

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
Version 1.1	August 2017: Updated to reflect changes in version 4.1

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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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Toolbox 4.1 Installation Manual

1 Introduction

This document provides a summary description of the installation procedure of the QSAR Toolbox (version 4.1) 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 Background

The new QSAR Toolbox 4.1 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 4.1 is a major update to Toolbox and can be installed alongside version 4.0.

4 Installed components

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

5 Installation package

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.

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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/>.

Execute the "StartInstall.exe" file in the root directory (Figure 1). This executable is going to provide a dialog from which the user can install PostgreSQL, Database and the QSAR Toolbox application.

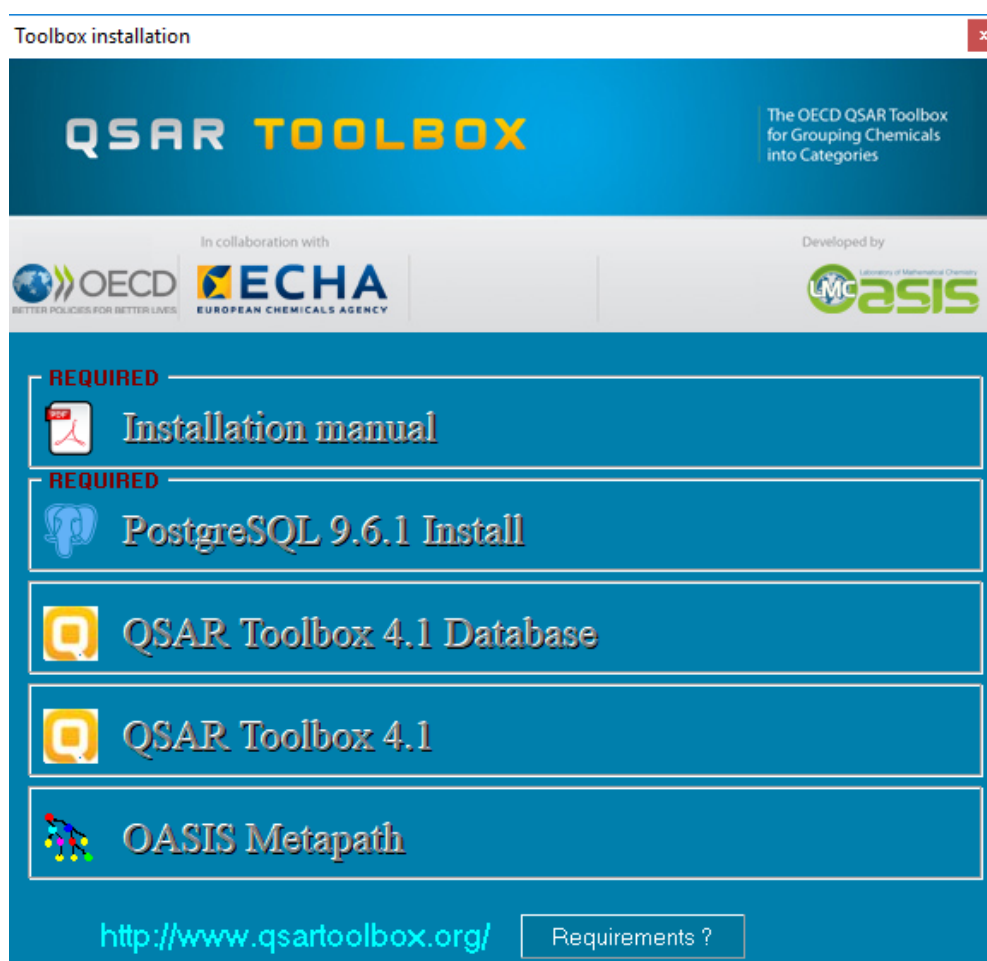


Figure 1: Installation startup screen

6 Installation sequence

6.1 PostgreSQL installation

If you have an existing PostgreSQL installation, versions 9.4, 9.5 or 9.6, you could use it - you would need to provide the port and postgres superuser password - otherwise continue reading this section.

Click on **PostgreSQL 9.6.1 Install** button and follow the on the screen.

You will be asked to select an installation folder (Figure 2), leave the default setting.

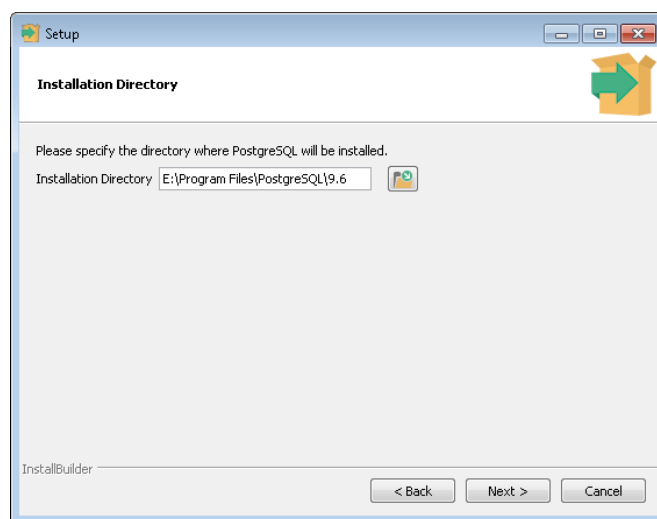


Figure 2: PostgreSQL install folder.

Next you will be asked to set the **Data** folder (Figure 3). Make sure the Data folder is on a drive that has at least 5GB of free space.

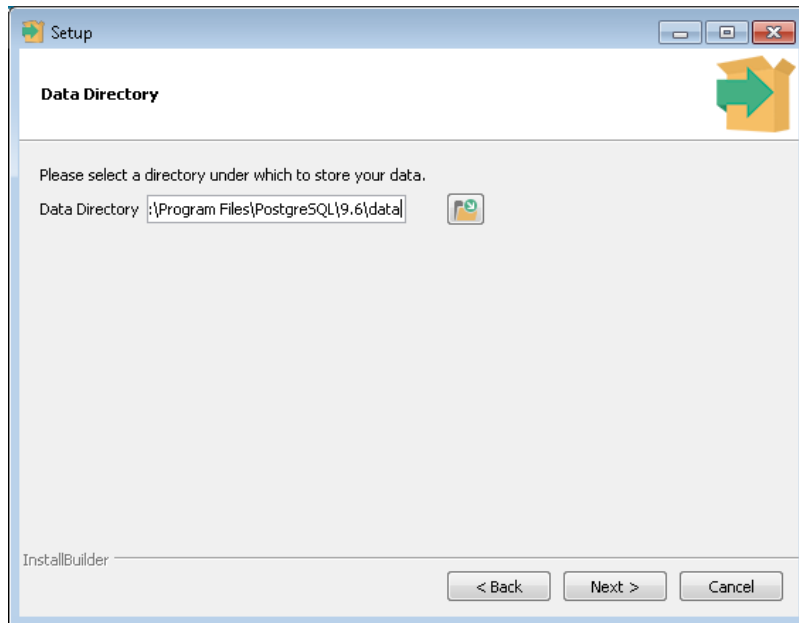


Figure 3: PostgreSQL Data folder

Next you will be asked to enter the password for the superuser password (Figure 4). Whatever you decide to put here **make sure you write it down or memorise it** as it will be needed later in the installation procedure and generally throughout the PostgreSQL installation’s lifetime.

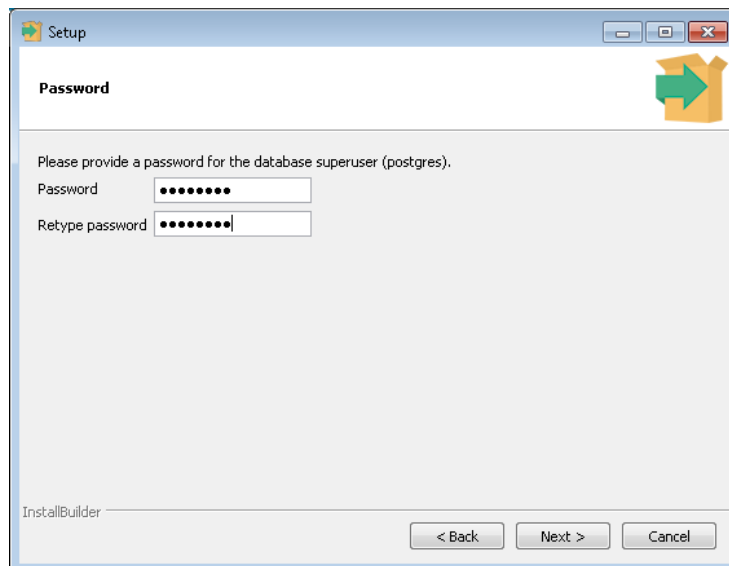


Figure 4: Superuser password.

Next you need to specify the port the PostgreSQL server would listen to (Figure 5). The default provided is 5432. If you have an already installed version of PostgreSQL (e.g 9.0)

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this port may be taken. Whatever port you decide on **make sure you write it down or memorise it** as it will be needed later in the installation procedure and generally in throughout the PostgreSQL installation’s lifetime.

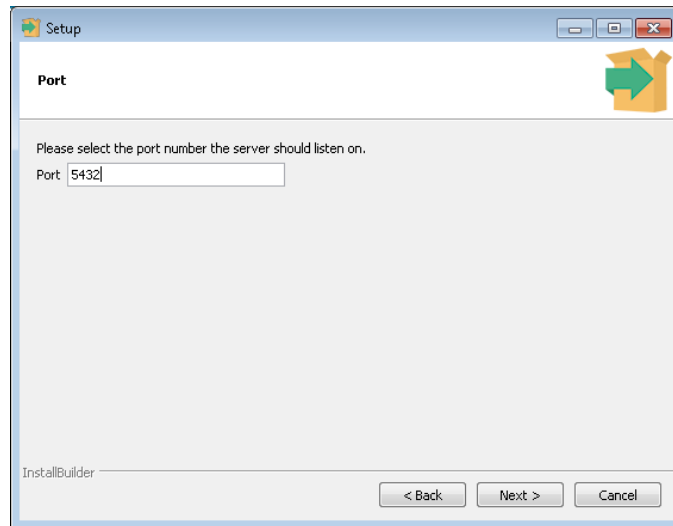


Figure 5: PostgreSQL listen port.

Next you will be asked to select locale. Just leave it as default.

On the final stage uncheck the **“Launch Stack Builder at exit?”** at the end of the installation. Even if you leave it checked you can always close the stack builder afterwards.

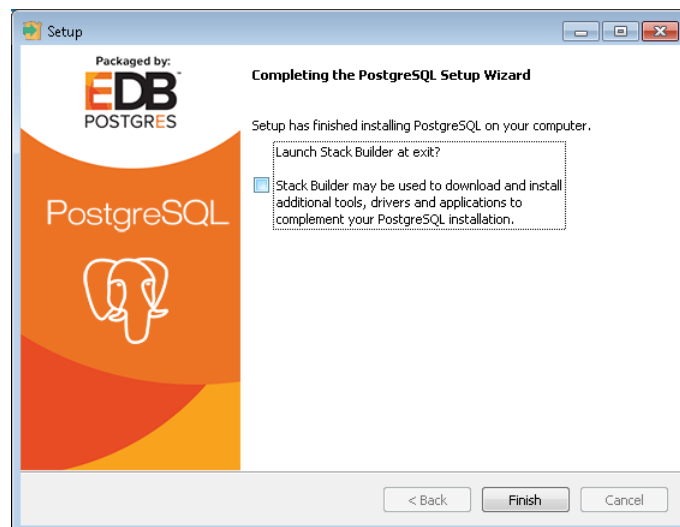


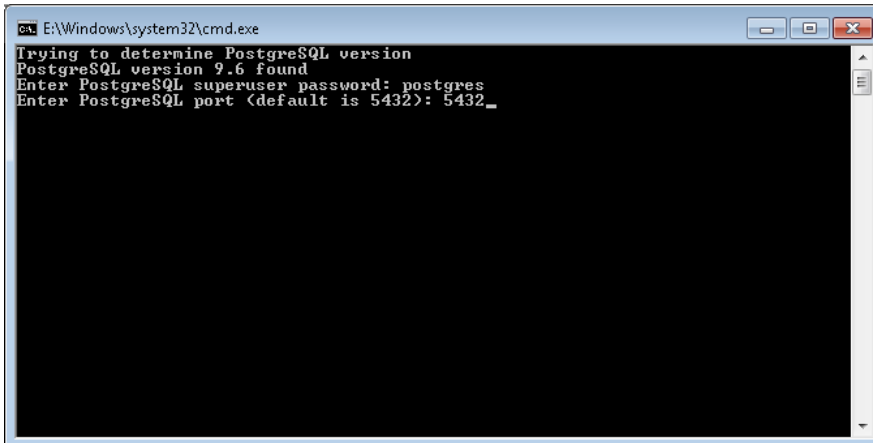
Figure 6: Launch stack builder prompt

6.2 QSAR Toolbox database(s) installation

The QSAR Toolbox Database layer consists of three separate PostgreSQL databases. One is the data repository, one is the EPI reports cache and one is the bio-library data (downloaded from <http://itis.gov> and slightly modified for performance reasons).

Note: A prerequisite for the database deployment step is that there is a functional PostgreSQL server listening. Whether you are using an existing PostgreSQL deployment or one that was just deployed you need to check that the PostgreSQL service is up and running before continuing with database deployment. You could do 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.

To install the databases click on the **QSAR Toolbox 4 Database** button. You will be asked (Figure 7) to provide the PostgreSQL superuser password and listen port (see **PostgreSQL installation** section of this manual).



```
E:\Windows\system32\cmd.exe
Trying to determine PostgreSQL version
PostgreSQL version 9.6 found
Enter PostgreSQL superuser password: postgres
Enter PostgreSQL port (default is 5432): 5432_
```

Figure 7: Set PostgreSQL password and listen port.

After you enter the password and port the database deployment will commence. It is a lengthy operation (up to 15 min depending on computer configuration) and it should not be interrupted.

After the databases have been deployed a **"Databases successfully deployed"** will be displayed and the process will pause until a key is pressed.

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Note: The QSAR Toolbox database is designed to be used by a single Toolbox Server. Please make sure than there is no concurrent access to the same Postgres database from different instances of Toolbox server.

6.3 QSAR Toolbox applications installation

The QSAR Toolbox application consists of the two layers of the QSAR Toolbox – the client and server. To install them click on the **QSAR Toolbox 4** of the bootstrap installer. You will be asked for a destination folder (Figure 8)

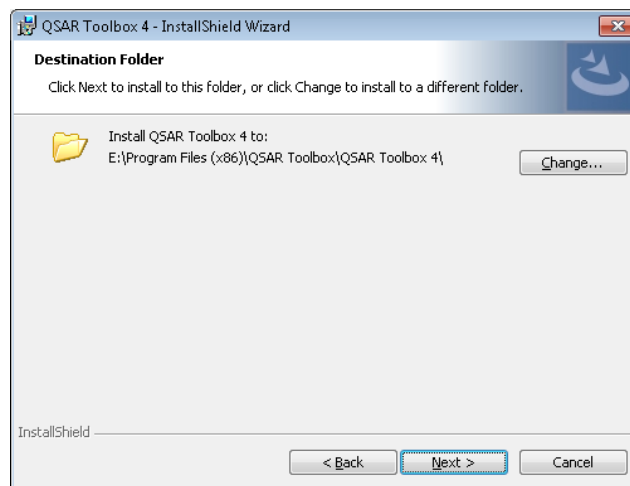


Figure 8: Destination folder for the QSAR Toolbox 4 client and server

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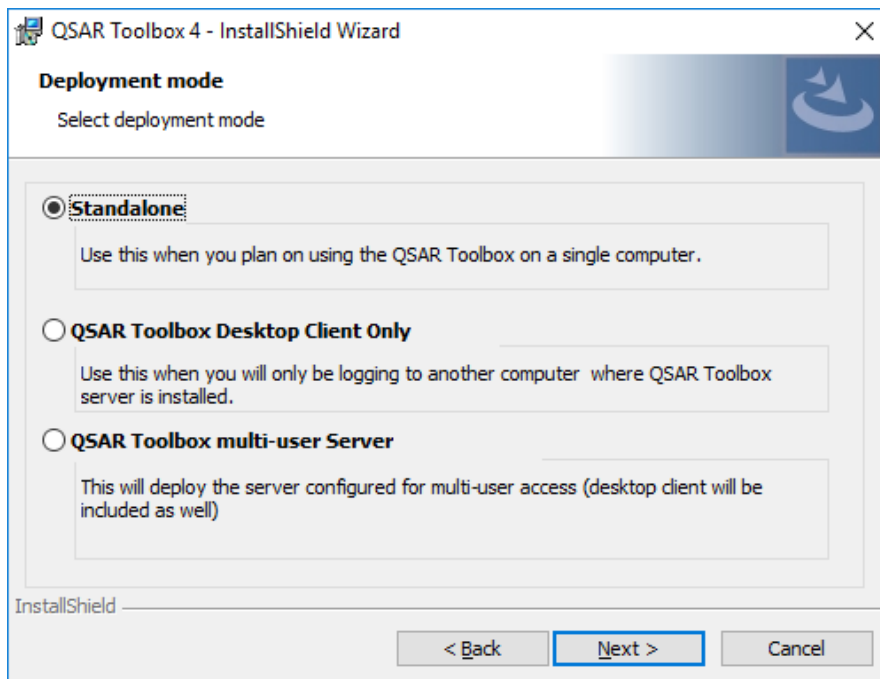


Figure 9: Deployment mode

After you’ve specified the destination folder 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** – 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).

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After you’ve specified the deployment mode you will be prompted to enter the connection parameters (Figure 10) for the Client and Server applications. These include both the host and port that the Client connects to the Server and the host and the port that the Server uses to connect to the PostgreSQL database. Some of the controls will be disabled based on the selected deployment mode.

The parameters are:

- **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(see below)
- **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).

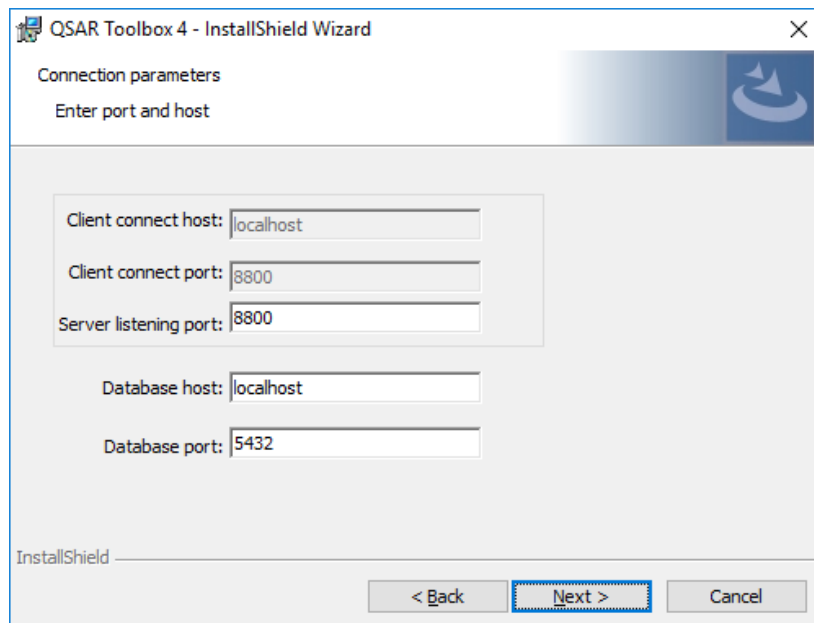


Figure 10: Connection parameters for QSAR Toolbox client and server

6.4 OASIS Metapath

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

7 Known issues

7.1 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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