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QSAR TOOLBOX

The OECD QSAR Toolbox
for Grouping Chemicals
into Categories

User manual

Deploying the Toolbox WebServices engine

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Document history

Version	Comment
Version 1.0	31/07/2017, first version

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

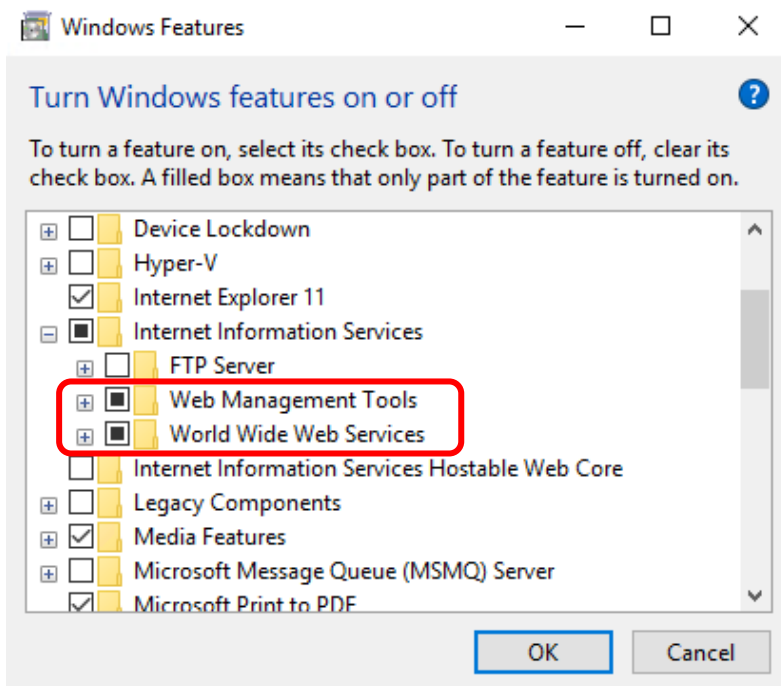
To deploy the WebServices engine, you would need:

- 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 WeServices engine

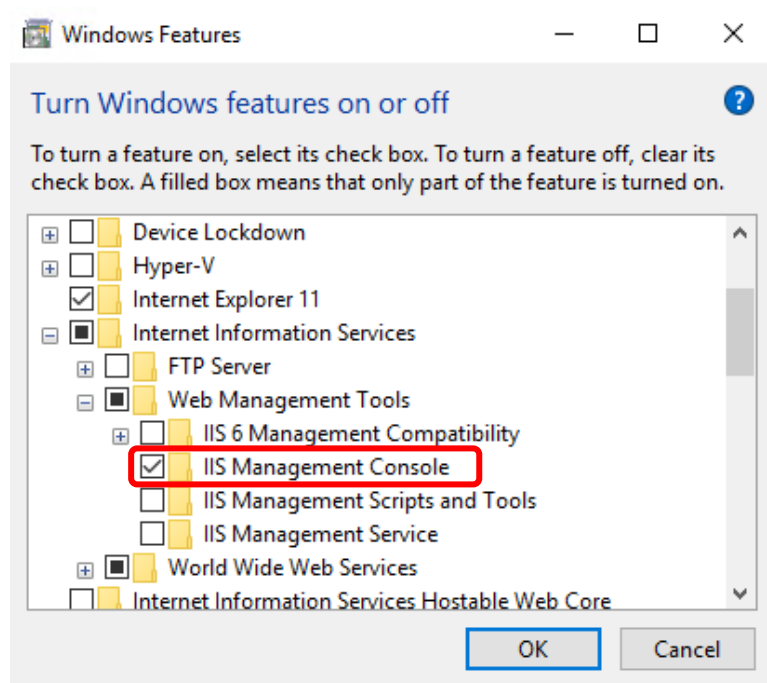
3. Enabling IIS Manager and related components (Windows 7, 8, 8.1, 10)

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**

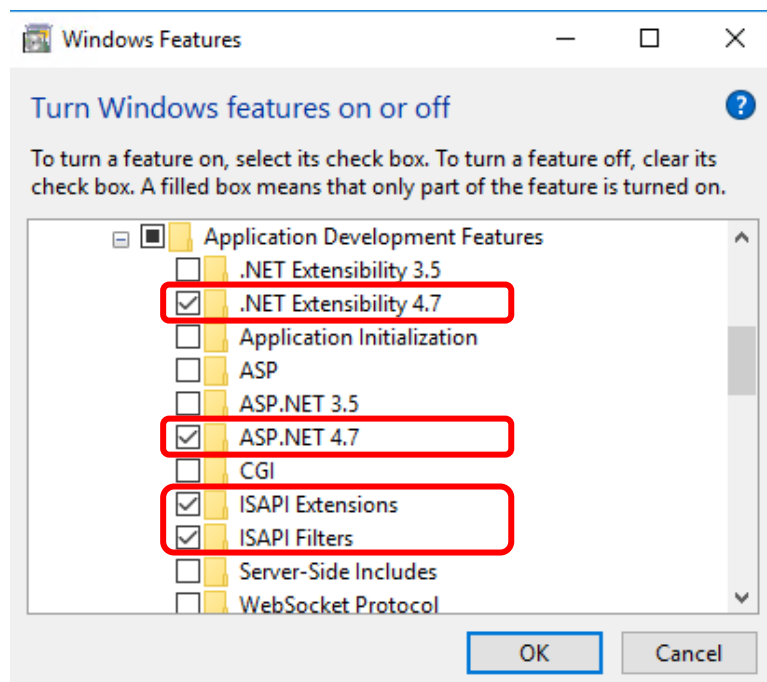


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- Expand **Web Management Tools** and make sure **IIS Management Console** is checked

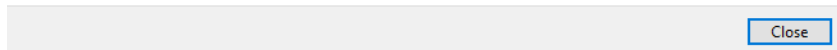
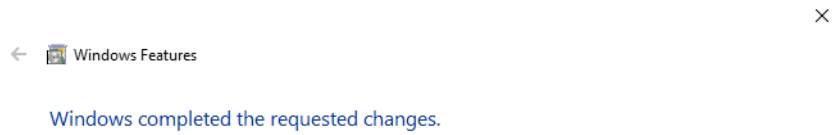


- Expand **World Wide Web Services**, then expand **Application Development Features** and make sure **.NET Extensibility 4.5** (or later), **ASP.NET 4.5** (or later), **ISAPI Extensions** and **ISAPI Filters** are all checked



Deploying the Toolbox WebServices engine

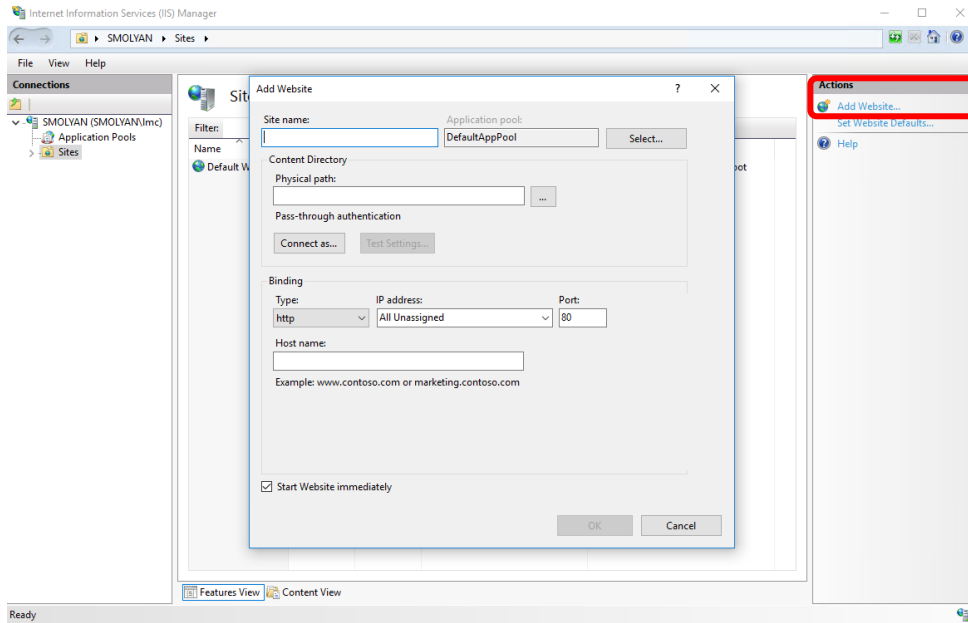
6. Click **OK**. Windows will then install the selected components. Once they are installed, click **Close**.



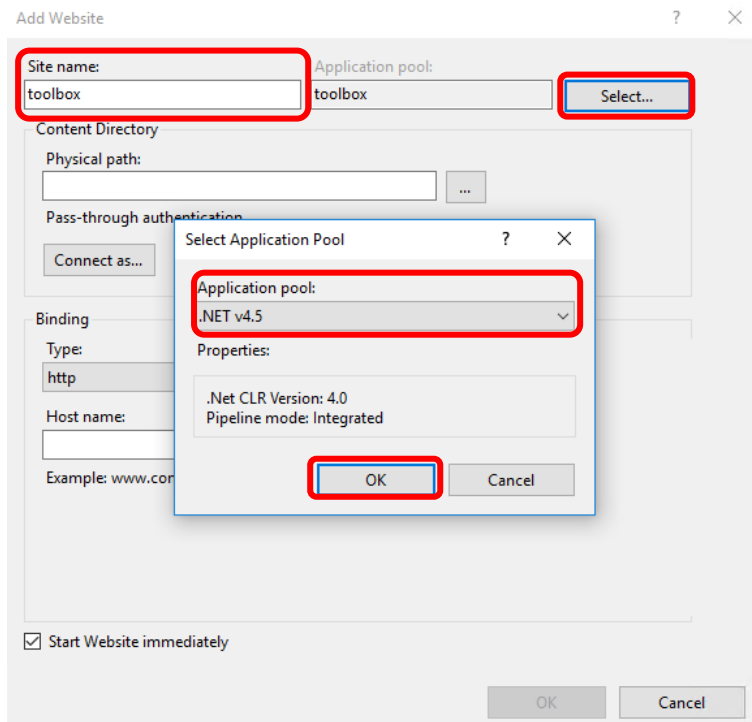
Deploying the Toolbox WebServices engine

4. Deploying TBWSe in IIS

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

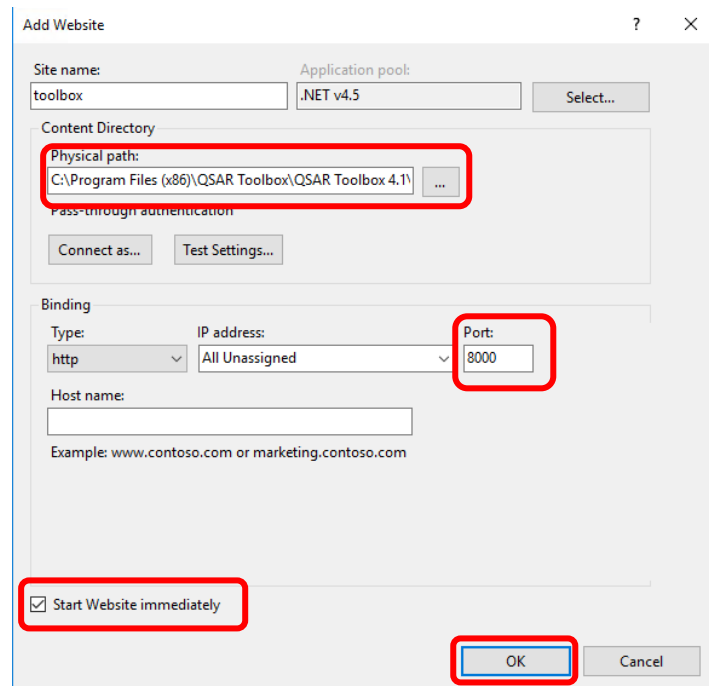


3. Enter a **Site name** of your choice, e.g. *toolbox*
4. Click the **Select...** button right of **Application Pool**, select **".NET v4.5"** from the **Select Application Pool** window and click **OK**



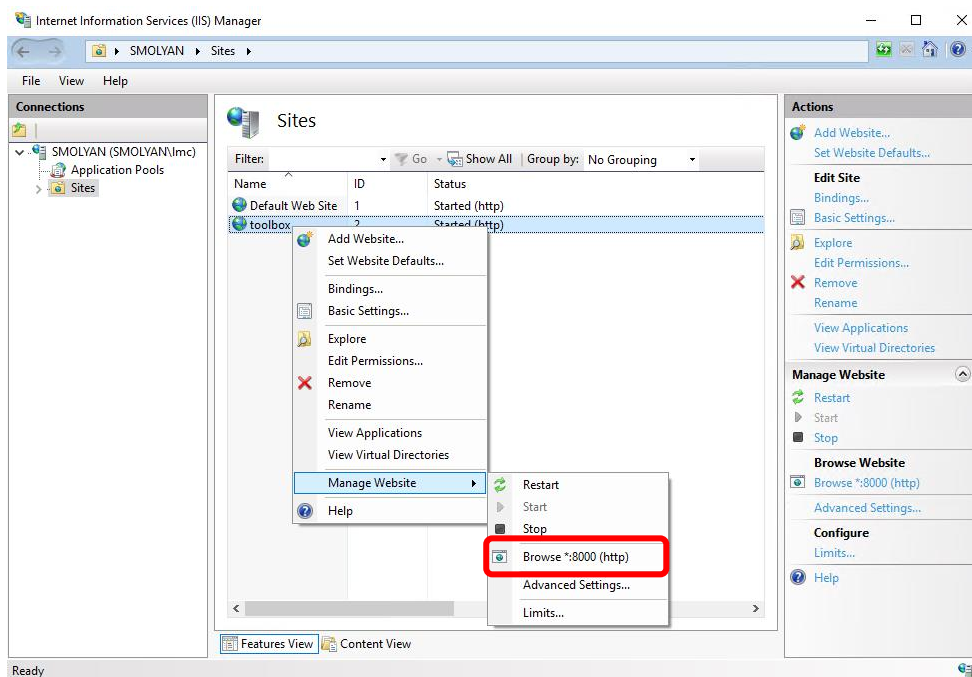
Deploying the Toolbox WebServices engine

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. Keep the **Start Website immediately** checkbox checked and click **OK**

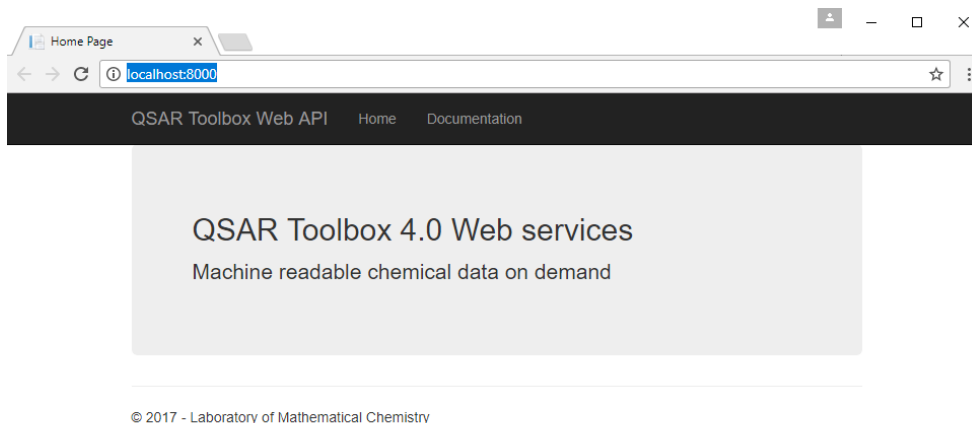


8. Right-click on the newly created website, select **Manage Website** and then click on **Browse *:8000 (http)** - this should load the TBWSe welcome page in your browser.

Deploying the Toolbox WeServices engine



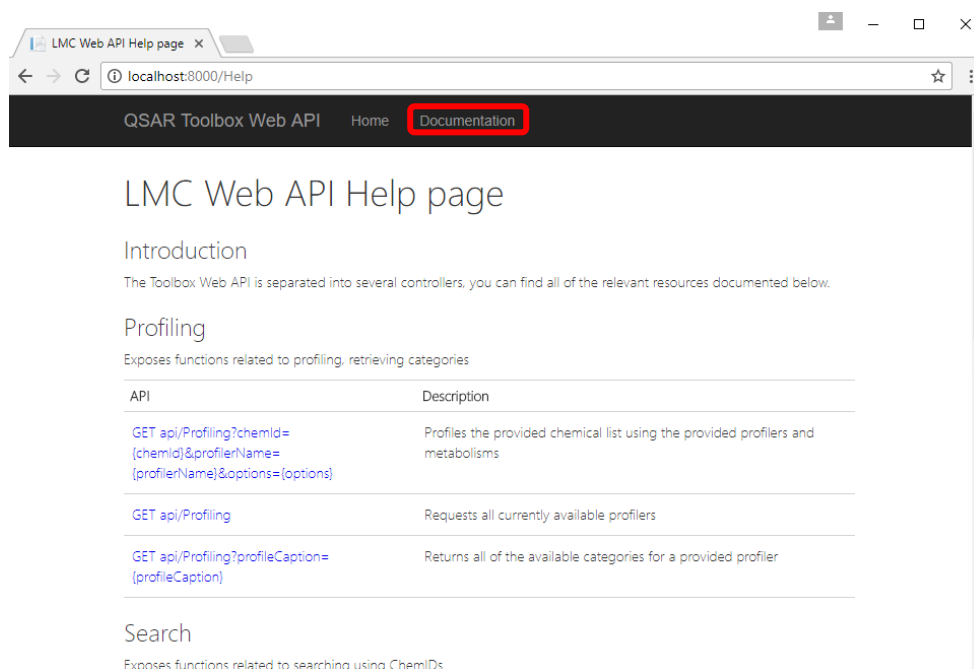
- Allow anywhere from 2 to 10 minutes for the TBWSe to load if this is the first start of the system.



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](#).