



Byosphere[®] Automated Processor Guide

October 2025

5.11

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Introduction

The Protein Metrics Byosphere® Automated Processor is a server-based product which automatically generates analyses from MS files as they are written to source directories. When MS files are copied to designated source folders, workflows are generated in a designated directory and the MS files used in them are automatically uploaded to the Byosphere server and compressed to the proprietary *.pacq format. New workflows are then generated which use the server sample references and these workflows are then submitted to the server.

The product contains two parts:

- **Watchers** identify newly added or updated MS files and generates workflows based on provided templates, FASTA files and specialized instructions. Different Watchers can be used to create different kinds of workflows based on the kinds of MS files and their source directories.
- **Automation Service**, when in AutoProcess mode, identifies workflows created by the Watchers, uploads and compresses the MS files and submits equivalent workflows as analyses, using the server versions of the MS files. The same Automation Service, when in AutoUpload mode, serves as the Data Uploader, which is available with all Byosphere systems.

For more information about the Data Uploader, see **Byosphere 05 Data Uploader Guide.pdf**.

System Requirements

The minimum hardware/software requirements for the machine that will host the Data Uploader is listed below:

CPU	Memory	Storage	OS	Network
>= 2 cores	>= 16 GB	>= 100 GB	Windows Server 2022	>= 1 GB/s

The machine will require access to the file system with the files/folders to be uploaded.

Install the Automation Server Package

Ideally, the Automation Server should be installed in an environment that is independent from the Analysis Service so that they do not compete for the same resources.

1. Download the Automation Server installer to the local environment and run the installer.
2. On the local environment, run Byosphere to initialize the server URL in the configuration file and test the connection:
 - a) Run `\ProteinMetrics\PMI-Byosphere-Client\Base\PMI-Byosphere-Client.exe`
 - b) Choose **Server > Configure**, enter the Byosphere server URL, and click **OK**

Configure the Automation Server

Modify `appsettings.json` in the installed `PMIAutomationService` directory as follows:

Parameter, Req'd & Default value	Note
<i>Parameter:</i> Host <i>Required:</i> Yes	Byosphere Application Server IP address
<i>Parameter:</i> UseAPIToken <i>Required:</i> Yes, if using API Token	If true, set Windows Credential to use API token set on Application Server (see below). An API token is recommended for Byosphere v 4.1 and above.
<i>Parameter:</i> KeychainNameSpace <i>Default:</i> PmiAutomationCredentials	Must be consistent with the credentials set up using <code>PMI-Keychain-Manager.exe</code> in Windows Credential Store; see notes below
<i>Parameter:</i> LocalWorkingPath <i>Default:</i> <code>Environment.GetFolderPath(Environment.SpecialFolder.CommonApplicationData)\ProteinMetrics\AutomationServer</code>	Folder location to store temporary files generated and then deleted during uploads. The default value will be used if the customer value is not specified or accessible.
<i>Parameter:</i> ExecPath <i>Default:</i> <code>Environment.GetFolderPath(Environment.SpecialFolder.ProgramFiles)\ProteinMetrics\PMI-Byosphere-Client\Base</code>	The <code>console.exe</code> executable path from the Protein Metrics Byosphere Client software installation
<i>Parameter:</i> BaseDir <i>Required:</i> On prem only	This is a required parameter for OnPrem only. This is the NAS mount drive. This setting in Windows must match its counterpart in App Server's <code>base_dir</code> in Linux. Example: <code>"BaseDir": "C:"</code>
<i>Parameter:</i> AutomationConfigurationID	The value is the Automation configuration ID in the Admin Portal. This is a required parameter for Data Uploader and Auto Processor. It is not required for Watcher.

Parameter, Req'd & Default value	Note
<i>Parameter:</i> ProjectUploadFolderID <i>Required:</i> Yes <i>Default:</i> 0	ID of the Byosphere server destination folder for submitted analyses using the Automated Processor; The user specified by the API token must be a Super User to create a root-level folder (the default value ID=0), or have File Editor, Folder Editor and Viewer privileges for a specified Byosphere Web Client folder. For the Automated Processor, project files created by the analysis are uploaded to this folder tree. Output Folder and ProjectUploadFolderID can be the same folder. To find a folder's ID, see the Find Byosphere Upload Folder ID section below.
<i>Parameter:</i> AutomatedMode	This parameter is required for Watcher. To run the executable as a Watcher, set it as: <code>"AutomatedMode": "BuildWflw",</code> In this mode, samples, workflow templates and other inputs are used to generate workflows in the directory defined by the Output parameter (see the Configure the Watcher section below).

Parameter, Req'd & Default value	Note
<i>Parameter:</i> SearchPattern <i>Required:</i> Yes	Extensions of all files (including MS files) to be uploaded. all other file types will be ignored. If AutoProcess is true, only MS files will be uploaded.
<i>Parameter:</i> Comment	Optional text to save in the Comment field of the uploaded file version
<i>Parameter:</i> DeleteAfterUpload <i>Default:</i> false	If true, input file or directory will be deleted upon successful upload to save space. Only SearchPattern/MSFile matched files/folders are deleted.
<i>Parameter:</i> WriteLastScan <i>Default:</i> false	If true, last scan time will be auto-created / updated by the program and written to the configuration file. Note: when set to true, the LastScanTime line should be removed (along with the comma after "WriteLastScan": true) before restarting the service.
<i>Parameter:</i> LastScanTime <i>Required:</i> No	This this value is auto-created / updated by the last program run. If both Modified After and LastScanTime exist, later of the two values will be in use. Format is "yyyy-MM-dd HH:mm:ss" Example: "LastScanTime": "2021-06-01 19:58:56" (HH is a 24 hour clock)
<i>Parameter:</i> RollingWindowDelta	The unit is second. The Automation will check for new data using time stamp setup in Modified After or LastScanTime. However, sometimes NAS data is not immediately available for cloud instance to be picked up. The delta window makes the Modified After or LastScanTime more tolerant in such cases. If there is data with timestamp 12-20-22 11:50 AM, data will not be uploaded using "Modified After": "2022-12-20 12:30:00". Data will be uploaded using the following, given a 3600 second or 1 hour delta effectively checking the file against 12-20-22 11:30 AM. "RollingWindowDelta": 3600, "Modified After": "2022-12-20 12:30:00" If no value is specified, no delta window will be applied. Example: "RollingWindowDelta": 3600
<i>Parameter:</i> ApplyMetadataToExistingFile	When ApplyMetadataToExistingFile is true, additional metadata might be applied to a file already in Byosphere. When the value is false, the Byosphere file will not be updated with metadata. Default value is false. Example: "ApplyMetadataToExistingFile": true

Parameter: CustomSettings

CustomSettings is an array of custom codes. Custom code will be executed in the order they are listed. Parameter includes

- CustomCodeExePath, optional CustomCode, optional MetadataPath. This set is executed for each sample.
- CustomCodeExePathBefore, optional CustomCodeBefore, optional MetadataPathBefore. This set is executed before Automation starts scanning for new data.
- CustomCodeExePathAfter, optional CustomCodeAfter, optional MetadataPathAfter. This set is executed after Automation has processed current scan data.
- CustomCodeExePathAutomationTrigger, optional CustomCodeAutomationTrigger, optional MetadataPathAutomationTrigger. This set is executed for each Automation Trigger file.

MetadataPath can contain output from the custom code. Contact support@proteinmetrics.com for more information on integration with third party tools through custom codes.

Examples,

- First custom code executes python code,
- Second custom code executes python code with a parameter,
- Third example is an executable,
- Fourth example is an executable with a parameter and a metadata output path

```
"CustomSettings": [
  {
    "CustomCodeBeforeExePath": "py-
thon.exe",
    "CustomCodeBefore":
    "PMIGetMetadata.py"
  },
  {
    "CustomCodeAfterExePath": "py-
thon.exe",
    "CustomCodeAfter": "\"D:\\Test
Data\\PMIGetFasta.py\" --protein"
  },
  {
    "CustomCodeAutomationTrigger":
    "GenedataIntegration.exe"
  },
  {
```

	<pre> "CustomCodeExePath": "BioviaIntegra- tion.exe", "CustomCode": "-f", "MetadataPath": "E:\\Pro- gramData\\ProteinMetrics\\BioviaMetadata" }], </pre>
Parameter: ApplySampleMetadataToProject	False When True, the metadata for the first sample added to a workflow is automatically included in the project.
Parameter: LocalInputRoot (optional)	<p>Automation by default honors local folder hierarchy and will create a matching folder hierarchy in Byosphere. LocalInputRoot parameter allows user to define common path that will be skipped during Byosphere subfolder creation processor therefore redefine a root folder.</p> <p>LocalInputRoot is case insensitive. LocalInputPath and LocalInputRoot are expected to have the same path format of Windows, Linux, or UNC path.</p> <p>Examples in Linux or Windows filepath format:</p> <p>LocalInputPath c:/a/b/z, LocalInputRoot c:/a/b => common path c:/a/b -> data will be uploaded to Output Folder > z</p> <p>LocalInputPath c:/a/b, LocalInputRoot empty => no common path -> data will be uploaded to Output Folder > a > b</p> <p>LocalInputPath c:\a\b, LocalInputRoot c:\m => no common path -> data will be uploaded to Output Folder > a > b</p> <p>LocalInputPath c:\a\b\z, LocalInputRoot c:\a\b\z\y => common path c:/a/b/z -> data will be uploaded to Output Folder</p>
Parameter: UserGroupIds (optional)	<p>Specifies the ids of user groups that should be assigned to the new folders created when uploading a file. The groups will be assigned to all uploaded folders or to subfolders from the level specified by UserGroupSubfolderLevel.</p> <p>Example:</p> <p>"UserGroupIds": "2,3"</p>
Parameter: UserGroupSubfolderLevel (optional) Default: 1	<p>Specifies the level of LocalInputPath directory from where UserGroupIds should be applied when uploading folders.</p> <p>When this parameter is not provided or its value is less than or equal to 1, UserGroupIds will be applied to all new folders.</p> <p>Examples:</p> <p>"LocalInputPath": "C:/a/b/c/d/e",</p> <p>"UserGroupIds": "2,3"</p>

	<p>Example 1:</p> <p>"UserGroupSubfolderLevel ": 1</p> <p>Result: User groups will be applied to all subfolders: a,b,c,d,e</p> <p>Example 2:</p> <p>"UserGroupSubfolderLevel ": 3</p> <p>Result: User groups will be applied to the following subfolders: c,d,e</p> <p>Example 3 (when LocalInputRoot is provided):</p> <p>"LocalInputRoot": "C:/a/b/c",</p> <p>"UserGroupSubfolderLevel ": 3</p> <p>Result: User groups will be applied to the following subfolders: d,e (subfolder 'c' will not be uploaded due to LocalInputRoot value)</p>
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Note: The Automation Server supports metadata. The configuration can be customized so that the folder and file names are parsed into strings which can be saved with the file to specific metadata fields. For information about metadata customization, contact support@proteinmetrics.com.

Configure the Watcher

The installed PMIAutomationService folder is also used by the Watchers. After configuring this folder for the Automation Service, make a copy of the folder for each Watcher and name them accordingly. Next, configure the `appsettings.json` in each of the Watcher directories. Most of the Watcher `*.json` parameters that are shared with the Automation Server `*.json` parameters above will be assigned the same values. There are also specialized parameters for the Watchers to configure as follows:

Parameter, Req'd & Default value	Note
<i>Parameter:</i> LocalInputPath <i>Required:</i> Yes	The path of the folder or root folder of subfolders containing the MS files to be uploaded and processed as analyses.
<i>Parameter:</i> SubFolderLevel <i>Default:</i> 1	The subfolder level of the LocalInputPath directory where the MS files are found. For a value of 1, the MS files are found in the LocalInputPath directory; for a value of 2, the MS files are in folders under that directory, etc.
<i>Parameter:</i> ProcessEntireFolder <i>Default:</i> false	If true, all the MS files in folder at the SubFolderLevel as well as its subfolders are loaded into a single workflow Note: This must be set to false for *.raw and *.d folder samples.
<i>Parameter:</i> WflwOutputDir <i>Required:</i> Yes	The directory where workflows are generated when BuildWflw is set to true, typically the LocalInputPath directory specified for the Automation Service
<i>Parameter:</i> WflwTemplate <i>Required:</i> Yes	The path or file name of the workflow file containing the workflow parameters, apart from samples, which are loaded from the LocalInputPath tree, and sequences, which are loaded from the Sequence path and fasta file.
<i>Parameter:</i> Sequence <i>Required:</i> Yes	The path or file name of the fasta file(s) containing any sequences to load.
<i>Parameter:</i> ReportConfig <i>Required:</i> No	The full path and file name of the report configuration *.rptc file to be loaded into the workflows. If no report configuration is specified, the default report for that project type (*.blgc, *.ntms or *.bmap) Note: Local report configuration files can be added directly to the workflow templates. This is recommended if the Watcher applies to more than one workflow with different report types. In that use case, use absolute paths since relative paths are not supported.
<i>Parameter:</i> SampleProteinCSV <i>Required:</i> No	The full path and file name of the sample-protein *.csv file to be loaded into the workflow.
<i>Parameter:</i> CustomJS <i>Required:</i> Yes	The path and file name of a Custom.js file containing instructions for naming and parsing files and workflows. For help with customizing generated workflows, contact support@proteinmetrics.com
<i>Parameter:</i> AutomationTrigger <i>Required:</i> No	When ProcessEntireFolder is true , a more precise way to trigger the Watcher is to use an automation trigger file. A sub-folder will be processed if and only if the filename designated as the AutomationTrigger is present in the folder. Example: "AutomationTrigger": "WatersmabEnd.raw"

Parameter: ContinueAfterCustomCode Required: No Default: true	If true, we will continue with BuildWflw after custom code is executed. If false, no action will be taken after the custom code is executed.
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Find Byosphere Upload Folder ID

Byosphere folder IDs are displayed when uploading to or downloading from a selected folder. To identify the folder ID, do the following:

1. Create the upload folder in Byosphere. If the Keychain credentials for the Data Uploader is not a Super User, then add a user group for that user name with File Editor, Folder Editor and Viewer privileges.
2. In Byosphere Desktop, login to the server and choose **File > Upload**.
3. In the **Server file/folder** cell, click the "..."/>

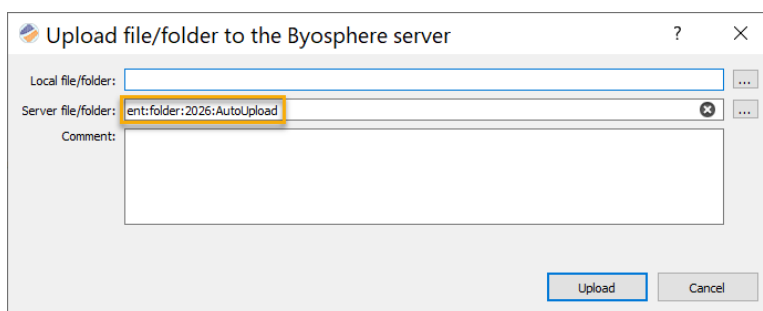


Figure 1: Identify the Byosphere upload folder ID

Run as Windows Service

The Protein Metrics Automation Server and the Watchers are recommended to run as Windows Services rather than as console applications. The executable sc.exe in CMD can also be used to create, start, stop, or delete a Windows Service:

:: Create a Windows Service for the Automation Server

```
sc create PmiAutomationService DisplayName="PMI Automation Server"
binPath="C:\Program Files\ProteinMetrics\Pmi-Automation-
Service\PmiAutomationService.exe"
```

:: Start a Windows Service

```
sc start PmiAutomationService
```

:: Stop a Windows Service

```
sc stop PmiAutomationService
```

:: Delete a Windows Service

```
sc delete PmiAutomationService
```

Repeat these steps for each Watcher Server. After configuring and verifying the setup, it is recommended to set the Protein Metrics Automation Server **Start Type** to **Auto**. Windows services can be managed in the Windows Services App:

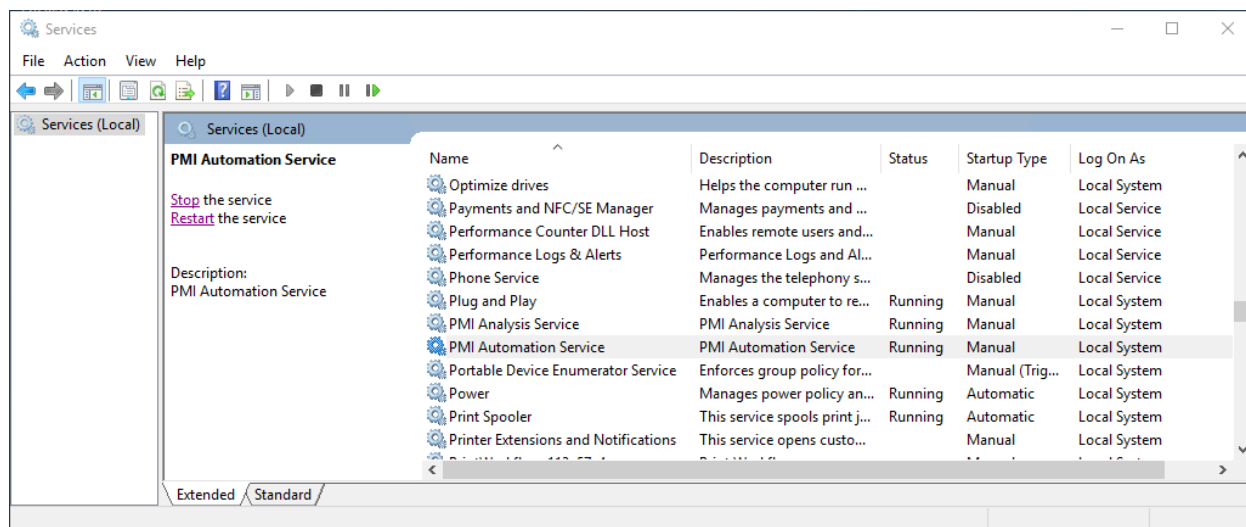


Figure 2: Window Services App

The Log On account for Protein Metrics Automation Service can be a Local Service:

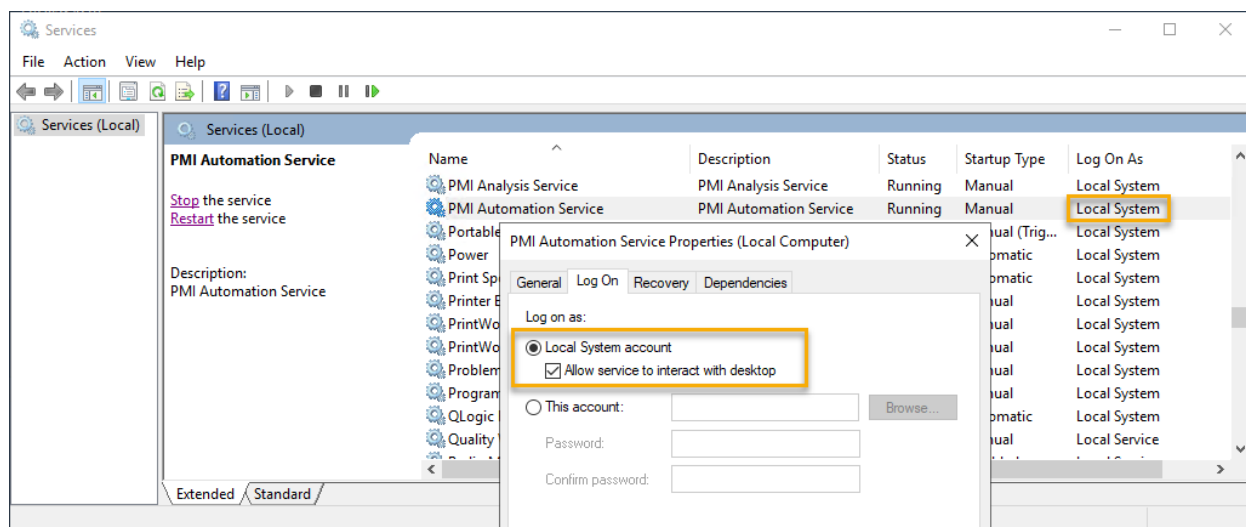


Figure 3: Protein Metrics Automation Service Local logon account

Alternatively, the Log On account for Protein Metrics Automation Service can be an individual user:

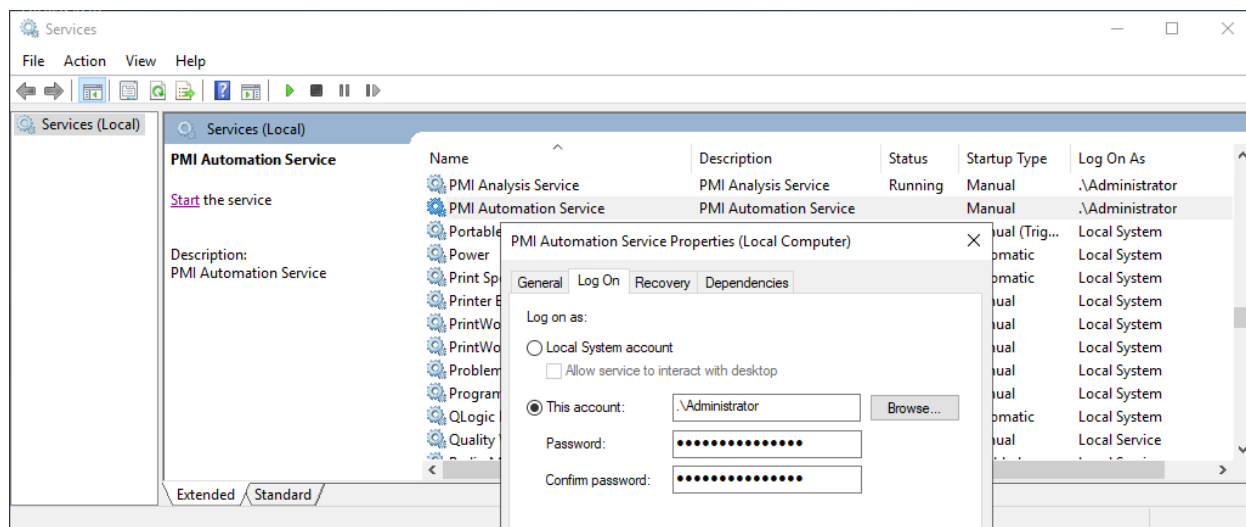


Figure 4: Protein Metrics Automation Service Administrator logon account

Note: After verifying the setup, Automation Server failure recovery can be adjusted according to Company IT policies.

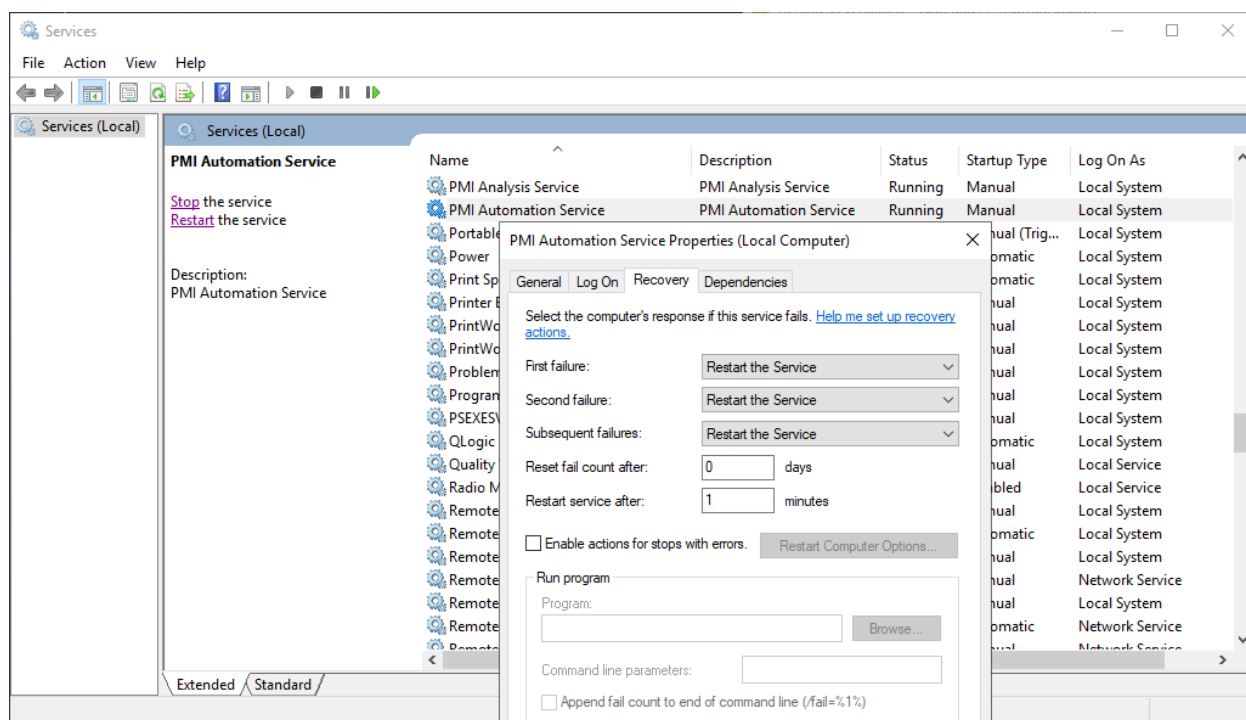


Figure 5: Automation Server failure recovery

Windows Credential for Automation Server

Automation Server uses Windows Credential Store to avoid exposing user passwords in the configuration. Commands are run in the CMD console. For Administrator log on services, a simple CMD window is used. For Local System log on services, there are many tools to access Local System account. One way is to use <https://docs.microsoft.com/en-us/sysinternals/downloads/pstools>

- Start CMD, Run as administrator

- Execute the following command:
`psexec -i -s cmd.exe`
- This will launch a new CMD window granting Local System account access
- Windows Credentials setup can be executed from the Local System account

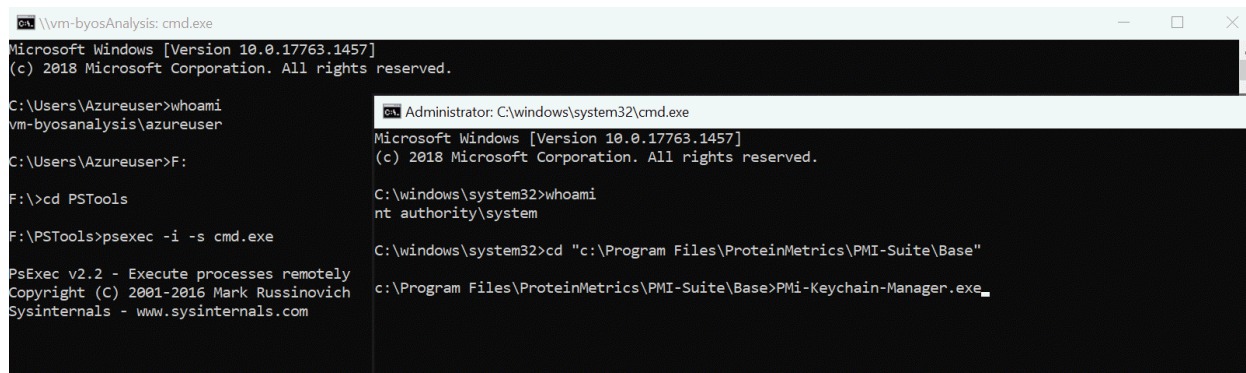


Figure 6: Accessing Local System account

To configure the password used in App Server authentication for Automation Server:

- Follow App Server Guidance on setup API Token
- Open a CMD window as shown above.
- Customize and run the following commands:

```
PMi-Keychain-Manager --delete --namespace=PmiAutomationCredentials
PMi-Keychain-Manager --add --namespace=PmiAutomationCredentials --
key=server --value="https://byosphere.company.com"
PMi-Keychain-Manager --add --namespace=PmiAutomationCredentials --
key=api-token --value=ABCDEabcde
PMi-Keychain-Manager --read --namespace=PmiAutomationCredentials --
key=api-token --context-data="server=https://byosphere.company.com"
```

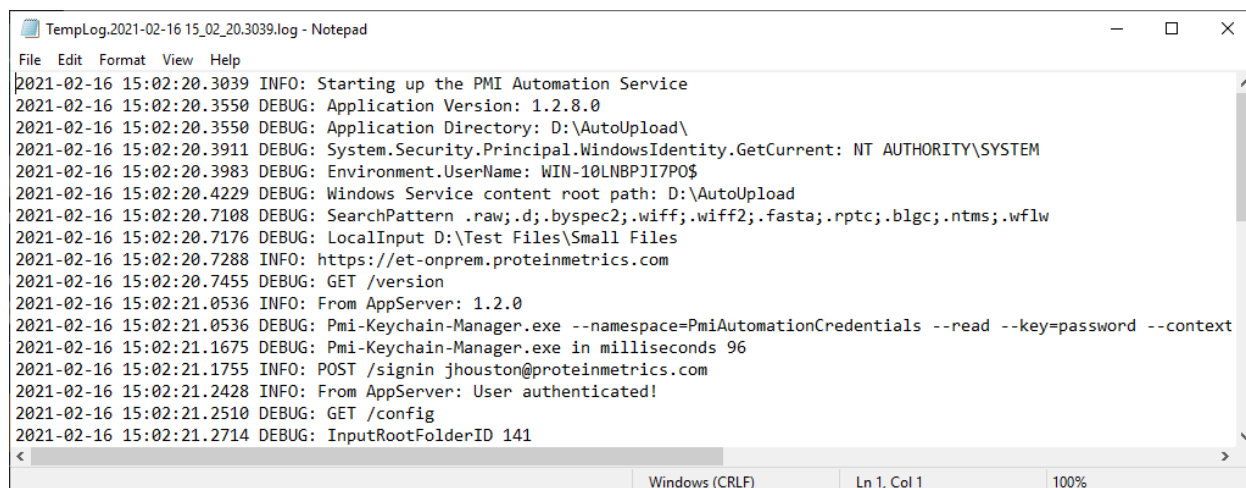
The final line will display the API Token value for the Byosphere server URL. This user account assigned to the API Token requires the Super User privilege and the Contributor entitlement.

Note: Credentials only need to be setup one. In the future updates, run the last line to verify.

Note: Automation Server is set to log on as **Local System** by default. Depending on Company IT policies, Windows Credential might be necessarily to setup from Local System account. To find out more, please refer to <https://docs.microsoft.com/en-us/windows/win32/services/localsystem-account> and

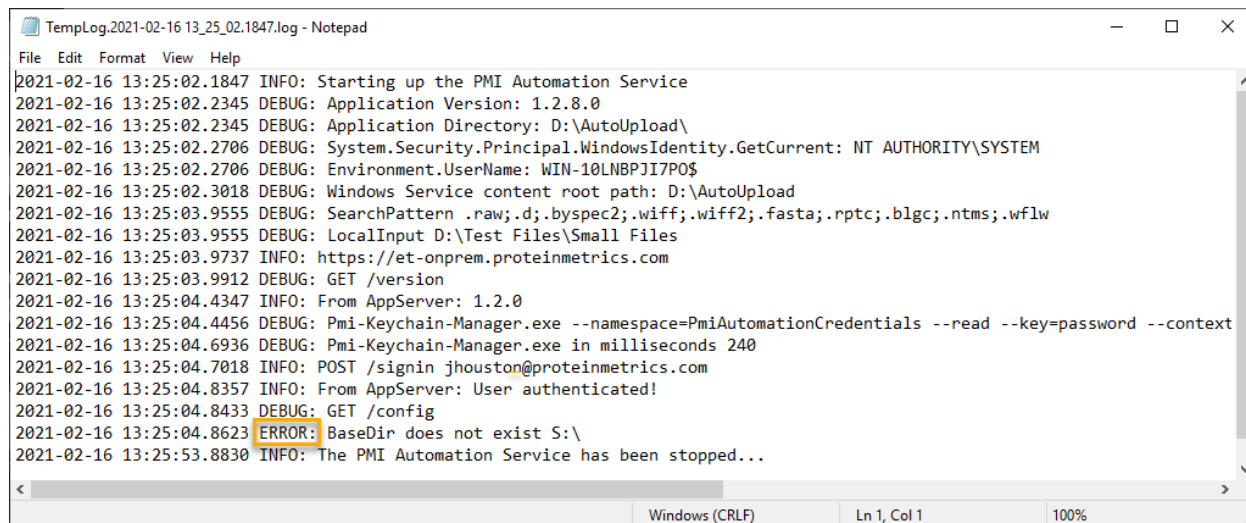
<https://docs.microsoft.com/en-us/windows/win32/ad/the-localsystem-account>

Example of a successful Automation Server startup using username and password: expect to see no errors:



```
TempLog.2021-02-16 15_02_20.3039.log - Notepad
File Edit Format View Help
2021-02-16 15:02:20.3039 INFO: Starting up the PMI Automation Service
2021-02-16 15:02:20.3550 DEBUG: Application Version: 1.2.8.0
2021-02-16 15:02:20.3550 DEBUG: Application Directory: D:\AutoUpload\
2021-02-16 15:02:20.3911 DEBUG: System.Security.Principal.WindowsIdentity.GetCurrent: NT AUTHORITY\SYSTEM
2021-02-16 15:02:20.3983 DEBUG: Environment.UserName: WIN-10LNBPJ17P0$
2021-02-16 15:02:20.4229 DEBUG: Windows Service content root path: D:\AutoUpload
2021-02-16 15:02:20.7108 DEBUG: SearchPattern .raw;.d;.byspec2;.wiff;.wiff2;.fasta;.rptc;.blgc;.ntms;.wflw
2021-02-16 15:02:20.7176 DEBUG: LocalInput D:\Test Files\Small Files
2021-02-16 15:02:20.7288 INFO: https://et-onprem.proteinmetrics.com
2021-02-16 15:02:20.7455 DEBUG: GET /version
2021-02-16 15:02:21.0536 INFO: From AppServer: 1.2.0
2021-02-16 15:02:21.0536 DEBUG: Pmi-Keychain-Manager.exe --namespace=PmiAutomationCredentials --read --key=password --context
2021-02-16 15:02:21.1675 DEBUG: Pmi-Keychain-Manager.exe in milliseconds 96
2021-02-16 15:02:21.1755 INFO: POST /signin jhouston@proteinmetrics.com
2021-02-16 15:02:21.2428 INFO: From AppServer: User authenticated!
2021-02-16 15:02:21.2510 DEBUG: GET /config
2021-02-16 15:02:21.2714 DEBUG: InputRootFolderID 141
```

Figure 7: Example of Successful Automation Server startup



```
TempLog.2021-02-16 13_25_02.1847.log - Notepad
File Edit Format View Help
2021-02-16 13:25:02.1847 INFO: Starting up the PMI Automation Service
2021-02-16 13:25:02.2345 DEBUG: Application Version: 1.2.8.0
2021-02-16 13:25:02.2345 DEBUG: Application Directory: D:\AutoUpload\
2021-02-16 13:25:02.2706 DEBUG: System.Security.Principal.WindowsIdentity.GetCurrent: NT AUTHORITY\SYSTEM
2021-02-16 13:25:02.2706 DEBUG: Environment.UserName: WIN-10LNBPJ17P0$
2021-02-16 13:25:02.3018 DEBUG: Windows Service content root path: D:\AutoUpload
2021-02-16 13:25:03.9555 DEBUG: SearchPattern .raw;.d;.byspec2;.wiff;.wiff2;.fasta;.rptc;.blgc;.ntms;.wflw
2021-02-16 13:25:03.9555 DEBUG: LocalInput D:\Test Files\Small Files
2021-02-16 13:25:03.9737 INFO: https://et-onprem.proteinmetrics.com
2021-02-16 13:25:03.9912 DEBUG: GET /version
2021-02-16 13:25:04.4347 INFO: From AppServer: 1.2.0
2021-02-16 13:25:04.4456 DEBUG: Pmi-Keychain-Manager.exe --namespace=PmiAutomationCredentials --read --key=password --context
2021-02-16 13:25:04.6936 DEBUG: Pmi-Keychain-Manager.exe in milliseconds 240
2021-02-16 13:25:04.7018 INFO: POST /signin jhouston@proteinmetrics.com
2021-02-16 13:25:04.8357 INFO: From AppServer: User authenticated!
2021-02-16 13:25:04.8433 DEBUG: GET /config
2021-02-16 13:25:04.8623 ERROR: BaseDir does not exist S:\
2021-02-16 13:25:53.8830 INFO: The PMI Automation Service has been stopped...
```

Figure 8: Example of Failed Automation Server startup

Application Notes

- New files are identified by content, not by name. If a file is edited, it will be uploaded as new version over the existing file with that name.
- Files which have MS sample extensions but are not recognized by the Byos application as MS files or folders (for example, corrupted data) are uploaded but not compressed into *.pacq format. Multiple versions of these files may then be generated.
- Log files written to the PMIAutomationService\Logs directory can be renamed or configured by editing the file PMIAutomationService\NLog.config. For more information, please refer to <https://github.com/nlog/nlog/wiki/Configuration-file> or contact Protein Metrics support. Note that log level can be Debug, Info, Warning, Error, and Fatal. It is recommended to start with Debug level logging during initial deployment to enable Protein Metrics to better troubleshoot any issues. It is recommended to use Info in normal operation; Warning or high to minimize logging. User can delete log files at PMIAutomationService\Logs subdirectory if log information is no longer needed.