

2/6/2020

QSAR TOOLBOX

The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

User manual

Deploying the Toolbox WebServices engine

Deploying the Toolbox WebServices engine

Document history

Version	Comment
Version 1.0	31/07/2017, first version
Version 1.1	02/06/2020, first revision (updated the <i><u>Deploying TBWSe in IIS</u></i> section)

Deploying the Toolbox WebServices engine

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Deploying the Toolbox WebServices engine

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

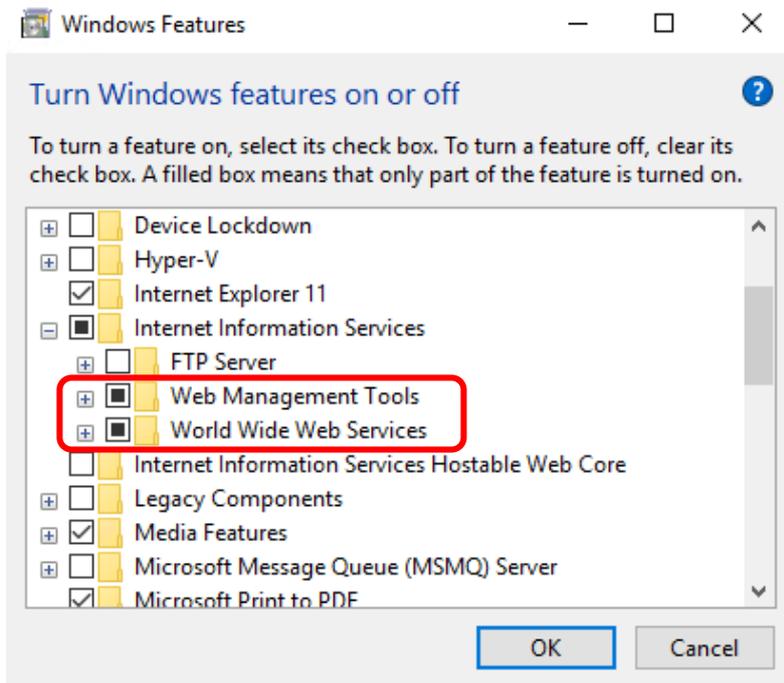
To deploy the WebServices engine, you would need:

- 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

Deploying the Toolbox WebServices engine

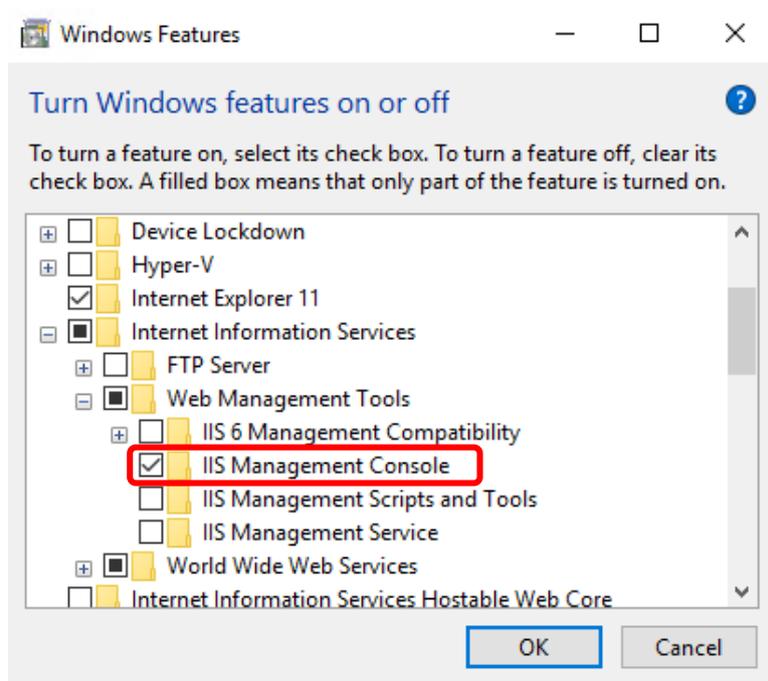
3. Enabling IIS Manager and related components (Windows 7, 8, 8.1, 10)

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**

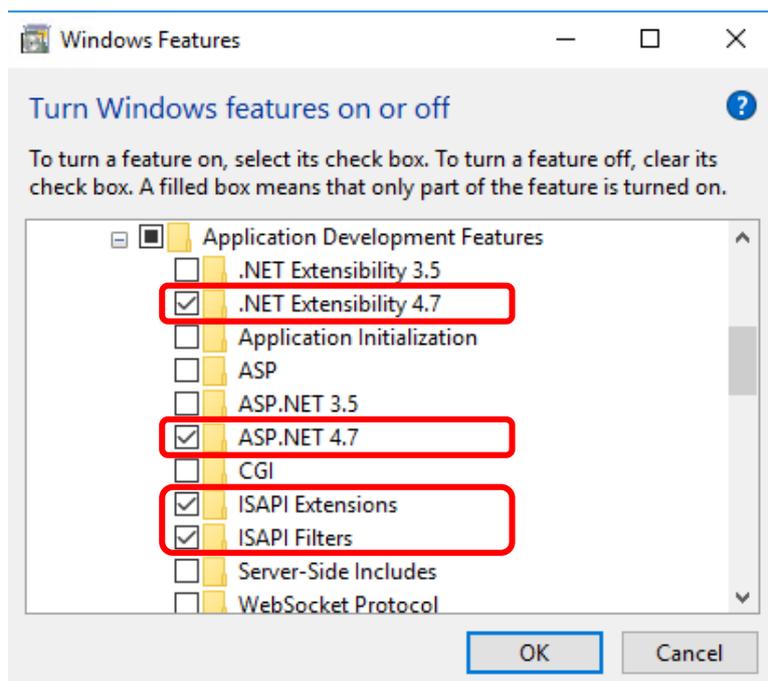


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- Expand **Web Management Tools** and make sure **IIS Management Console** is checked

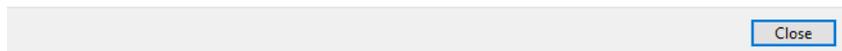
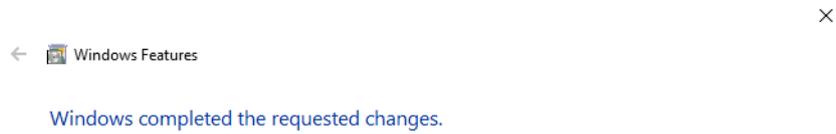


- Expand **World Wide Web Services**, then expand **Application Development Features** and make sure **.NET Extensibility 4.5** (or later), **ASP.NET 4.5** (or later), **ISAPI Extensions** and **ISAPI Filters** are all checked



Deploying the Toolbox WebServices engine

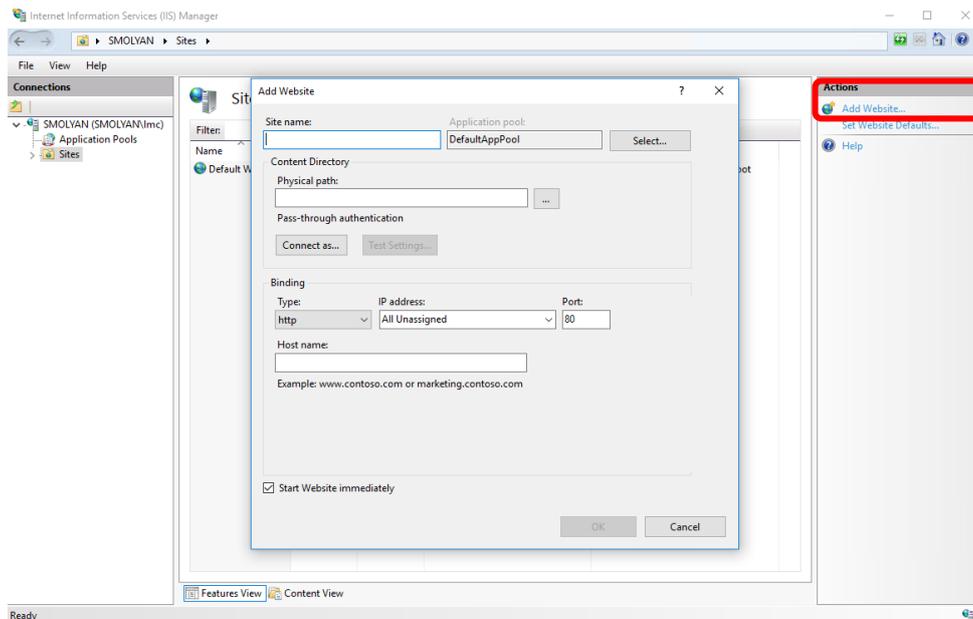
6. Click **OK**. Windows will then install the selected components. Once they are installed, click **Close**.



Deploying the Toolbox WebServices engine

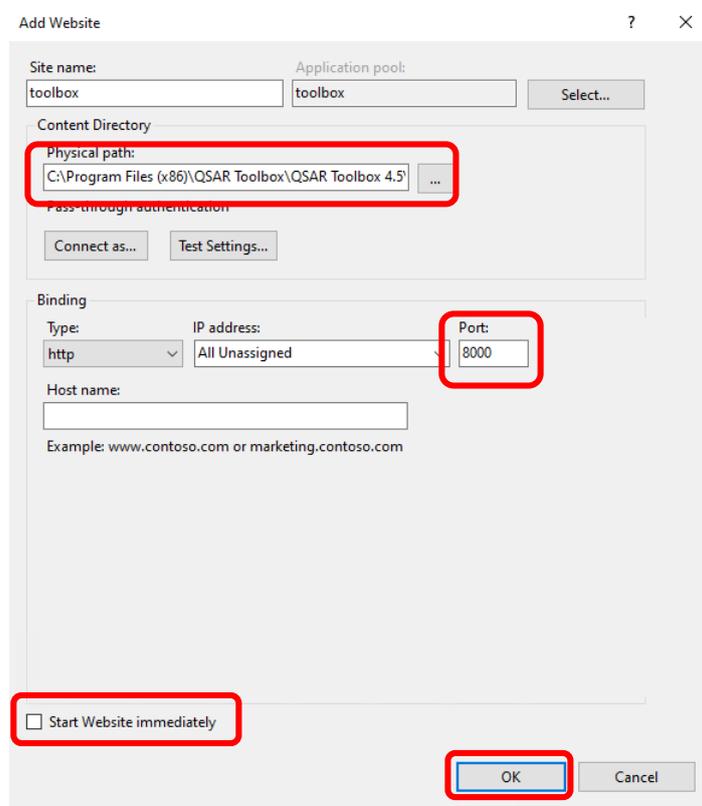
4. Deploying TBWSe in IIS

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

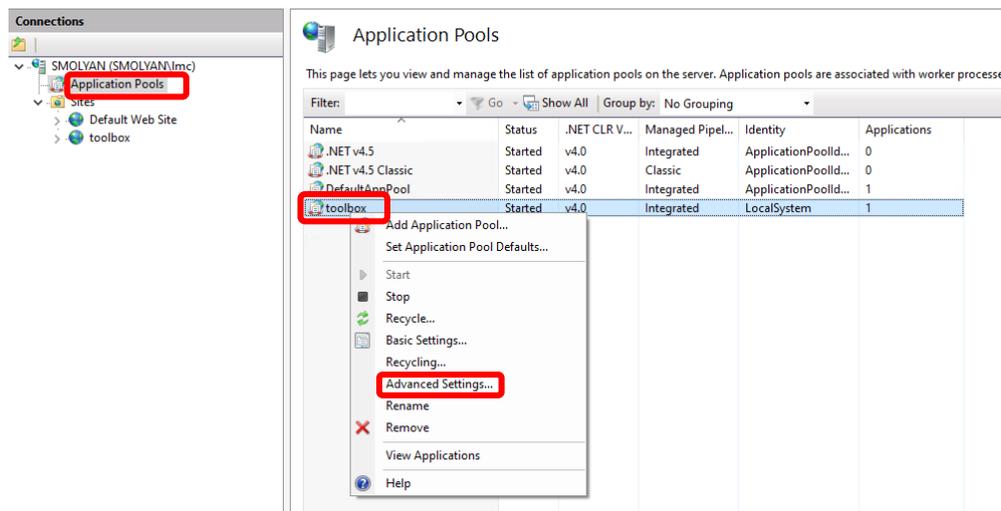


3. Enter a **Site name** of your choice, e.g. *toolbox*
4. By default, the website will be placed in an application pool with the same name. Nevertheless, check the value of the **Application Pool** as it is needed for step 8
5. Enter **Physical path**. This is the path to the directory where the Toolbox 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**

Deploying the Toolbox WebServices engine



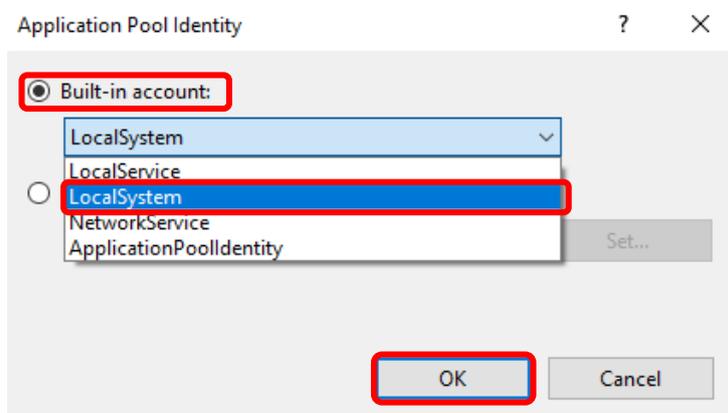
- Click on the Application Pools item under the root of your IIS Manager, locate the pool from step 4 (usually **toolbox**) and right click on it. From the context menu, choose **Advanced Settings...**



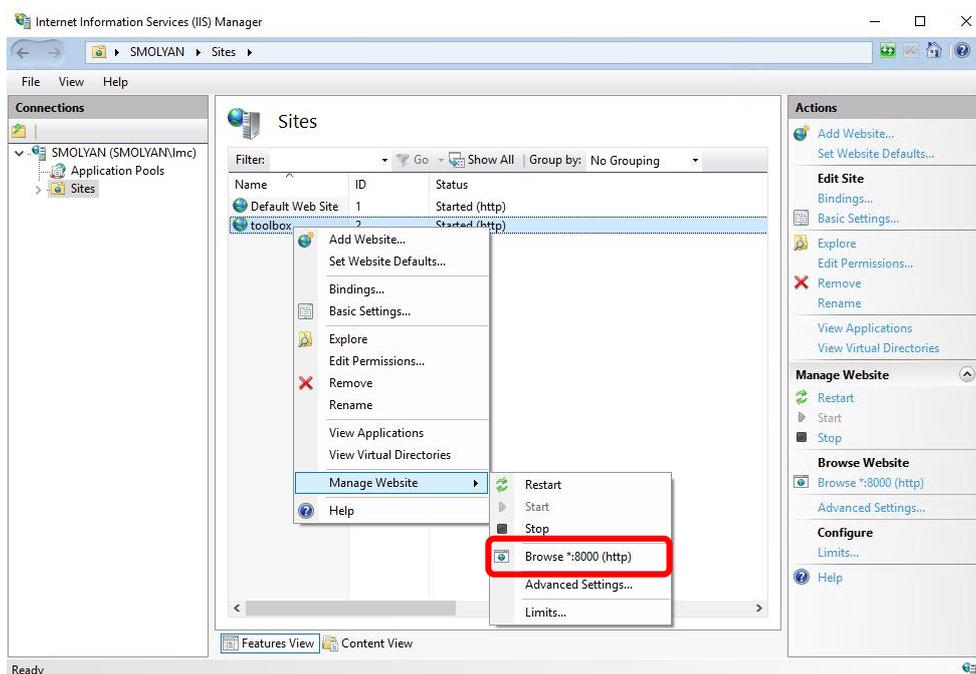
- Under **Process Model**, locate **Identity** and click on the button with the three dots on the right of it
- In the **Application Pool Identity** dialog, make sure the **Built-in account** option is selected. From the drop-down menu select **LocalSystem** and then click OK to close the dialog. Click **OK** again to close the **Advanced Settings** window.

Deploying the Toolbox WeBServices engine

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.

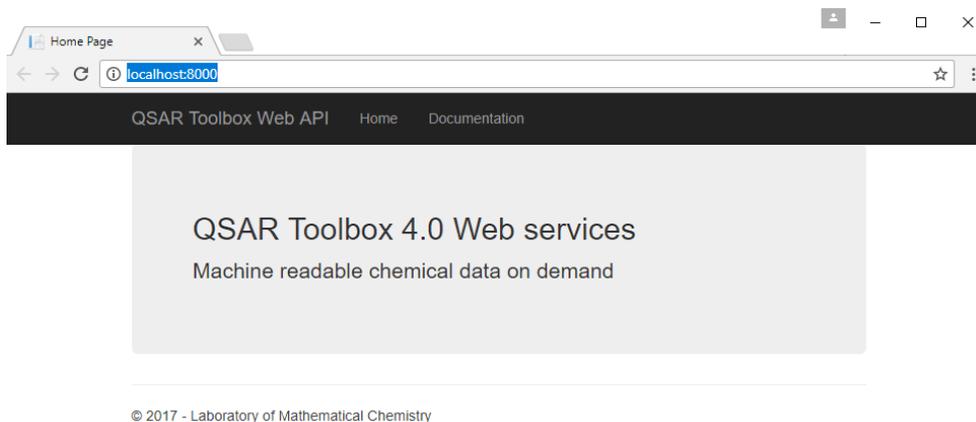


- Back under **Sites**, right-click on the newly created website, select **Manage Website** and then click on **Start**. Then right-click again and from the **Manage Website** menu click on **Browse *:8000 (http)** - this should load the TBWSe welcome page in your browser.



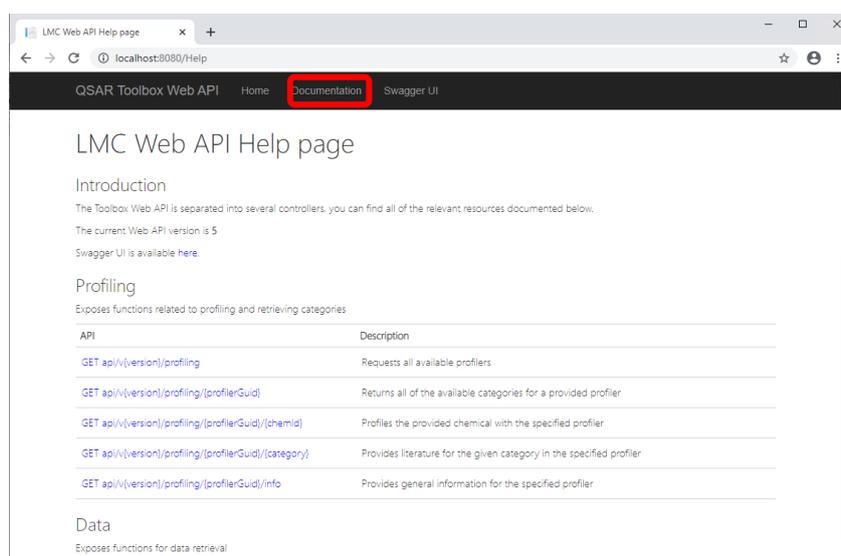
- Allow anywhere from 2 to 10 minutes for the TBWSe to load if this is the first start of the system.

Deploying the Toolbox WeServices engine



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](#).