User manual

Deploying the Toolbox WebServices engine
Document history

<table>
<thead>
<tr>
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<th>Comment</th>
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</thead>
<tbody>
<tr>
<td>Version 1.0</td>
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<td>Version 1.1</td>
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</tr>
</tbody>
</table>
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Contents

Document history ............................................................................................................................... 1
1. Purpose .......................................................................................................................................... 4
2. Prerequisites .................................................................................................................................. 4
3. Enabling IIS Manager and related components (Windows 7, 8, 8.1, 10) ................................. 5
4. Deploying TBWSe in IIS .................................................................................................................. 8
5. Documentation of the available functions ..................................................................................... 11
6. Support .......................................................................................................................................... 11
1. Purpose

The Toolbox WebServices engine (TBWSe) exposes a set of Toolbox functions via a RESTful API. It gives third-party applications access to the substances, profilers and calculators available in the QSAR Toolbox.

2. Prerequisites

To deploy the WebServices engine, you would need:

- Toolbox Server installed on the same host (see the QSAR Toolbox Installation Manual)
- Internet Information Services (IIS) version 8 or later – installation is described in the next section
3. Enabling IIS Manager and related components (Windows 7, 8, 8.1, 10)

1. Go to Control Panel → Programs → Turn Windows features on or off
2. Locate and expand the Internet Information Services node
3. Check both Web Management Tools and World Wide Web Services
4. Expand **Web Management Tools** and make sure **IIS Management Console** is checked.

5. Expand **World Wide Web Services**, then expand **Application Development Features** and make sure **.NET Extensibility 4.5** (or later), **ASP.NET 4.5** (or later), **ISAPI Extensions** and **ISAPI Filters** are all checked.
6. Click **OK**. Windows will then install the selected components. Once they are installed, click **Close**.

Windows completed the requested changes.
4. Deploying TBWSe in IIS

1. Open IIS Manager (run `inetmgr.exe`)
2. From the Actions pane, click View Sites and then Add Website

3. Enter a Site name of your choice, e.g. `toolbox`
4. By default, the website will be placed in an application pool with the same name. Nevertheless, check the value of the Application Pool as it is needed for step 8
5. Enter Physical path. This is the path to the directory where the Toolbox Server has been installed. The default location is `C:\Program Files (x86)\QSAR Toolbox\QSAR Toolbox 4.1\Toolbox Server`
6. Pay attention to the Port field – enter an unoccupied port of the local host, eg. 8000
7. Uncheck the Start Website immediately checkbox and click OK
8. Click on the Application Pools item under the root of your IIS Manager, locate the pool from step 4 (usually toolbox) and right click on it. From the context menu, choose Advanced Settings...

9. Under Process Model, locate Identity and click on the button with the three dots on the right of it.

10. In the Application Pool Identity dialog, make sure the Built-in account option is selected. From the drop-down menu select LocalSystem and then click OK to close the dialog. Click OK again to close the Advanced Settings window.
This option is necessary because the Toolbox server relies on several Profilers, Metabolism simulators and Parameter calculators that are utilized via COM Server access which requires specific access rights.

11. Back under Sites, right-click on the newly created website, select Manage Website and then click on Start. Then right-click again and from the Manage Website menu click on Browse *:8000 (http) - this should load the TBWSe welcome page in your browser.

12. Allow anywhere from 2 to 10 minutes for the TBWSe to load if this is the first start of the system.
5. Documentation of the available functions

The TBWSe is self-documented meaning that the documentation of the available functions is contained within the engine itself. It can be accessed from the Documentation link on the start page.

6. Support

Support can be obtained via the QSAR Toolbox Helpdesk.