Spectrum Mill Installation v7.11 onto a Windows 2016 Server

Contents

Compute Requirements:	1
Operating systems:	1
Partitions:	2
Processors: > 8 CPU, when counting cores keep in mind 2 CPU/core	2
RAM: >16 GB (>24 GB for no enzyme searches)	2
Storage: > 300 GB	2
Installation	2
In the Word version of this document, for all of the Blue headings clicking on the blue arrow at left will collapse/expand each section	2
Step 0. Uninstall prior version of Spectrum Mill, if present.	2
Step 1. Install Microsoft Internet Information Services (IIS)	4
Step 2. Install PERL – Strawberry Perl	4
Step 3. Install Java*	4
Step 4. Install Thermo Fisher API MSFileReader for use with .RAW files from Thermo Fisher Scientific instruments.	6
Step 5. Install Python	6
Step 6. Install R	8
Step 7. Install Spectrum Mill v7.0	9
Step 8. Install Public Javascript Libraries	9
Step 9. Configure security for Spectrum Mill Web Access	9
Step 10. Share and configure security for the data folder (msdataSM), the database folder (SeqDB), and the user s parameters folder (millauto)	aved
Step 11. Test drive	13
Step 12 Update SRM configuration to match CPUs on your VM	14
Step 13 Restore custom modifications and saved parameter sets from prior version of Spectrum Mill.	14
Troubleshooting	14
If the Select Data Directory button doesn't work:	14
If PERL does not work:	15
If you are prompted to download "faindex.cgi"	15
If you are denied permission to update the database list	15

Compute Requirements:

Operating systems:

- Windows Server 2016 (encouraged)
- Windows 10 (single-user environment)

Partitions:

Although one can configure a single C: drive, the following is recommended. A dedicated SM partition allows for greater flexibility in adjusting storage requirements as server usage grows.

C:\ for OS

D: \for Spectrum Mill

Processors:≥ 8 CPU, when counting cores keep in mind 2 CPU/coreRAM:≥16 GB (≥24 GB for no enzyme searches)Storage:≥ 300 GB

Rules of thumb:

- keep a 2:1 ratio of RAM:CPU for running tryptic peptide searches
- keep a 3:1 ratio of RAM:CPU for running no enzyme searches ie. Immunopeptidomics of HLA peptides

Practical Example - Broad Institute usage:

To support a lab of ~30 people we currently run 3 Spectrum Mill servers on virtual machines (VMs)

- 2 servers: 24 CPU, 48 GB, 300 GB RAM
- 1 server: 16 CPU, 48 GB, 300 GB RAM

We keep the storage purposely low and move data off of the SM servers within 2 weeks of processing. This is because the cost of high performance storage on our VMs is ~10x more than offline utility storage.

Installation

Copy/download the folder **SM_install onto** the Spectrum Mill server.

- SM_install
 - SetupScripts
 - ThermoAPI_MSFileReader_3.0_SP2
 - ThermoAPI_MSFileReader_3.1_SP4
 - SpectrumMill_7.11.216_31_win-x86_64.exe
 - InstallGuide_SMv7.11_Clauser_20220401.pdf
 - strawberry-perl-5.32.1.1-64bit.msi
 - jre-8u202-windows-x64.exe
 - jre-8u202-windows-i586.exe
 - R-4.1.0-win.exe
 - R-4.1_libs_for_SM.zip
 - Anaconda3-2019.10-Windows-x86_64.exe

While logged onto the desktop of the SM server as administrator, perform the following: If upgrading from v6.0 or v7.0, then steps 1 and 5 can be skipped.

In the Word version of this document, for all of the Blue headings clicking on the blue arrow at left will collapse/expand each section.

Step 0. Uninstall prior version of Spectrum Mill, if present.

- Stop the Spectrum Mill SRM service Click StartMenu > Windows Administrative Tools > Services For prior version < 6.0 Select Agilent Spectrum Mill Workflow, click stop For prior version > 7.0 Select Spectrum Mill Workflow, click stop
- Make a backup copy of the prior version.
 From the folder /SpectrumMill/ copy all but the following directories to a backup location called /SpectrumMillprior, to serve as a backup
 - a. msdataSM

- 3. For extra backup protection rename the following two directories.
 - a. /SpectrumMill/msdataSM to /SpectrumMill/msdataSMold
 - b. /SeqDB to /SeqDBold
- 4. Uninstall the prior version.
 - a. Click Settings > Apps & Features
 - b. Scroll down and select Spectrum Mill, click Uninstall as shown below.
 - c. Select Remove and click next as shown further below.

← Settings		- 0	×
යි Home	Apps & features		
Find a setting	Snip & Sketch Microsoft Corporation	8.00 KB 11/14/2019	
Apps	Spectrum Mill Proteomics Workbench B.07.01	75.4 MB	
IΞ Apps & features	7.01.0000	2) 1/2020	
⊒+ Default apps	Modify	Uninstall	
때 Offline maps	Sticky Notes Microsoft Corporation	16.0 KB 3/7/2020	
Apps for websites	Strawberry Perl (64-bit)	533 MB	
D Video playback	Thermo Foundation 3.1	2,12/2020	
☐ Startup	Theres FreeChile 11	1/31/2020	



 In the Spectrum Mill directory after uninstalling the following should remain afterward. msdataSM/* (user data) millsrm/*.log millbin/*.tlb (API for Agilent Extractor) results_msedman The following are also expected to be retained if the user created custom modifications, saved correction factors, saved parameter sets, and sequence database with the prior version: msparams_mill/smconfig.custom.xml msparams_mill/reporterIon.corrections.txt millauto/* /SeqDB/*

Step 1. Install Microsoft Internet Information Services (IIS)

- 1. From the folder **SM_install/SetupScripts** right-click the file **DISM-IIS.bat**, and then select **Run as Administrator**. This step can take several minutes.
- 2. After installation, review the results, then close the window.
- 3. From an Internet browser, go to http://localhost to verify that the IIS is properly installed. The IIS welcome screen appears if properly installed.

Step 2. Install PERL – Strawberry Perl

- 1. From the folder SM_install, double-click the file strawberry-perl-5.32.1.1-64bit.msi.
- 2. Follow the instructions to install PERL to the default location of **C:\Strawberry**. Continue to click **Next** or **Install** until the installation is done.
- 3. Install two additional Perl packages from the public repository CPAN:
 - Win32::Shortcut.pm
 - Math:MatrixReal.pm

These are used to calculate iTRAQ/TMT ratios with isotopic correction, using SM's afRICA correction method.

- a. Click StartMenu >Strawberry Perl> CPAN Client
- **b.** Enter and execute two separate commands at the prompt: **cpan>**
 - (Copy each command below and paste by right clicking in the client window)
 - i. cpan> install Win32::Shortcut.pm
 - ii. cpan> install Math:MatrixReal.pm
- c. When successfully completed, 2 files will have been installed at:
 - i. C:\Strawberry\perl\site\lib\Win32\Shortcut.pm
 - ii. C:\Strawberry\perl\site\lib\Math\MatrixReal.pm
- Note: SM > v 7.0 The version of Perl in use for SM is configured via the following line now present in the file SpectrumMill/web.config
 - <add name="Perl-CGI" path="*.pl" verb="*" modules="CgiModule" scriptProcessor="C:\Strawberry\perl\bin\perl.exe "%s" %s" resourceType="File" requireAccess="Script" responseBufferLimit="0" />
 - For SM < v7.0 one had to instead configure IIS to run PERL scripts. From the folder SM_6.0_install/IIS Setup Scripts), right-click the file Perl64IIS.bat, and then select Run as Administrator.

Step 3. Install Java*

When using Spectrum Mill, the only modules which require JAVA are the Sherenga *de novo* sequencing program and the Spectrum Viewer applet (which also inconveniently requires client-side Internet Explorer installed on users computers). If you do not anticipate using those modules, you can proceed without installing JAVA.

- 1. If an older version of Java is installed, remove the program. If older 32-bit and 64-bit versions are installed, remove them both.
- 2. From the folder **SM_install**, right-click the file jre-8u202-windows-x64.exe, and then select **Run as Administrator**.
- 3. Follow the instructions to install the Java Runtime Environment to the default location. If you are warned that a newer version of Java is available, continue anyway. Upon completion, the Java installer will open the browser to verify the Java version. Note that on Windows 10 this step runs the Microsoft Edge browser, which does not support add-ons. Simply close the browser and continue.
- 4. Repeat steps 2-3 with jre-8u202-windows-i586.exe. When encountering the screen below, click **Not Now** and/or consult below, *Notes on JAVA licensing, and consider consulting IT support within your organization for JAVA licensing status.

ava Setup - Uninstall out-of-date versions -	_		×
Java GRACLE			
Out-of-Date Java versions Detected			
Keeping out-of-date Java versions installed on your system may present a security risk.			
✓ Java 8 Update 202 (64-bit)			~
Click "Uninstall" to uninstall the selected Java versions. Warning: Uninstalling out-of-date versions of Java may cause some older Java applications to no longer r information	un. <u>M</u>	<u>ore</u>	
Not Now	Ur	ninstall	>

If you are updating from a different version of JAVA:

- 1. Click Start > Control Panel > Programs > Java. (For Windows 10, click the Control Panel icon , then click Programs, then click Java.)
- 2. In the Java Control Panel, click the Java tab, then click View.
- 3. In the Java Runtime Environment Settings dialog box, make sure that the version that you just installed is enabled.
- 4. Simplest is to install both 32-bit and 64-bit on the SM server.
- 5. IE-defaults to running in 32-bit mode, so client computers should have at least 32-bit.

*Notes on JAVA licensing:

https://www.oracle.com/java/technologies/javase-jre8-downloads.html

Since the java 8 update at April 16, 2019 8u221, all versions and updates for (java 8,9,10,11,14) has no cost for personal use and development purposes. Any other use, needs a Commercial License. Since Spectrum Mill is distributed **without** any accompanying commercial sublicense for Java, we provide the last so called "free" version from January 15, 2019.

Java SE Runtime Environment 8u202: <u>https://www.oracle.com/java/technologies/javase/javase8-archive-downloads.html</u>

Spectrum Mill server administrators are expected to be accountable for their own licensing compliance with subsequent JAVA updates from Oracle.

Step 4. Install Thermo Fisher API MSFileReader for use with .RAW files from Thermo Fisher Scientific instruments.

If you intend to use Spectrum Mill only with data generated on Agilent instruments you may skip this step.

- 1. From the folder SM_install\ThermoAPI_MSFileReader_3.0_SP2\MSFileReader_x86_x64 right-click the file MSFileReader_x86_x64.exe*, and then select Run as Administrator.
- Follow the instructions to install MSFileReader to the default location of C:\Program
 Files\Thermo\MSFileReader along with Microsoft redistributable libraries suggested by the installer. Continue
 to click Next or Install until the installation is done.
- 3. From the folder SM_install\ThermoAPI_MSFileReader_3.1_SP4 right-click the file MSFileReader_x64.exe*, and then select Run as Administrator.
- 4. Without uninstalling v3.0 SP2, follow the instructions to install the 64-bit version **MSFileReader** to the default location of **C:\Program Files\Thermo\MSFileReader** along with Microsoft redistributable libraries suggested by the installer. Continue to click **Next** or **Install** until the installation is done.

*Note: The above installer programs were created by Thermo Fisher Scientific and were downloaded from: <u>https://thermo.flexnetoperations.com/control/thmo/login?</u>

by Karl Clauser, and 3.1 SP4 was verified to be the most recent version as of 3/1/2021. The SM Thermo Data Extractor program v7.07.213 and beyond was compiled using the MSFileReader 3.1 SP4 DLL: XRawfile2_x64.dll.

As one progresses thru the above steps the following files will be installed.

C:\Program Files\Thermo\MSFileReader	after 3.0 SP2 install	after 3.1 SP4 install
Fileio_x64.dll	8/8/2014	1/17/2017
fregistry_x64.dll	8/8/2014	8/8/2014
XRawfile2_x64.dll	8/8/2014	1/17/2017

The Spectrum Mill Thermo Data Extractor will not work if fregistry_x64.dll is absent. It will be absent if you install only 3.1 SP4, or inadvertently uninstall 3.0 SP2 while installing 3.1 SP4.

Step 5. Install Python

- 1. From the folder SM_install, right-click the file Anaconda3-2019.10-Windows-x86_64.exe, and then click Run as Administrator.
 - a. Choose Install for All user (not Just Me)
 - b. When reaching this screen. Check both boxes despite the scary warning. Click Install.

O Anaconda3 2019.10 (64-	bit) Setup			\times	
	Advanced Installation Options Customize how Anaconda integrates	s with Windows			
Advanced Options					
🗹 Add Anaconda to	my PATH environment variable				
Not recommended. I menu and select "An Anaconda get found cause problems requ	nstead, open Anaconda with the Windo aconda (64-bit)". This "add to PATH" op before previously installed software, b iring you to uninstall and reinstall Anaco ta as my default Python 3.7	ows Start otion makes out may onda.			
This will allow other programs, such as Python Tools for Visual Studio PyCharm, Wing IDE, PyDev, and MSI binary packages, to automatically detect Anaconda as the primary Python 3.7 on the system.					
Anaconda, Inc. ————	< Back	Install	Canc	el	

- 2. Restart the VM to make the path available to IIS and the SM applications.
- Note: Python is properly run directly from SM webpages because of the following line in the file spectrumMill/web.config

<add name="Python 3.7" path="*.py" verb="*" modules="CgiModule" scriptProcessor="C:\ProgramData\Anaconda3\python.exe %s %s" resourceType="File" />

However, some SM Python scripts are started by Perl scripts, which is like running Python from the command line. Checking the scary checkbox above automatically takes care of what is described below, and thus enables running Python from the command line without having t manually execute these steps.

Manually enabling command-line Python

Add the 4 Anaconda lines shown below to the PATH environment variable (for the system, not the user) on the VM, from the System control panel.

- Detailed instructions:
 - Click StartMenu > Control Panel > System > Advanced system settings
 - On the Advanced tab click the Environment Variables button. In the lower system variables pane (not the upper user pane) select Path and click Edit. Click the new button, and add the above line.
 - Move the Python lines to above the existing Perl lines.

Edit environment variable	×
C:\ProgramData\Anaconda3	New
C:\ProgramData\Anaconda3\Library\mingw-w64\bin	
C:\ProgramData\Anaconda3\Library\usr\bin	Edit
C:\ProgramData\Anaconda3\Library\bin	Luit
C:\ProgramData\Anaconda3\Scripts	
C:\Program Files (x86)\Common Files\Oracle\Java\javapath	Browse
%SystemRoot%\system32	
%SystemRoot%	Delete
%SystemRoot%\System32\Wbem	
%SYSTEMROOT%\System32\WindowsPowerShell\v1.0\	
C:\Strawberry\c\bin	Move Up
C:\Strawberry\perl\site\bin	
C:\Strawberry\perl\bin	Move Down
C:\Program Files\R\R-3.6.2\bin\x64\	MOVE DOWN
	Edit text
OK	Cancel
- OK	Curreer

o Click OK on each of the several open menus to exit.

Step 6. Install R

Sorry folks this step is a real nuisance. I haven't yet had the perseverance to automate it.

- 1. Uninstall prior version of R if present. See Step 0 for how to uninstall a windows application.
- 2. From the folder **SM_install**, right-click the file **R-4.1.0-win.exe**, and then click **Run as Administrator**.
- 3. Install external public R packages used in SpectrumMill

Unzip the file SM_install/R-4.1_libs_for_SM.zip

From the folder SM_install/R-4.1_libs_for_SM copy all the packages to the folder

C:\Program Files\R\R-4.1.0\library

Notes:

On first execution the scripts themselves would download the necessary external packages automatically if the username which controls the webserver (IUSR) had write permission to the directory. Since that would be an unwise security practice, we do it the above way. If the libraries were not provided (or one sought to later upgrade R and install updated versions of the packages), one could instead open RGui from the start menu (right-click to run as administrator). Then, under the file menu select source R code. Sourcing the following two scripts would install all the external R packages currently in use.

SpectrumMill\millR\plotRatioDistributions.r SpectrumMill\millR\plotBoxDeNovoMetrics.r SpectrumMill\millR\normalizeReporterRatios.r

Alternatively, one could also do the following: To the file: C:\Program Files\R\R-4.1.0\library\base\R\Rprofile Add the following lines to the end of the file. myPaths <- c('D:/SpectrumMill/millr/R/R-4.1_libs_for_SM') .libPaths(myPaths) Then copy the R packages there. Add the following line to the PATH environment variable (for the system, not the user) on the VM, from the System control panel.

C:\Program Files\R\R-4.1.0\bin\x64\

Detailed instructions:

Click StartMenu > Control Panel > System > Advanced system settings

On the Advanced tab click the Environment Variables button. In the lower system variables pane (not the upper user pane) select Path and click Edit. Click the New button, and add the above line. Move the line to above the existing Perl lines. Click OK on each of the several open menus to exit.

5. Restart the VM to make the path available to IIS and the SM applications.

Step 7. Install Spectrum Mill v7.0

- 1. From the folder SM_install, double-click the file SpectrumMill_7.09.215_28_win-x86_64.exe.
- 2. If you are asked to install .NET 2.0, click No.
- 3. If the .NET 4.51 Installation panel appears, click **Install**, accept the agreement, and click **Next** in each screen to accept default values until .NET 4.51 is installed. After the system reboots, the installation continues.
- 4. In the welcome screen, click **Next**.
- 5. If you get a message that says you have an unsupported version of PERL, then remove PERL from your system and install it according to the instructions in "Step 2. Install PERL".
- 6. If you get a message that says you have only a 32-bit version of JAVA, continue anyway.
- 7. If your server does not have the recommended disk volume configuration, then you will be warned. Click **Yes** to continue, or click **No** to partition your drive volumes to the recommended configuration. For details, see the *Spectrum Mill Getting Started Guide*,

https://proteomics.broadinstitute.org/millhtml/SM_instruct/SpectrumMillQuickStartGuide.pdf.

- Skip OR Carefully read the License Agreement, particularly the "Confidentiality Terms and Conditions" section.
 a. If you accept the terms, click **Yes** to continue.
- 9. On the Spectrum Mill Software and MS Data Files Location page, click the drive with the most amount of disk space, then click **Next**.
 - a. The Spectrum Mill software and data must reside on the same partition. The installation program defaults to the largest partition because data requires the most space for storage. You do not see this page of installation if you have only one partition.
- 10. On the Protein Sequence Database Location page, either:
 - a. Click the same drive as Spectrum Mill Software and MS Data Files or click the drive with the second most amount of space available, then click **Next**.
 - b. If the disk has 2 or more partitions, avoid the use of C: for SeqDB.
 - c. Depending on your requirements, the disk space required for your databases can grow to a range of 50 to more than 100 GB.

Step 8. Install Public Javascript Libraries

1. Copy the folder SM_install\JavascriptLibsPublic to the SM server \SpectrumMill\JavascriptLibsPublic.

Step 9. Configure security for Spectrum Mill Web Access

By default, Spectrum Mill configures IIS for Anonymous access. The Internet guest account (IUSR) has all the appropriate permissions to access Spectrum Mill.

Do this step only if Integrated Windows Authentication is required by your organization.

- 1. Open an elevated command window. (run as administrator)
- $2. \quad Go \ to \ the \ \ Spectrum Mill\ \ milladmin \ folder.$
- 3. For each user who needs access:
 - Run smSetPermissions.pl.

- Run smSetmsdataSMPermissions.pl.
- 4. Read the comments inside of these script files for details. Contact your IT department to assist in the proper configuration of security.
- 5. Close the command window.

These scripts can be customized. See the **readme.txt** file in the **\SpectrumMill\milladmin** folder for additional information.

With Integrated Window Authentication, a logon is required to access the

Spectrum Mill site. You can set Windows file and directory access permissions for directories under **SpectrumMill\msdataSM** so that access to data is restricted for only those users and groups that have read and write

permissions. Set the permission on a directory and all of its subdirectories, with the msdataSM directory accessible by all users. For more information on configuring security on the Microsoft Internet Information Services (IIS), refer to http://www.iis.net.

Step 10. Share and configure security for the data folder (msdataSM), the database folder (SeqDB), and the user saved parameters folder (millauto)

You must share the folder **msdataSM** so that data files can be copied to the SM server for processing. You can share the folder **SeqDB** if you want users to be able to update the sequence databases on the server from a different computer. You can share the folder **millauto** if you want users to be able to delete saved parameter files on the server or move them between multiple SM servers.

If you are upgrading from a prior version of Spectrum Mill and left these 3 directories in place prior to uninstalling you should be able to skip this step. If you moved or renamed them before uninstalling, then go to step 13 before continuing with this step.

CAUTION

You must use the Computer Management console to share the **msdataSM**, **SeqDB**, and **millauto** folders. If you share them in any other way, permission settings for Spectrum Mill files will be set incorrectly.

Windows 10 and Windows Server 2016

- 1. Log in as an administrator.
- 2. Click StartMenu > Windows Administrative Tools > Computer Management
- 3. In the navigation pane, expand **Shared Folders**.

*			Computer	Management		_ _ X
File Action View Help						
🗢 🏟 🙇 🔜 🙆 🚺	FT 🛐					
🜆 Computer Management (Local	Share Name	Folder Path	Туре	# Client Connections	Description	Actions
⊿ System Tools		C:\Windows	Windows	0	Remote Admin	Shares
I ask Scheduler Event Viewer	gga CS	C:/	Windows	0	Default share	More Actions
⊿ 🙀 Shared Folders	IST ES	D:\	Windows	0	Default share	
🔬 Shares	2 IPCS	E:\	Windows	0	Remote IPC	
8 Sessions	Gau					
Open Files						
Performance						
🚔 Device Manager						
⊿ 🔄 Storage						
Windows Server Backup Disk Management						
Services and Applications						
- Andrew Statistics						
< III >						
l,						

- 4. Right-click Shares, and then click New Shares.
- 5. In the Welcome to the Create a Shared Folder Wizard page, click Next.
- 6. In the Folder Path page, click Browse, locate and select SpectrumMill\msdataSM, and then click Next.
- 7. In the Name, Descriptions, and Settings page, click Change.
- 8. In the Offline Settings page, select No files or programs from the shared folder are available offline.



9. Click OK, then click Next.

10. In the Shared Folder Permissions page, select the kind of permissions that you want for the shared folder.

- a. To customize settings for your organization, click **Customize permissions**.
- b. See your system administrator or the Windows Help for more information.

At the Broad Institute we customize to simply allow full permissions for the user group in which all Spectrum Mill users have an institutional login:

Charles\proteomics

See the permissions and select users screenshots below for steps 12 c-f.

- 11. Click Finish. Repeat steps 4-10 for SeqDB and millauto
- 12. To enable users to delete files from the **msdataSM**, **SeqDB**, **and millauto** directories, you must also configure Security for the user group. The Computer Management window shown in step 3 that should now have 3 additional items for **msdataSM**, **SeqDB**, **and millauto**. Follow steps a-f below for each of the 3 shares.
 - a. Right-click on the share name and choose properties.
 - b. Go the security tab and click edit. (see screenshots below)
 - c. In the Permissions window, Click add. (see screenshots below)
 - d. In the Select Users Window, enter the object name of the desired user group (see screenshots below) Click Check Names, and Click Ok.
 - e. In the Permissions window, Click Full Control allow to set the Permission and Click Apply. Click OK.
 - f. In the Properties window Click Ok.

퉣 shiva - Remote Desktop Connectio	'n							_		×
Re File Action View Help										^
🗢 🔿 🔂 🔂 🔂	?					Permissions for msdataSM			×	
 Computer Management (Local Vissem Tools Task Scheduler Intervent Viewer Shared Folders Shares Sessions Open Files Noral Users and Groups 	Share Name Share	Folder Path C:\Windows C:\ D:\ D:\SpectrumMill\ D:\SeqDB	Type Windows Windows Windows Windows Windows	# Client Connec 0 0 1 0 2 2 2	ctions	Security Object name: D:\SpectrumMi Group or user names: CREATOR OWNER St IUSR St SYSTEM St Administrators (SHIVA) Adm	II\msdataSM			
M > N Performance	General Publi	sh Share Permissions	Security		`	Users (SHIVA\Users)	in instructors y			
 Storage Windows Server Backup Disk Management Services and Applications 	Object name: Group or user CREATC CREATC CREATC CREATC CREATC CREATC	D:\SpectrumMill\msda names: JR OWNER 1 ators (SHIVA\Administrat missions click Fritt	ors)	* *		Permissions for CREATOR OWNER Full control Modify Read & execute List folder contents	Add Allow	Remove Deny		
	Permissions fo	or CREATOR OWNER	Allow	Edit	Select	Read	ints, or Groups		/	×
	Modify Read & exe List folder o Read	ontents		v	Select Users From ti	t this object type: s, Groups, or Built-in security principals this location:	3	<u>0</u>	bject Types.	
	For special pe Advanced.	missions or advanced se	ttings, click	Advanced	Enter t	ı.mir.eau the object names to select (<u>examples</u> <u>omics]</u>):		Locations heck Names	s
< >		ОК	Cance	Apply	Ad	lvanced		OK	Cancel	
<										>:

Step 11. Test drive

If the server name has been added to your institutional Domain Name Service (DNS) database: point your browser to your server's SM home page. The following are representative examples:

http://shiva/millhome.htm

If not, type ipconfig at a dos prompt on the server, then use the IP address.

http://192.168.196.42/millhome.htm



Or, Double-click the Spectrum Mill Home icon on the SM server's desktop.

- 1. Check that the server, PERL, and CGI.pm are working:
 - a. Open the site <u>http://yourcomputer.yourdomain/millhtml/hello.htm</u> with your browser.
 - b. Click Print PERL is working.
 - c. If PERL is working correctly, you will see these statements:
 - Hello World.

If you can see this PERL is working.

If you can see this CGI.pm is working.

- d. If you get a message that PERL is not working, see "If PERL does not work" in the Troubleshooting section below.
- 2. If you wish to configure a different default instrument other than ESI-QEXACTIVE-HCD-v4-30-20:
 - a. Open the file D:\SpectrumMill\ millhtml\SM_js\smCustomFlags.js with a text editor, such as Notepad.

- b. Replace the value for **defaultInstrument** with the appropriate instrument variable, such as ESI-QTOF-AGILENT.
- Try your own dataset or benchmark against the SM developers by downloading Example Data and Sequence Databases. Choose a dataset from the SpectrumMill_releases/ExampleData directory on the Cloud Platform SM was obtained from, download, and consult the SM Quick Start Guide:

https://proteomics.broadinstitute.org/millhtml/SM_instruct/SpectrumMillQuickStartGuide.pdf

- a. ExampleData\Thermo\Exploris480_JurkatQC
- b. ExampleData\Agilent\QTOF6550_Hela120

Step 12 Update SRM configuration to match CPUs on your VM

- 1. The Spectrum Mill installer sets the value of maxConcurrentTask to be 1 less than the number of logical processors your VM is configured with. If you change the number of CPUs allocated to your server after you run the Spectrum Mill installer then you will need to edit the configuration file for the Spectrum Mill service request manager (SRM) service in order to use all CPUs. Update the SRM configuration to match the number of processors on your server. Edit the file SpectrumMill/millsrm/SMSRM.Config. For example: change the value of maxConcurrentTask="7" to be 1 less than the number of logical processors your VM is configured with. This should be revised anytime you change the number of processors allocated to the VM.
- 2. Restart the service, Spectrum Mill workflow service request manager.
 - a. Click StartMenu > Windows Administrative Tools > Services
 - b. Select Spectrum Mill Workflow, click restart.
 - c. This step re-initiates the SRM using the SpectrumMill/SMSRM.Config.

Step 13 Restore custom modifications and saved parameter sets from prior version of Spectrum Mill.

Uninstalling a prior version of SM followed by installation of a new version of SM is expected to retain user created custom modifications, saved parameter sets, and sequence databases from the prior version. If there was a problem, now is the time to reverse the backup steps undertaken in Step 0 above. Replace the following with the backup copies made before uninstalling.

- 1. Copy from /SpectrumMillprior to /SpectrumMill:
 - a. msparams_mill/smconfig.custom.xml
 - b. millauto/*
 - c. /SeqDB/*
- 2. If you undertook the extra backup protection step 0.3 reverse it now.

In order to preserve the permissions and sharing status on your original directories, delete the empty installer created directories, msdataSM and SeqDB, then rename your backups as shown below

- a. /SpectrumMill/msdataSMold to /SpectrumMill/msdataSM
- b. /SeqDBold to /SeqDB
- 3. If there are problems with permissions and sharing status on these directories revisit step 9.

Troubleshooting

This section describes some possible problems that you might encounter when installing Spectrum Mill. Refer also to the online help for additional troubleshooting information. See "Tips and Tricks" at http://your_server/millhtml/SM_instruct/tips.htm#IIS

If the Select Data Directory button doesn't work:

- Check that PERL is working correctly.
 - See "If PERL does not work"

- Check that all data files are under subfolders of msdataSM.
 - If Spectrum Mill finds data files in the msdataSM folder or in folders above that level, it will stop looking for data files and not find the ones that are under msdataSM.
- Check that security has been set up.

See "Step 9. Configure security for Spectrum Mill Web Access".

Check that cookies are enabled in your web browser.

If PERL does not work:

- Make sure that the IIS Perl mappings are correctly set:
 - See Note: under "Step2. Install PERL" for details.
- ✓ Make sure permissions are properly set for **millscripts** and **millbin**.
 - From the **SpectrumMill\milladmin** folder, as administrator, run these PERL scripts:
 - smConfigureIIS.bat
 - smSetPermissions.pl

If you are prompted to download "faindex.cgi"

See the second bullet under "If PERL does not work" about permissions.

If you are denied permission to update the database list

Check that the file spectrumMill\millhtm\sm_js\dbnames.js has Modify permissions for IUSR. See "Step 9. Configure security for Spectrum Mill Web Access".