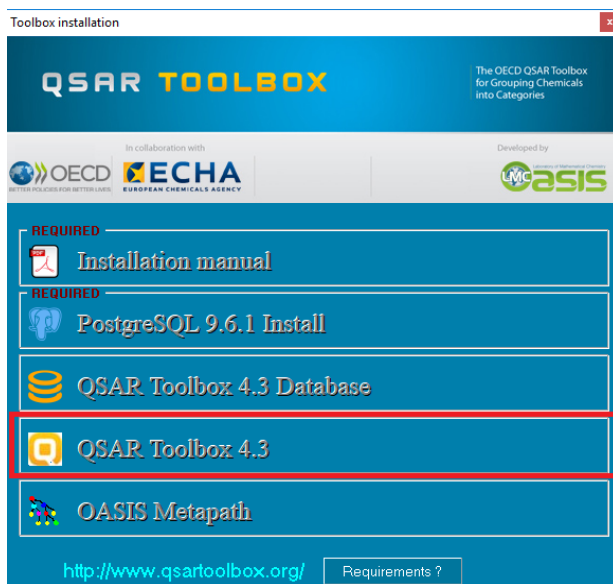


Figure 9. Start installation of the Toolbox application

Step 2.2. Start the installation of Toolbox by clicking Next (Figure 10)

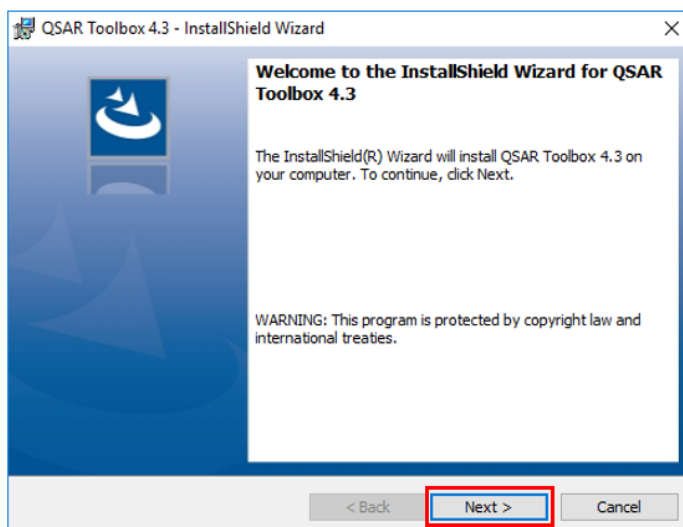


Figure 10. InstallShield Wizard screen

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Step 2.3. Accept the terms of the license agreement in order to continue with the Toolbox installation (Figure 11)

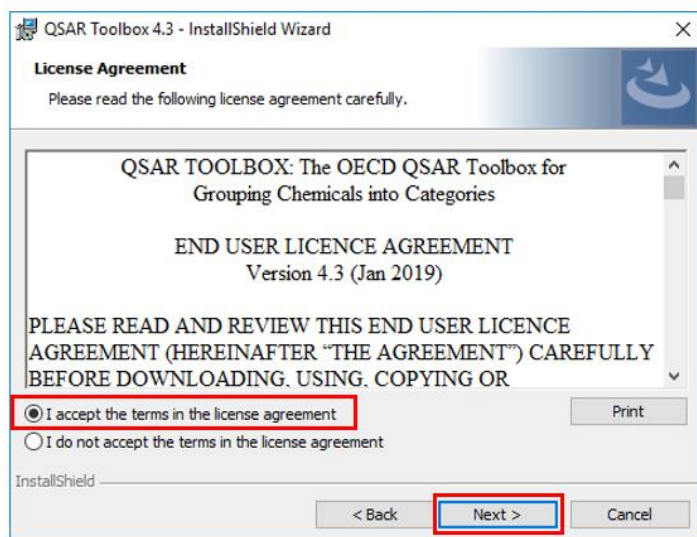


Figure 11. License agreement

Step 2.4. You will be asked for a destination folder of the Toolbox. Click **Next** to install the Toolbox to the default directory (Figure 12)

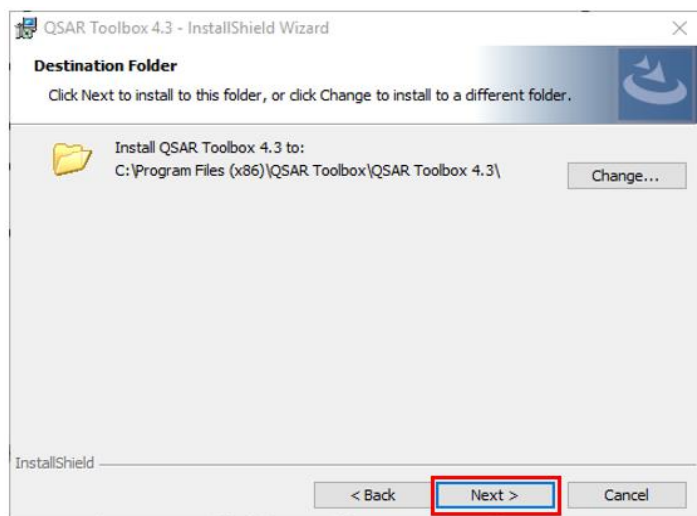


Figure 12. Selection of Toolbox destination folder

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Step 2.5. Then you will be prompted to select the deployment mode for the installation suite. There are three deployment modes for available for QSAR Toolbox 4 - Standalone, Client only or Multi-user server.

- **Standalone** – This deployment mode should be used on a single computer. This deployment mode allows for creation of new profiling schemes, importing of databases and creation of new QSARs. This is the recommended deployment mode for users who will be developing profiling schemes, QSARs, databases.
- **QSAR Toolbox Desktop Client Only** - This mode will install only the Toolbox client. It will have to be connected to a separate deployment of a QSAR Toolbox multi-user Server.
- **QSAR Toolbox multi-user Server** - This deployment mode is similar to the standalone deployment, in that it installs both Server and Client layers of the QSAR Toolbox, however it configures the Server in multi-user mode. When connected to a multi-user server the user will have restrictions on certain features, such as creation of new profiles and importing of databases.

Note: In order to open a port for incoming connections the multi-user server needs to be started with administrative permissions (or equivalent).

Select the **Standalone** deployment mode used for a single computer and click **Next** (Figure 13)

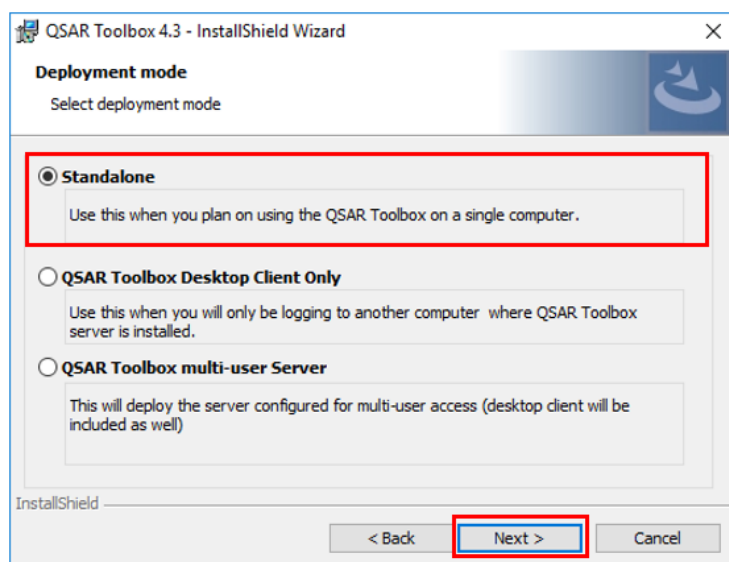


Figure 13. Selection of deployment mode of Toolbox

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Step 2.6. Next you will be prompted to enter the connection parameters for the Client and Server applications. Make sure the database port is the same (**5432** by default), click **Next** (Figure 14) and then finish the installation.

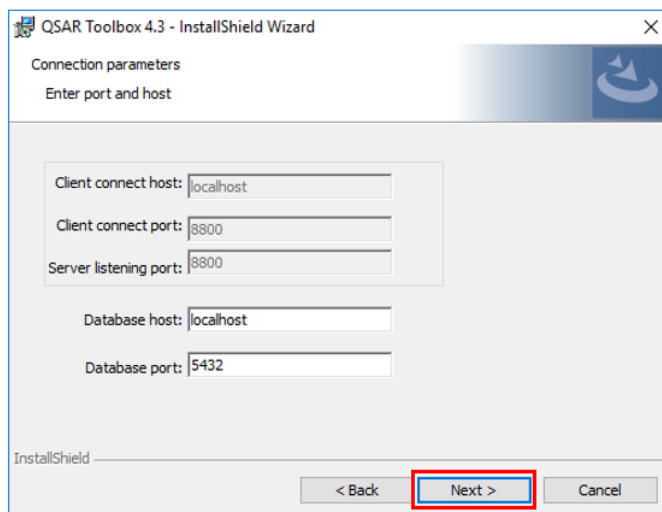


Figure 14. Entering connection parameters

Meaning of the parameters:

- **Client connect host:** This specifies the computer that the client will connect to.
- **Client connect port:** This is the port the client will use to connect to the Server. It should match the **listening port** that the Server was configured to listen to.
- **Database host:** This specifies the host computer where the PostgreSQL database is located.
- **Database port:** This specifies the port the PostgreSQL database server listens to (see **PostgreSQL installation** section).
- **Server listening port:** This is the port the QSAR Toolbox Server will listen on (and Toolbox Client will try to contact on).

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Step 2.6. Finalize the Toolbox application install by click on “Install” and then “Finish” (Figure 15)

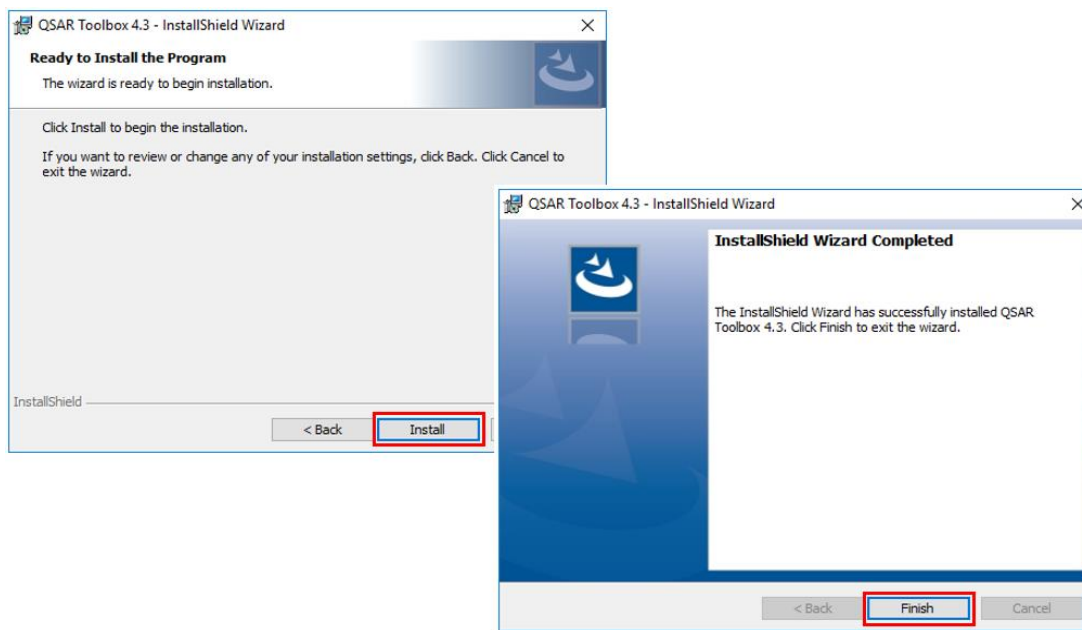


Figure 15. Finalizing of the Toolbox Application installation

Now all needed components for the properly work of Toolbox are installed and you can run the system.

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III. How to transfer custom items from previous Toolbox versions into the new one?

1. Transfer custom items from QSAR Toolbox 3.x to QSAR Toolbox 4.3

Two tools allowing to transfer custom items (profilers and databases) from QSAR Toolbox 3.x to QSAR Toolbox 4.3 are available.

a. Transfer custom profilers

Package with a *Scheme Migrator App* (i.e. the tool allowing transferring of custom profiling schemes) could be downloaded from the following link:

<http://toolbox.oasis-lmc.org/downloads/tools/SchemeMigratorApp.zip>

After extracting the content of the package, the *SchemeMigratorApp.exe* file should be manually placed in the COM34 folder created by the QSAR Toolbox 3.4 installation.

The default path to the COM34 folder is %PROGRAMFILES(X86)%\OASIS-LMC\COM34 (e.g. C:\Program Files (x86)\OASISLMC\COM34) (Figure 16).

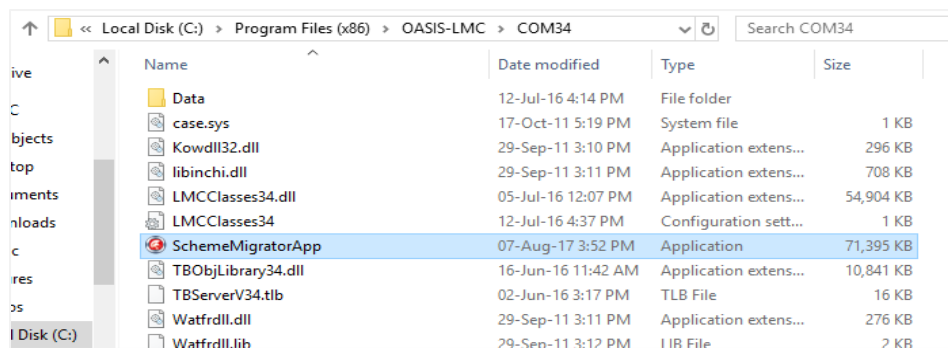


Figure 16. *Scheme Migrator App* executable in the default directory of the COM34 folder (QSAR Toolbox 3.4)

Start the program by running the *SchemeMigratorApp.exe* file. Multiple Toolbox 3.x schemes can be loaded with the "Load schemes" button (1) (Figure 17). Sequential loading of schemes adds them to the list. The list of loaded schemes can

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be cleared by using the "Clear list" button (2). Once the scheme(s) have been loaded, they can be converted by clicking the "Convert!" button (3).

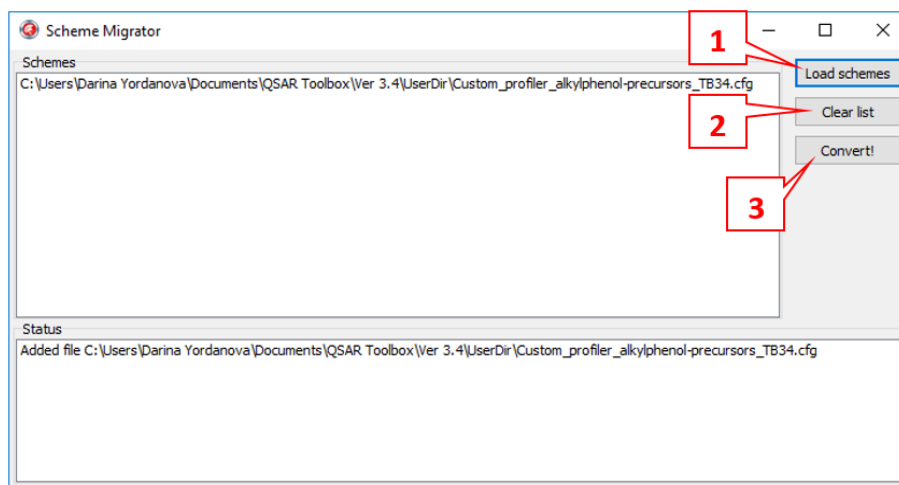


Figure 17. *Scheme Migrator App* screen

The conversion process may take from seconds to several minutes depending on the count, size and complexity of the input schemes, as well as on the computer hardware. Once the conversion process has been completed, a status log for each scheme is displayed in the Status pane informing whether the operation has succeeded.

In case of successful conversion, a new file (.plugin.config) will be created for each converted scheme. In order to be able to work with the converted schemes in QSAR Toolbox 4.3, they need to be placed in the CONFIG folder. Its default path is:

C:\Program Files (x86)\Common Files\QSAR Toolbox
4.3\Config\Addins\LMC.Toolbox.Server.Profiling

More details about the *Scheme Migrator App* could be found in the user manual included in the downloaded package.

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b. Transfer custom databases

Package with a *Database Migration Tool* (i.e. the tool allowing transferring of old Toolbox database) could be downloaded from the following link:

<http://toolbox.oasis-lmc.org/downloads/tools/DatabaseCopy4.3.zip>

The *Database Migration Tool* is an application with a very basic, easy to use user interface that is built to transfer user databases and inventories to the existing database.

Once the tool is downloaded, extract the content of the package and double click the *ToolboxDatabaseCopy4* executable (Figure 18)

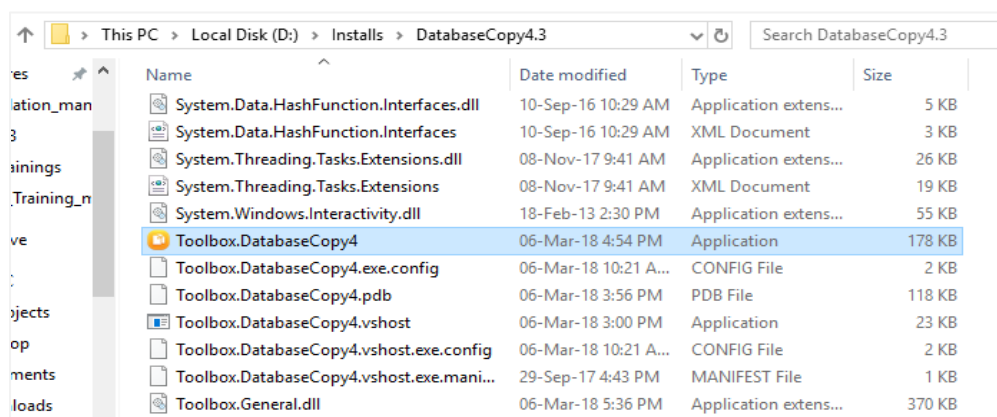


Figure 18. *Database Migration Tool* executable

The user interface of the *Database Migration Tool* includes three sections (Figure 19). The first section called *Source Database* (1) allows selecting the source database file by the “Open” button (the default location of the database is: C:\Program Files (x86)\Common Files\QSAR Toolbox\Ver 3.4\DB). The next section called *Toolbox 4.3 database* (2) shows the database to which the source database is transferred to. By default the application is preconfigured to connect to the installation database (e.g. toolboxv20). The third section lists the custom databases/inventories object of transferring (3). Once the database file is selected (in the first section), then list with the available custom databases/inventories will be loaded automatically and the user could select if they want to transfer all or just some of them. The process of migration starts by clicking the “Start Transfer” button (4).

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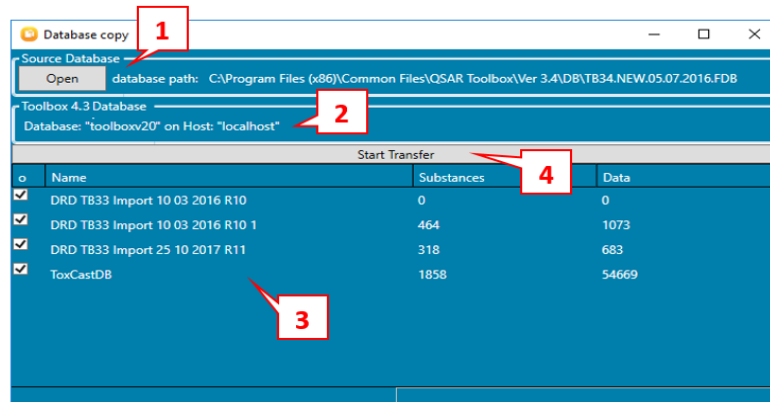


Figure 19. *Database Migration Tool* screen

Once started the process could not be cancelled until finished. The transfer process will take several minutes.

More details about the *Database Migration Tool* could be found in the user manual included in the downloaded package.

2. Transfer custom items from QSAR Toolbox 4.x to QSAR Toolbox 4.3

a. *Transfer custom profilers*

Currently there is no tool allowing automatically transferring of profilers from of Toolbox 4.x (i.e. Toolbox versions 4.0, 4.1 and 4.2) to Toolbox 4.3.

The users have to copy manually their custom profilers from the corresponding directory and to paste them into the profilers` directory in the Toolbox 4.3.

Default directory of the Toolbox 4.2 profilers: C:\Program Files (x86)\Common Files\QSAR Toolbox 4.2\Config\Profilers

Default directory of the Toolbox 4.3 profilers: C:\Program Files (x86)\Common Files\QSAR Toolbox 4.3\Config\Addins\LMC.Toolbox.Server.Profiling

b. *Transfer custom databases*

Currently there is no tool allowing automatically transferring of databases from of Toolbox 4.x (i.e. Toolbox versions 4.0, 4.1 and 4.2) to Toolbox 4.3.

The users have to import their databases/inventories manually in the Toolbox 4.3.

IV. How to remove the previous Toolbox version(s)?

1. Removing of QSAR Toolbox 3.x

Uninstall the available 3.x versions of Toolbox directly from the Control panel of your computer:

Control Panel\All Control Panel Items\Programs and Features

After the uninstallation of QSAR Toolbox, the database **will not** be removed. It should be deleted by hand.

2. Removing of QSAR Toolbox 4.x

The completely removing of QSAR Toolbox 4.x happens in two steps: 1) uninstallation of the program and 2) deletion of the database.

a. Uninstallation of QSAR Toolbox

Uninstall the available 4.x versions of Toolbox directly from the Control panel of your computer:

Control Panel\All Control Panel Items\Programs and Features

Uninstallation of QSAR Toolbox removes only the Toolbox application. The database should be further removed.

b. Removing of the Toolbox database

Preserving of the old Toolbox databases consume a lot of memory. In order to free some space on your computer, you could delete the old TB 4.x databases (i.e. the databases of Toolbox 4.0, 4.1 and/or 4.2) by using of the *Database removal tool*. The tool could be downloaded from the link below:

<http://toolbox.oasis-lmc.org/downloads/tools/ToolboxDatabaseManagement.zip>

Once the tool is downloaded, extract the content of the package and double click the *ToolboxDatabaseManagement* executable (Figure 20).

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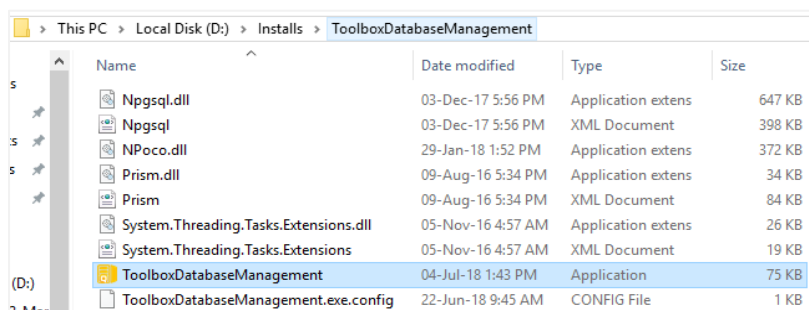


Figure 20. *ToolboxDatabaseManagement* executable

Enter the port and the password of the PostgreSQL (1) and click **Connect** (Figure 21).

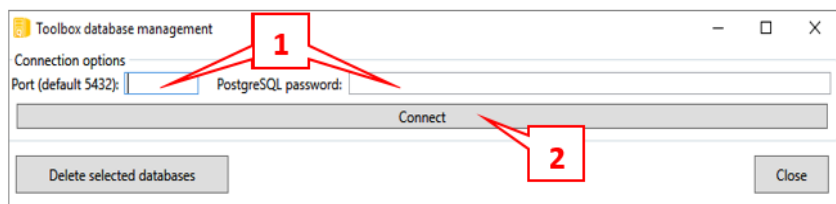


Figure 21. Enter the port and password of the PostgreSQL

The settings are: port: **5432** (by default); password: **postgres** (as recommended)

Note: If you have changed the password and you do not remember it, please follow the steps you will find at the following link in order to reset your PostgreSQL password:

<http://toolbox.oasis-lmc.org/content/documents/ResettingPostgreSQLPassword.pdf>

All available databases from Toolbox 4.x will appear. Select the old database(s) you want to delete (1) and click *Delete selected databases* (2) (Figure 22).

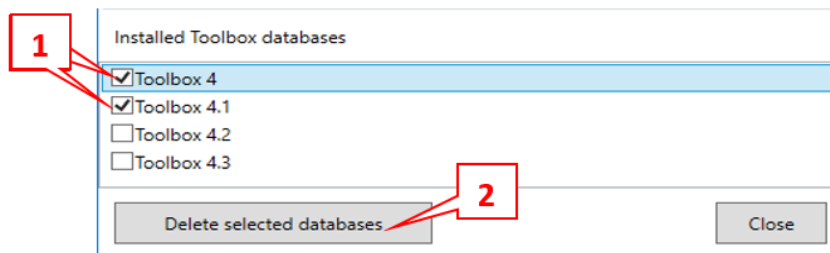


Figure 22. Selection of old database(s) to be deleted

V. OASIS Metapath

Click on the *OASIS Metapath* item of the bootstrap application and follow the onscreen instructions.

VI. Known issues

➤ Running the QSAR Toolbox on limited user accounts

The QSAR Toolbox server requires administrative permissions to run when running in Remote connect mode. They are necessary in order for the application to open a port and listen for client connection.

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