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>Deploying TBWSe in</i> <u><i>IIS</i></u> section)

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Deploying the Toolbox WebServices engine

1. Purpose

The Toolbox WebServies 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

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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

👿 Windows Features	_		×
Turn Windows features on or off			?
To turn a feature on, select its check box. To turn check box. A filled box means that only part of th	a feature (ne feature i	off, clear it is turned o	ts in.
💿 🗌 Device Lockdown			^
🕀 🗖 Hyper-V			
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Internet Information Services			
🕀 🗖 FTP Server			
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Internet Information Services Hostable	Web Core	2	
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🗉 🔲 Microsoft Message Queue (MSMQ) Se	rver		
Microsoft Print to PDF			Υ.
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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

Windows Feature	25		_		×
Turn Windows	features on or off				?
To turn a feature on, check box. A filled b	select its check box. To ox means that only part	turn of th	a feature o e feature i	off, clear s turned	its on.
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	.NET Extensibility 3.5				
	.NET Extensibility 4.7				
	Application Initialization	n			
	ASP				
	ASP.NET 3.5				
	ASP.NET 4.7				
	CGI				
	ISAPI Extensions				
	ISAPI Filters				
	Server-Side Includes				
	WebSocket Protocol				¥
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6. Click **OK**. Windows will then install the selected components. Once they are installed, click **Close**.

Windows Features
 Windows completed the requested changes.

Close

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4. Deploying TBWSe in IIS

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

→ SMOLYAN → Sites →		1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
e View Help encetions Application Pools Sites Default	Add Website ? × Site name: Application pool Content Directory. Physical path: Pass-through authentication Connect as Tet Settings. Binding Type: P address: Port: Http: All Unassigned v 80 Host name: Example: www.contoso.com or marketing.contoso.com Sate Vebsite immediately CK Cancel	Actions Set Website Set Website Defaults P Help

- 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. Nevertherless, check the value of the **Application Pool** as it is needed for step 8
- 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

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Add Website	?	×
Site name: Application pool: toolbox toolbox		
Content Directory		
Physical path: C:\Program Files (x86)\QSAR Toolbox\QSAR Toolbox 4.5)		
Connect as Test Settings		
Binding		
Type: IP address: Port:		
http 🗸 All Unassigned 🔪 8000		
Host name:		
Example: www.contoso.com or marketing.contoso.com		
Start Website immediately		
ОК	Cancel	

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...**

Connections	Application Pc This page lets you view and ma	DOIS mage the list of a	pplication pool	s on the server. App	plication pools are asso	ciated with worker pr	ocesses
 SMOLVAN (MOLVAN)(mc) Application Pools Ster Default Web Site toolbox 	This page lets you view and ma Filter: Name Name NIET v4.5 NIET v4.5 NIET v4.5 Classic DefaultAngPool Control Start Stop Recycle Basic Setting Advanced Settin Rename Remove View Applicatio	nage the list of a Comparison of the list of a Comparison of the list of the	pplication pool NET CLR V v4.0 v4.0 v4.0 v4.0	s on the server. App by: No Grouping Managed Pipel Integrated Classic Integrated Integrated	Identity ApplicationPoolld ApplicationPoolld ApplicationPoolld LocalSystem	ciated with worker pr Applications 0 0 1	ocesses
	Remove View Applicatio Help	ns					

- 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.

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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.

Арр	lication Pool Identity		?	×
۲	Built-in account:			
	LocalSystem	~		
~	LocalService		1	
0	LocalSystem			
	NetworkService ApplicationPoolIdentity		Set	
	C	Ж	Cancel	

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.

ile View Help				
SMOLYAN (SMOLYAN\Imc)	Sites	• 🚏 Go - 🕻	Show All Group by: No Grouping -	Actions Add Website Set Website Defaults
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	0 н	elp	Start Stop	Advanced Settings Configure
	<		Browse *:8000 (http) Advanced Settings Limits	Limits Help

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

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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

C (i) localhost:8080/Help		\$
QSAR Toolbox Web API Home Documen	Swagger UI	
LIVIC WED API Help pag	je	
Introduction		
The Toolbox Web API is separated into several controllers, y	ou can find all of the relevant resources documented below.	
The current Web API version is 5		
Swagger UI is available here.		
Profiling		
Exposes functions related to profiling and retrieving categor	ies	
API	Description	
GET api/v(version)/profiling	Requests all available profilers	
GET api/v{version}/profiling/{profilerGuid}	Returns all of the available categories for a provided profiler	
${\sf GET api/v{version}/profiling/{profilerGuid}/{chemld}}$	Profiles the provided chemical with the specified profiler	
GET api/v{version}/profiling/{profilerGuid}/{category}	Provides literature for the given category in the specified profiler	
GET api/v(version)/profiling/(profilerGuid)/info	Provides general information for the specified profiler	

6. Support

Support can be obtained via the <u>QSAR Toolbox Helpdesk</u>.

Version 1.1 Release date (June 2020)