Toolbox v.4.5 - User manual

Document history

Version	Comment
Version 1.0	March 2017: Installation notes for Toolbox version 4.0
Version 1.1	August 2017: Updated to reflect changes in version 4.1
Version 1.2	January 2018: Updated to reflect changes in version 4.2
Version 1.3	February 2019: Updated to reflect changes in version 4.3
Version 1.4	February 2020: Updated to reflect changes in version 4.4
Version 1.5	September 2021: Updated to reflect changes in version 4.5
Version 1.6	March 2022: Updated to reflect changes in version 4.5 SP1

Issue date: March 2022

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

Contents

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 4.5) set-up kit on a local PC operating Microsoft® Windows®.

The new QSAR Toolbox 4.x 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 4.5 is a major update to Toolbox and can be installed alongside previous versions of 4.x.

Version 4.5 is quite different system from 4.4.1 in that it migrated both to a new database management system, PostgreSQL 13, and to .NET 5.0. This means that both these must be installed regardless of existing Toolbox installs which used PostgresSQL 9.6 and .NET Framework 4.7.

PostgreSQL install may be particularly tricky as its **port** setting may interfere with the previously installed version.

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 13
- Microsoft .NET 5.0

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.

> **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 may 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 v.4.5 is a major update to Toolbox and can be installed alongside previous versions of 4.x.

If you not have not installed any of the previous versions of Toolbox v.4. (i.e. versions 4.0, 4.1, 4.2, 4.3 and/or 4.4), you need to install the four basic components of QSAR Toolbox

      1) PostgreSQL 13

      2) .NET 5.0

      3) Database

      4) QSAR Toolbox application.

If you have previously installed PostgreSQL 13 and .NET5.0, skip Step 1 and 2 and start directly from Step 3. 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

1. Step 1. PostgreSQL

Step 1.1. Click on **PostgreSQL 13.3 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. In the **Select components** stage you can uncheck the "Stack builder" component, as it is not needed for Toolbox (Figure 3).
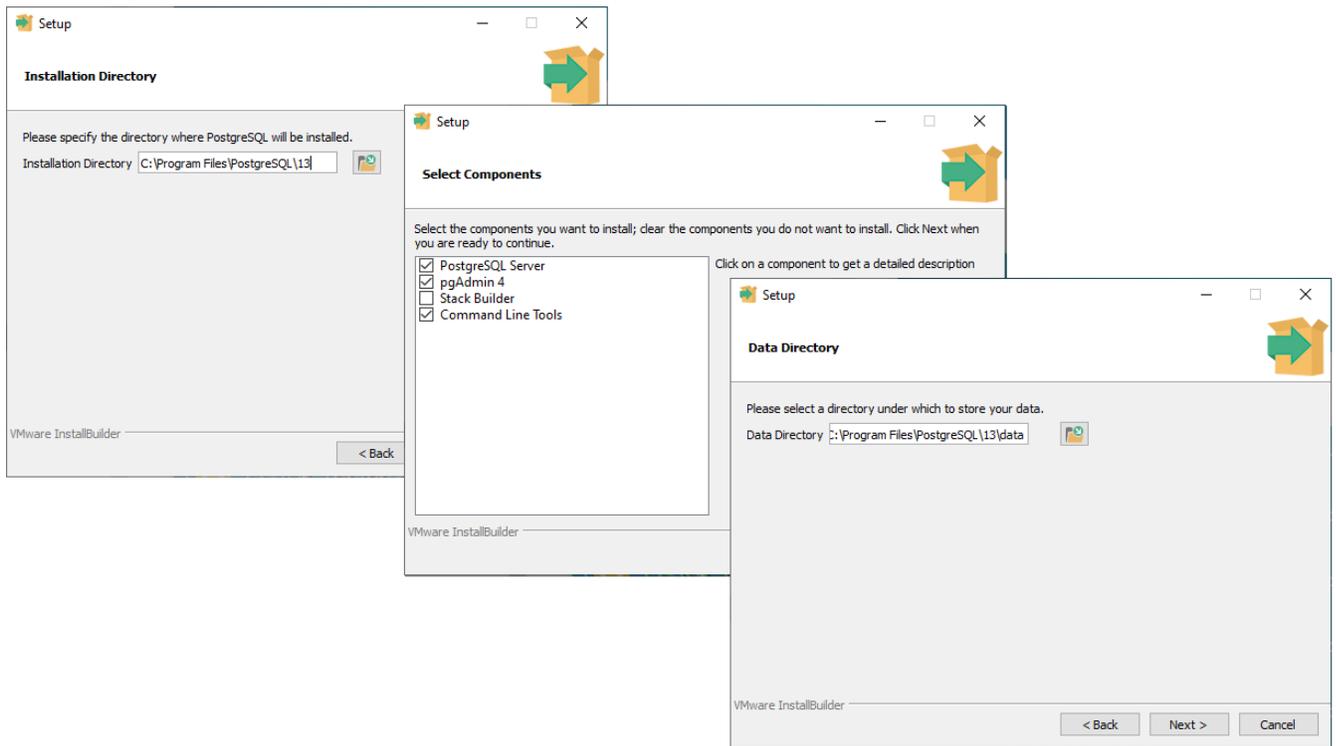
Figure 3. Selection of folders where the PostgreSQL should be installed and data stored

Note: Make sure the Data folder is on a drive that has at least **12 GB** of free space.

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

Password: **postgres** (recommended)

Port: **5432** (by default)

> **Important:** If you have previously installed Postgres (e.g. the previous version 9.6) port **5432** may be occupied. In that case, you need to select a different available port, for instance **5433**
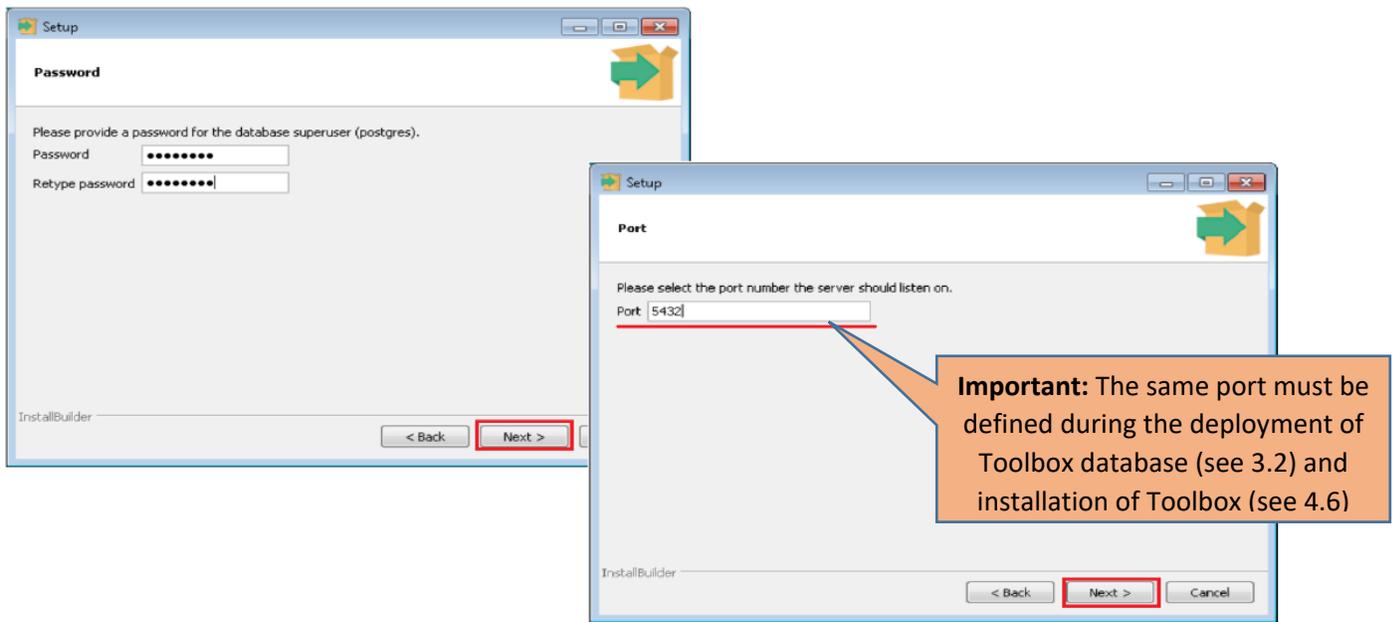

Figure 4. Specifying password and port for the PostgreSQL

> **Note:** Whatever you decide to put as a password and 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. You can simply click Next on Advanced Options and Pre Installation Summary, to click **Finish** (Figure 5)
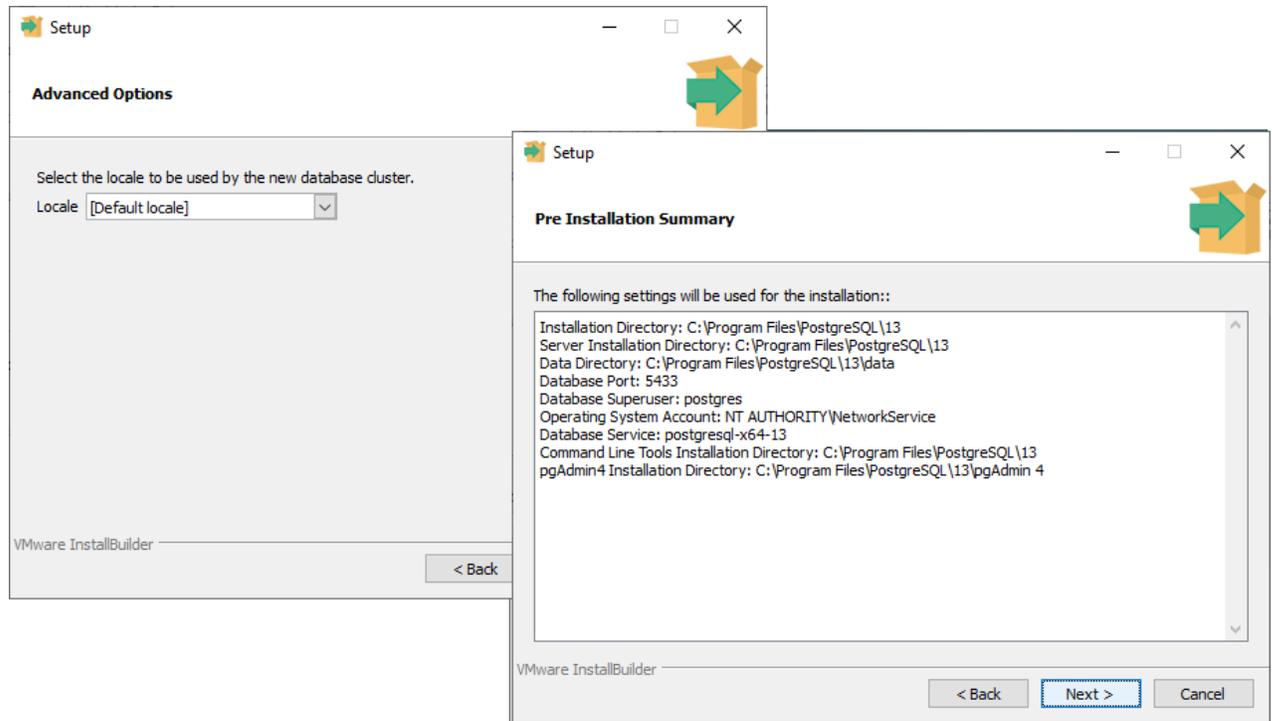

Figure 5. Advanced Options and Pre Installation Summary

Now PostgreSQL is installed and you can continue with the installation of the Toolbox database.
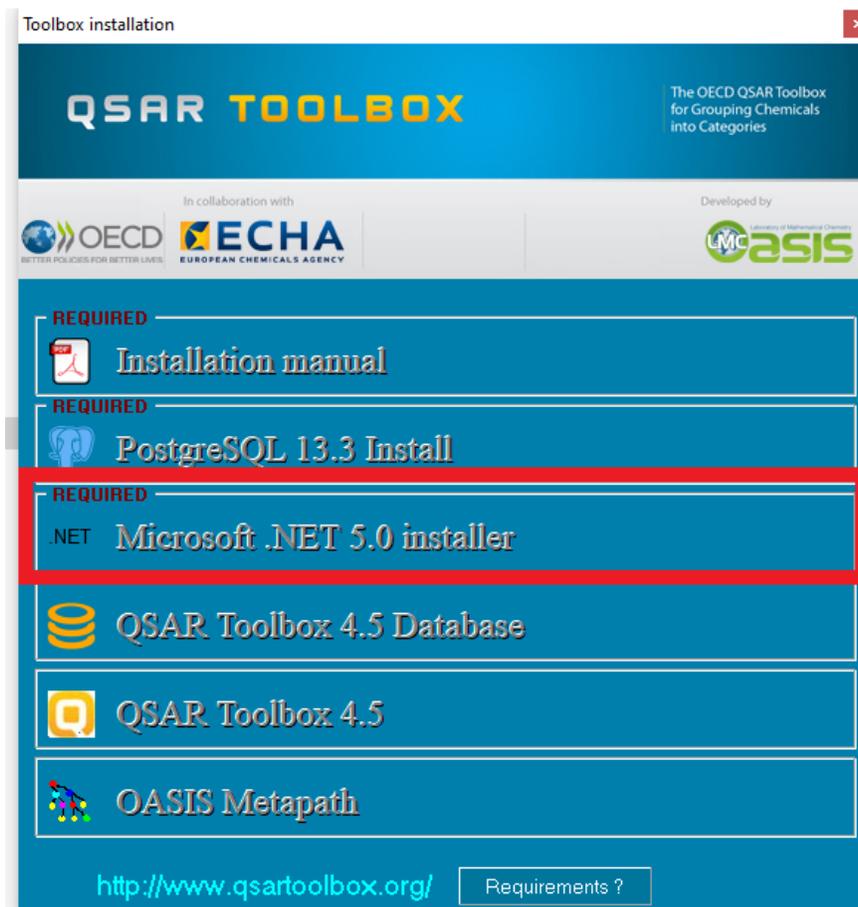
2. Step 2. Microsoft .NET 5.0

Figure 6. Install Microsoft .NET 5.0

Click on **Microsoft .NET 5.0 installer** and follow the onscreen instructions.

3. Step 3. Database

Step 3.1. Select *QSAR Toolbox 4.5 Database* (Figure 7)

Figure 7. Start installation of the Toolbox database

Step 3.2. You will be asked (Figure 8) to provide the PostgreSQL superuser password and listen port. (see 1.3):

- For password type the same password defined during PostgreSQL installation (see 1.3)

- For the port type **5432** (by default) and click the *Deploy* button. Be extra careful to enter the port you specified at step 1.3.
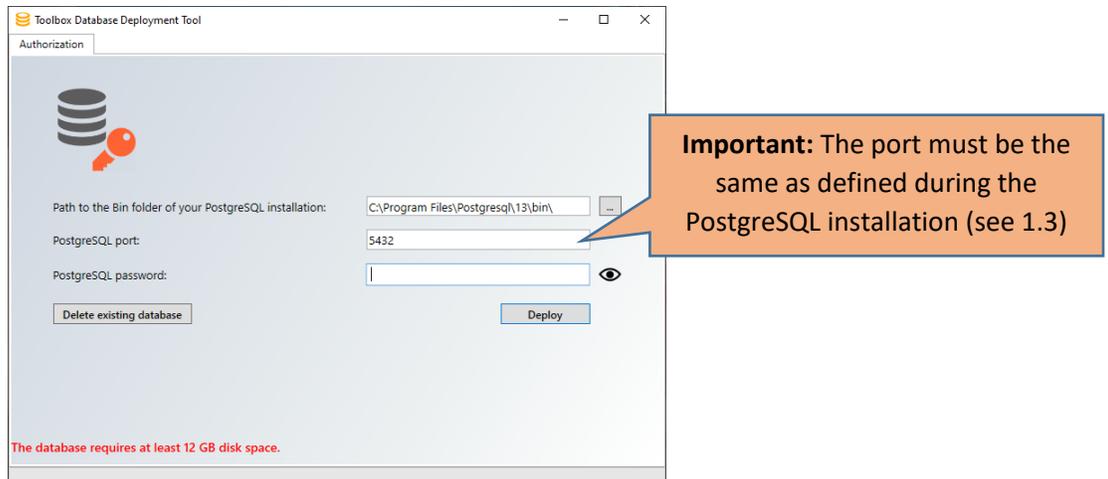

Figure 8. Start database deployment

> **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

Step 3.3. On the next confirmation message click on "Yes" (Figure 9). This warning message is related only to the same version of Toolbox. Deployment of the Toolbox v.4.5 database will not affect the previous databases.
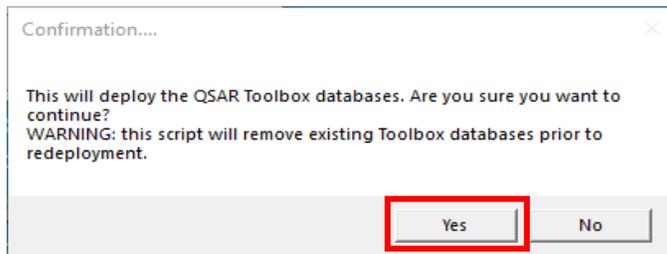

Figure 9. Confirmation message for starting database deployment

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"), it should have "Running" in the Status column.

Continue with the last step of the Toolbox installation.

4. Step 4. QSAR Toolbox

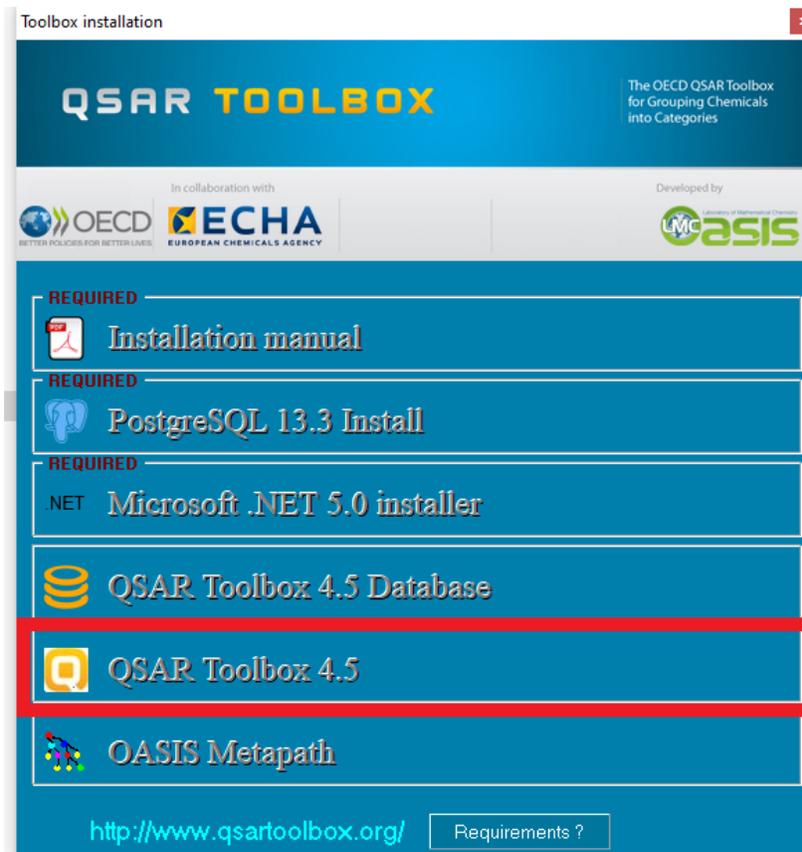**Step 4.1**. Select *QSAR Toolbox 4.5* (Figure 10)

Figure 10. Start installation of the Toolbox application

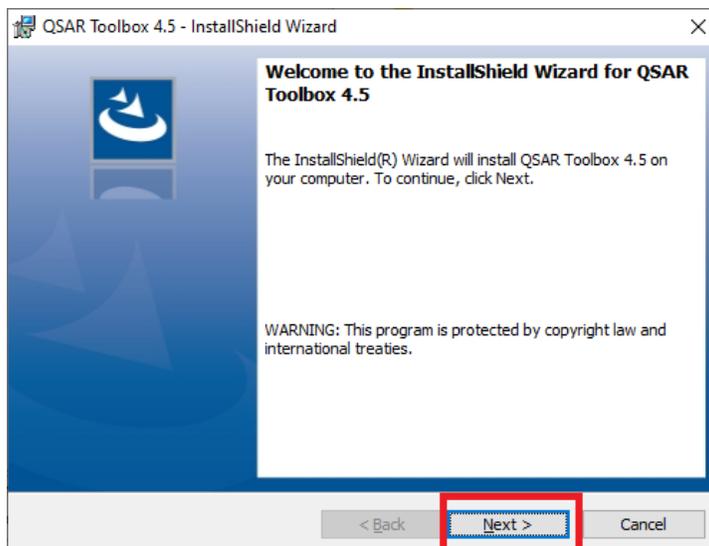**Step 4.2.** Start the installation of Toolbox by clicking Next (Figure 11)

Figure 11. InstallShield Wizard screen

Step 4.3. Accept the terms of the license agreement in order to continue with the Toolbox installation (Figure 12)
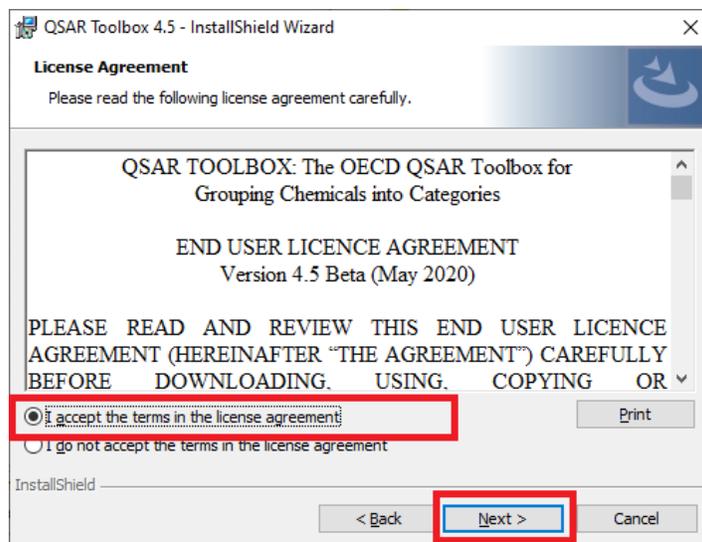

Figure 12. License agreement

Step 4.4. You will be asked for a destination folder of the Toolbox. Click **Next** to install the Toolbox to the default directory (Figure 13)
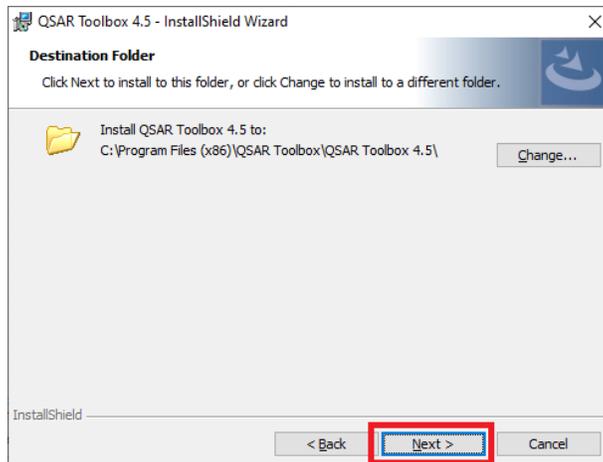

Figure 13. Selection of Toolbox destination folder

Step 4.5. 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 14)
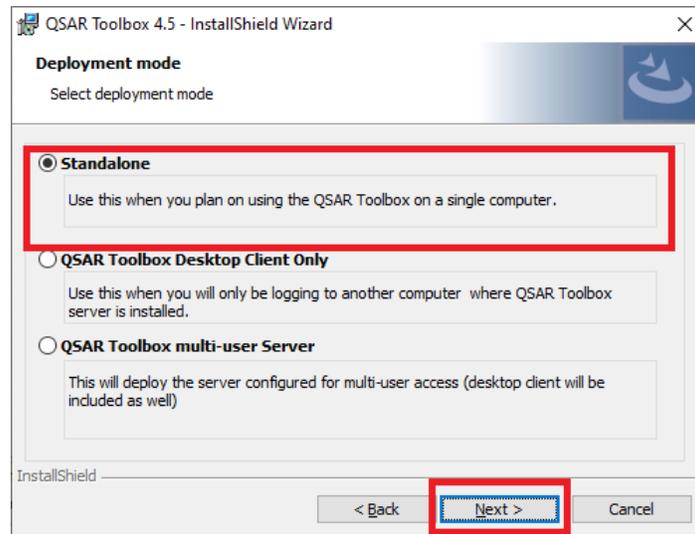

Figure 14. Selection of deployment mode of Toolbox

Step 4.6. 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.
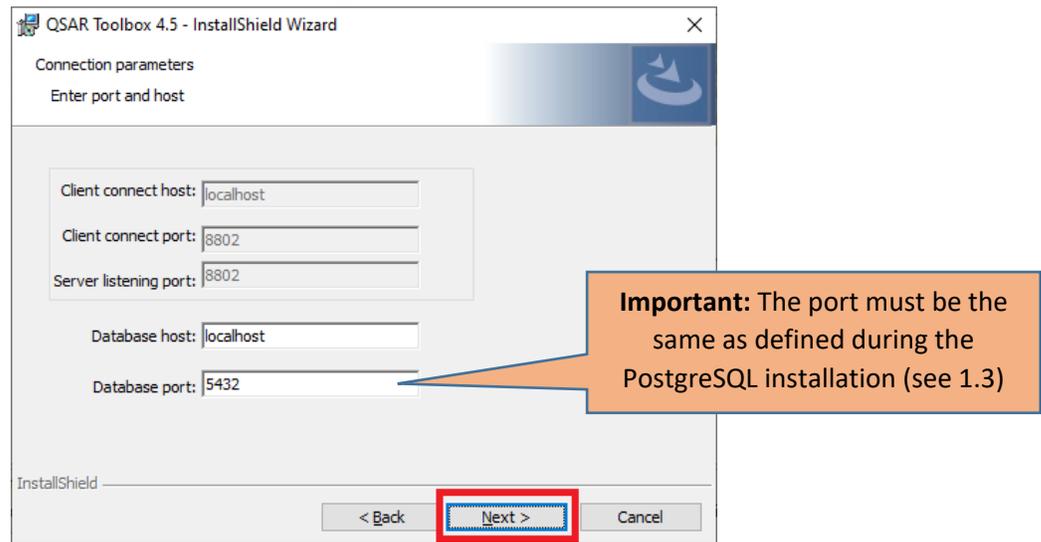

Figure 15. Entering connection parameters

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). **Server listening port** has a companion port, **SessionHealthMonitorPort,** which can be configured post installation, see the Note bellow)

Step 4.7. Finalize the Toolbox application install by click on "Install" and then "Finish" (Figure 16)
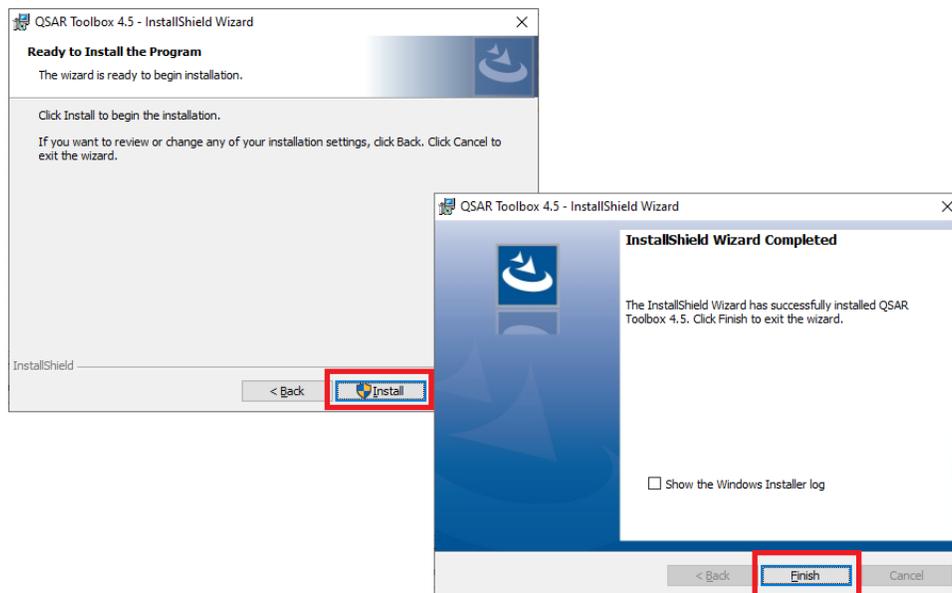

Figure 16. Finalizing of the Toolbox Application installation

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

> **Note:** If the QSAR Toolbox Client is configured to connect to a local server it will start QSAR Toolbox Server, if it is not already started.

> **Note:** The QSAR Toolbox also benefits from a service channel that can be configured in the config files of the Client and Server. It is set to port **8804** by default.
>
> To change it you'd need to search for the **SessionHealthMonitorPort** item and change the value to whatever you'd like. Here is what the configuration looks like:
> *<add key="SessionHealthMonitorPort" value="8804"></add>*
>
> Here are the names of the files where the port needs to be configured:
> *[InstallationFolder]*\Toolbox Client\bin\Toolbox.Desktop.Client.dll.config
> *[InstallationFolder]*\Toolbox Server\Bin\ToolboxServerApp.dll.config

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

1. Transfer custom items from QSAR Toolbox v.3.x to QSAR Toolbox v.4.5

Two tools allowing to transfer custom items (profilers and databases) from QSAR Toolbox v. 3.x to QSAR Toolbox v.4.5 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

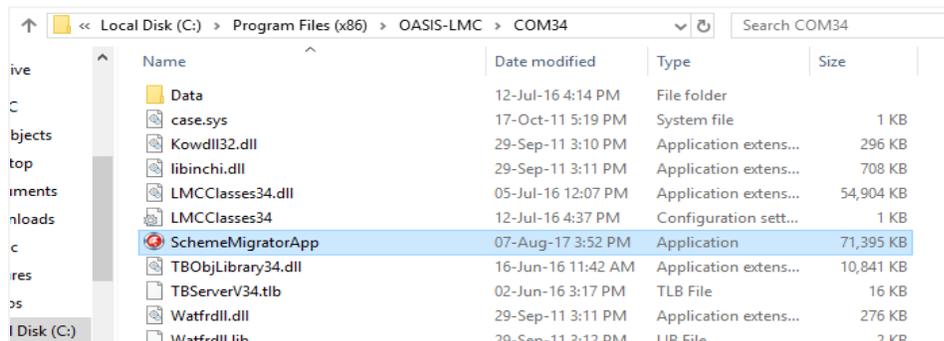(e.g. C:\Program Files (x86)\OASISLMC\COM34) (Figure 17).

Figure 17. *Scheme Migrator App* executable in the default directory of the COM34 folder (QSAR Toolbox v.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 18). Sequential loading of schemes adds them to the list. The list of loaded schemes can 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).
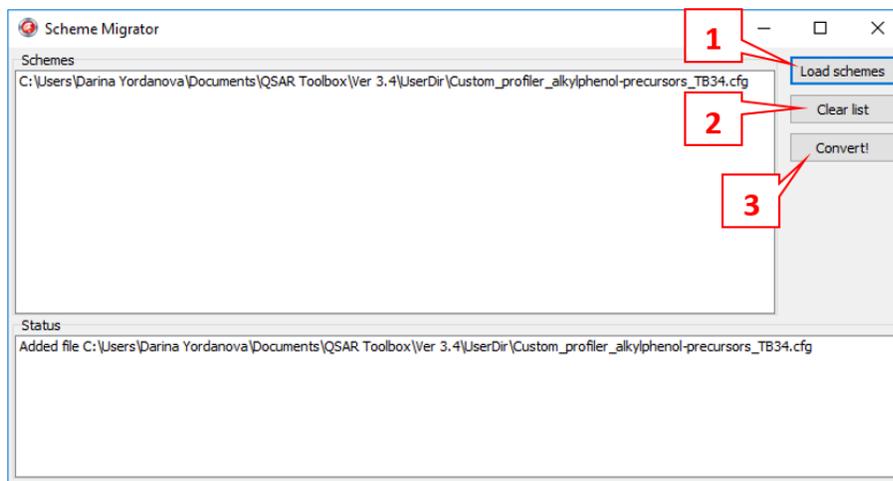

Figure 18. *Scheme Migrator App* screen

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 he 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 4.5, they need to be placed in the CONFIG folder. Its default path is:

C:\Program Files (x86)\Common Files\QSAR Toolbox 4.5\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.

b. *Transfer custom databases*

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

Download Database Migration tool

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 19)
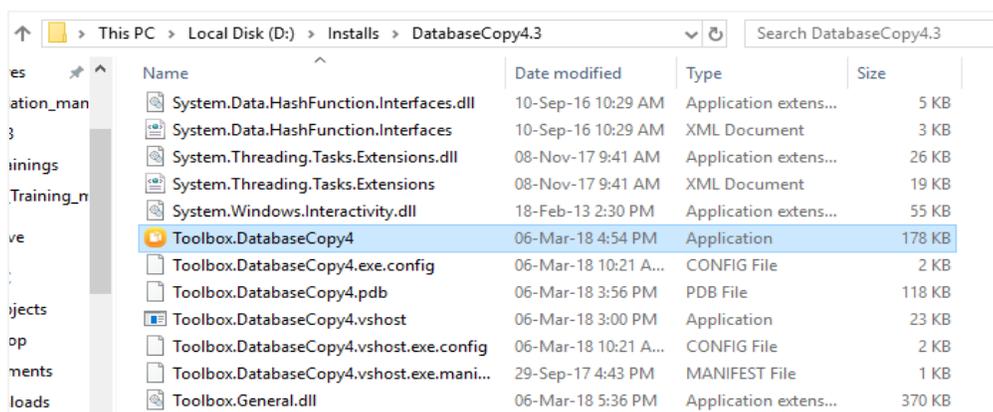

Figure 19. *Database Migration Tool* executable

The user interface of the *Database Migration Tool* includes three sections (Figure 20). 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 4.5* (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. toolboxv21). The third section lists the custom databases/inventories object of transferring (3). Once the database file is selected (in the first section), then the list with the available custom databases/inventories will be loaded automatically. Now the user could select all or just some of them to be transferred. The process of migration starts by clicking the "Start Transfer" button (4).
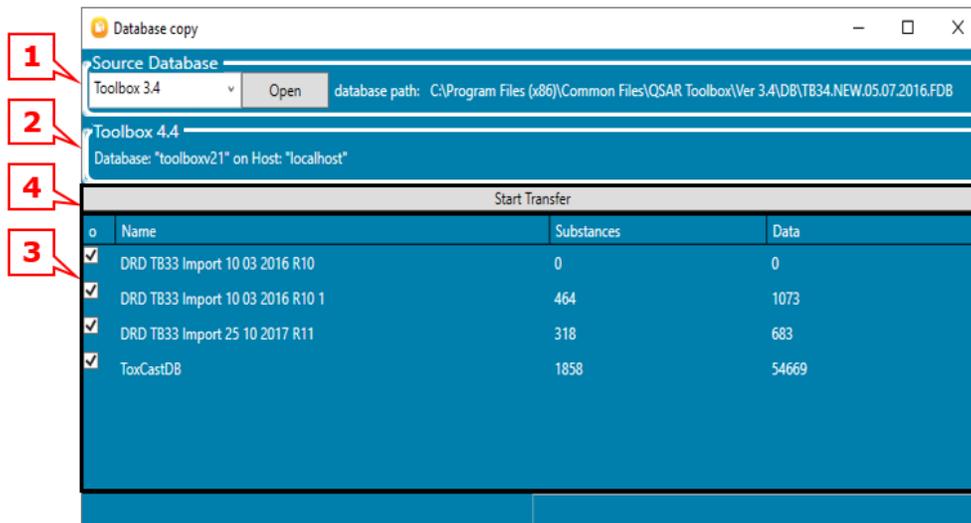
Figure 20. *Database Migration Tool* screen when transfer custom databases from Toolbox v.3.4

Once started the process could not be cancelled until finished. The transfer process will take several minutes depending on the size of custom databases selected for transferring.

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 v.4.x to QSAR Toolbox v.4.5

a. Transfer custom profilers

Currently there is no tool allowing automatically transferring of profilers from of Toolbox v.4.x (i.e. Toolbox versions 4.0, 4.1, 4.2, 4.3 and 4.4) to Toolbox v.4.5.

The users have to copy manually their custom profilers from the corresponding directory and to paste them into the profilers` directory in the Toolbox v.4.5.

Default directory of the Toolbox v.4.3 profilers: C:\Program Files (x86)\Common Files\QSAR Toolbox 4.3\Config\Profilers

Default directory of the Toolbox v.4.5 profilers: C:\Program Files (x86)\Common Files\QSAR Toolbox 4.5\Config\Addins\LMC.Toolbox.Server.Profiling

b. *Transfer custom databases*

The *Database Migration Tool* has been modified to transfer all custom databases from previous Toolbox versions (including Toolbox v.4.x) to the current version of Toolbox.

The *Database Migration Tool* could be downloaded from the following link:

Download Database Migration tool

The user interface of the *Database Migration Tool* includes three sections (Figure 21). The first section called *Source Database* (1) allows selection of the source database (the previous database that will be transferred to the current Toolbox version. All available Toolbox databases will be shown in the drop-down menu. Click on the "Connect" button identifies the exact version of the database. The next section called Toolbox 4.5 (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. toolboxv21). 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. Now 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).
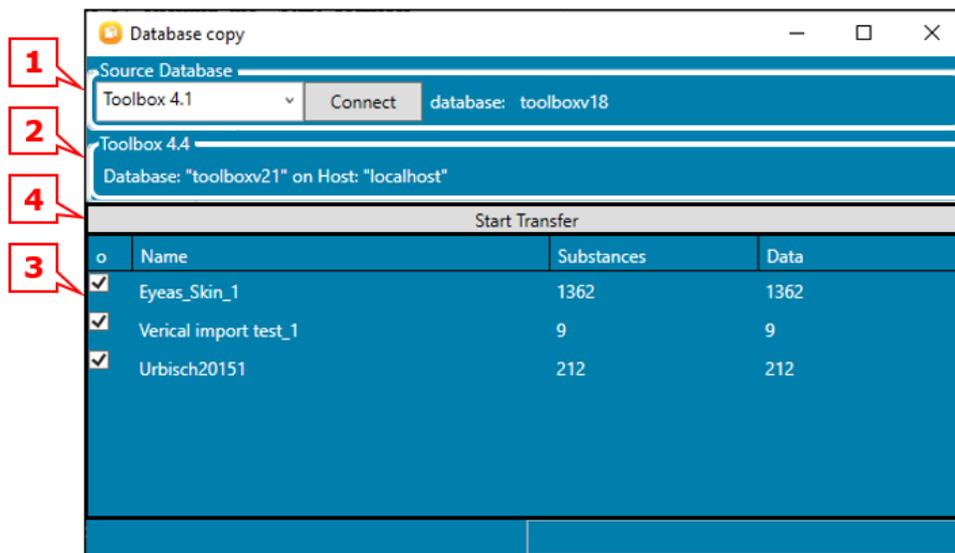

Figure 21. *Database Migration Tool* screen when transfer custom databases from Toolbox v.4.x

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

1. Removing of QSAR Toolbox v.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 v.4.x

The completely removing of QSAR Toolbox v.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 v.4.x databases (i.e. the databases of Toolbox v.4.0, v.4.1, v.4.2 and/or v.4.3) 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 22).
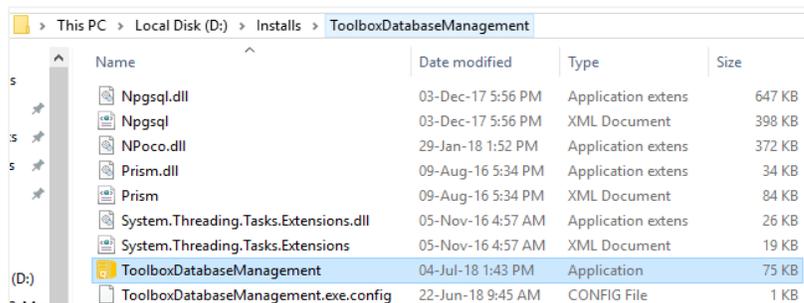
Figure 22. *ToolboxDatabaseManagement* executable

Enter the port and the password of the PostgreSQL (1) and click **Connect** (Figure 23) (see step 1.3).
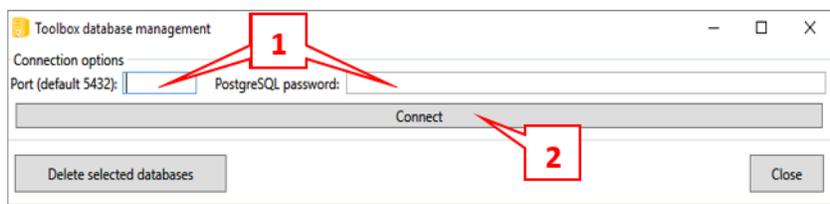

Figure 23. Enter the port and password of the PostgreSQL

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 v.4.x will appear. Select the old database(s) you want to delete (1) and click *Delete selected databases* (2) (Figure 24).
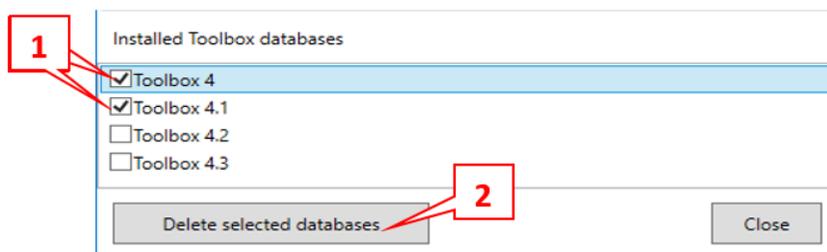
Figure 24. Selection of old database(s) to be deleted

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.

➤ Toolbox Client starts, displays splash screen, but the application window disappears after that, leaving a process in the Task Manager.

For a workaround of this issue please visit the Known Issues section of the QSAR Toolbox website at https://qsartoolbox.org/download/issues/

OECD

2, rue André Pascal

75775 Paris Cedex 16

France

Tel.: +33 1 45 24 82 00

Fax: +33 1 45 24 85 00

ehscont@oecd.org