User manual

QSAR TOOLBOX

The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

Document history

Version	Comment
Version 1.0	January 2019: QSAR Toolbox Server
Version 1.1	February 2020: Updated to reflect changes in version 4.4
Version 1.2	May 2020: Updated to reflect changes in version 4.5

Issue date: May 2020

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

1 Introduction

This document provides a description of the different deployment modes and usage scenarios for the QSAR Toolbox Server when used in multi-user context.

2 Background

The QSAR Toolbox is three tiered application. A PostgreSQL database tier provides database services to the QSAR Toolbox Server application (second tier) that contains the business logic which is then visualized and manipulated via the UI in the QSAR Toolbox Database Client (third tier). The technicalities of this separation, combined with the usage scenarios lead to a variety of deployment scenarios:

- **Standalone** - this is designed to be the simplest deployment. Just install the application on a single PC and run it.

- **QSAR Toolbox Desktop Client only –** this the lightweight deployment of the client for when there is a separate dedicated server machine.

- **QSAR Toolbox multi-user Server –** this is the deployment mode used when deploying for multiple users and the main focus of this document

3 Installation details

Whenever QSAR Toolbox Server is installed - **Standalone** or **QSAR Toolbox multi-user Server –** the Toolbox installer also deploys an accompanying Windows Service that can be used instead of the Server application. The Windows Service allows the server's administrator to start the server automatically, run under a secured acocunt, or otherwise administer the client-server deployment. The Service Name is **QSARToolbox4.5Server**.

> **Note:** The service is installed and configured with **Startup type** set to **Manual**. This is intentional. The QSAR Toolbox Server requires significant amount of resources, thus an explicit action by the system's administrator is required in order for it to start automatically.

This amounts to two entry-points for the server:

- QSAR Toolbox 4.5 Server appilication – this is the application that is familiar to users and can be started explicitly by the user or automatically by the Toolbox Desktop Client. The installer also creates shortcuts to this application in the start menu and the windows desktop.

- QSAR Toolbox Server windows service – this is a service can be started either by the windows system automatically (if a system's administrator has set it to Automatic), or by a user with administrative privileges via the service controller application.

4   Service controller

Toolbox installation package comes with a **QSAR Toolbox Service Controller** application which can be used to start/stop the service (Figure 1) as well as to monitor the server once the service has been started (Figure 2). Note that the controller application requires administrative privileges to run.
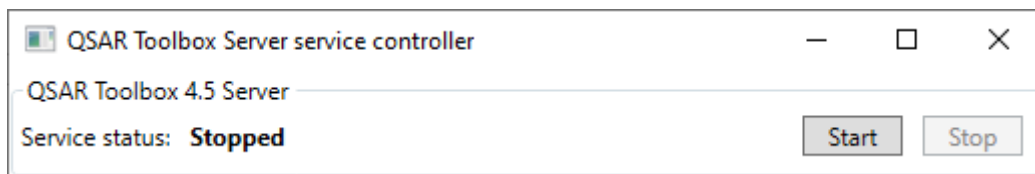

Figure 1: Service controller UI

Once the service is started the controller application will also display a UI modelled after the standalone QSAR Toolbox Server application:
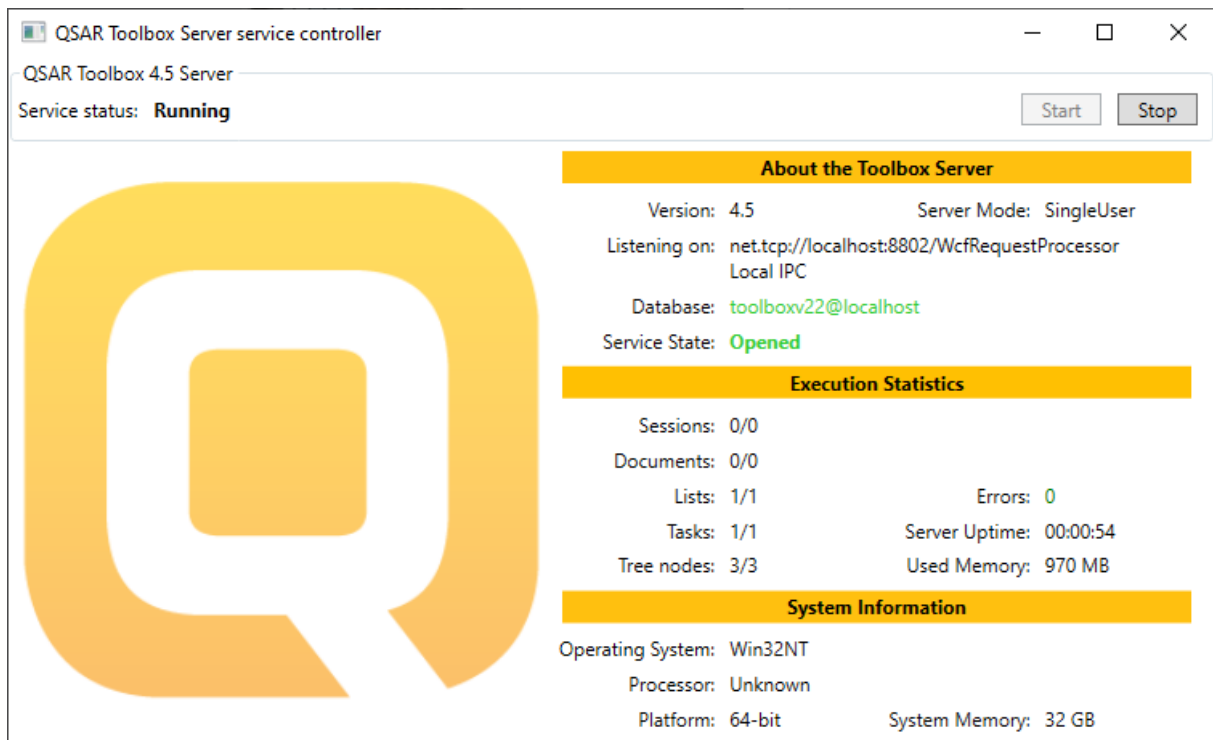
Figure 2: Service UI

An important distinction is that the service controller and the service itself are two separate things. Once the service is started the controller application can be closed and it will not affect the server's process. Additionally the service controller can be started at any point and if a server's window service is running it will connect to it and display a corresponding UI.

5 Microsoft Windows Server OS

When deploying in a Windows Server where on the same machine there will be one server running and multiple clients connecting from different session there is a particular set of cases that may arise.

The QSAR Toolbox Server was designed to run as a single instance per machine (additionally the Database was designed to service a single QSAR Toolbox Server). This is a fact one has to be cognisant of when setting up the server for multi-user access. Since the application and the windows service are basically two packages of the same thing they share the same contention. This can lead to the following scenarios when, for instance, deploying on a Windows Server operating system:

- server was started as a windows service and is running in the background. User tries to start the application from the shortcut and receives an "**Another instance of the Toolbox Server is already running**" message.

- server was started as an application by a user but another user, maybe an administrator, in a different session, tries to start the Windows Service. In this case the service start will just fail.

This means that the way QSAR Toolbox Server is used should be decided and clearly communicated to the users. A good rule of thumb can be:

- only a single user will start the server. All others just use their Desktop client.

- if multiple users should start the server they should do this by starting the windows service via the service controller application

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