

Agilent InfinityLab Purification Solutions

Administrator's
Quick Start Guide



Agilent Technologies

Notices

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A **WARNING** notice denotes a hazard. It calls attention to an operating procedure, practice, or the like that, if not correctly performed or adhered to, could result in personal injury or death. Do not proceed beyond a **WARNING** notice until the indicated conditions are fully understood and met.

In This Book

This manual contains information for administrators of the Automated Purification software.

1 The Role of the Administrator

This chapter describes the role of the administrator of the Automated Purification Software.

2 Setting Up Purification Users

This chapter gives step-by-step instructions on setting up the profiles for users of the Automated Purification software.

3 Checking and Editing User Privileges

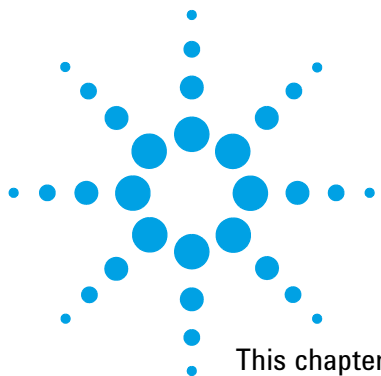
This chapter describes how to view the privileges associated with a user role, and edit them if necessary.

4 Purification Data File System

This chapter describes the data structure of the Automated Purification Software and how you organize it to suit your needs.

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1

The Role of the Administrator

This chapter describes the role of the administrator of the Automated Purification Software.

The Automated Purification Software supports two user modes: *Expert* and *Easy Prep*.

The user mode defines

- the menu items that are enabled in the Automated Purification Software
- the user interface items that are available
- access to Chemstation from the Automated Purification Software

The user modes are set up using the user authentication feature of the Agilent OpenLab Control Panel.

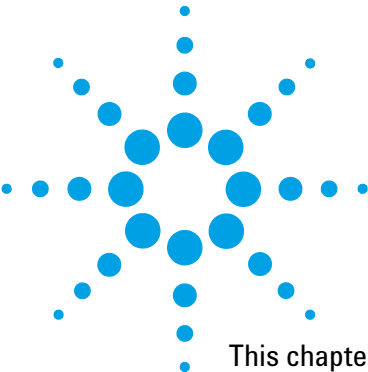
The role of the administrator is to:

- enable user authentication
- set up users
- assign roles to users
- check or edit the privileges of the user roles
- set up the data file system:
 - task folder structure
 - security settings
 - backup folders



1 **The Role of the Administrator**

In This Book



2 Setting Up Purification Users

This chapter gives step-by-step instructions on setting up the profiles for users of the Automated Purification software.

The Agilent Automated Purification software can support two types of user:

- Method Developers working in *Expert* mode have full access to all features of the software, including method editing.
- Operators working in *Easy Prep* mode have access to a reduced feature set that excludes method editing.

The user profiles are configured in the Agilent OpenLab Control Panel.

NOTE

If shared services is not configured for the different types of users, the Purification Software will automatically be controlled in *Expert* mode.

- 1 Open the Windows **Start** menu and navigate to the **OpenLab Control Panel** item.
 - a **Agilent Technologies > OpenLab > OpenLab Control Panel**The **OpenLab Control Panel** opens.
- 2 In the OpenLab Control Panel **Navigation** pane, select **Administration**.
- 3 From the **Administration** tasks in upper part of the **Navigation** pane, select **System Configuration**.

The **System Configuration** settings are displayed.
- 4 Click **Edit System Settings** in the toolbar.

The **Edit System Settings** dialog box is displayed.
- 5 Click the down-arrow of the upper field (for the authentication provider) and select **Internal** from the drop-down list and click **Next**.
- 6 In the **Authentication Parameters** section, click **Create Account**.

The form for the creation of the new account is displayed.



- 7 Complete the form with the details for the *Expert* user, including a password, and click **OK**.

The new account for the Method Developer is created.

- 8 Click **Next** to accept the new account, then click **Apply** to apply the configuration settings. Click **OK** when asked to confirm the changes to the system configuration.

Setup of the Method Developer user account is complete.

- 9 Close down the OpenLab Control Panel, reopen it and log in with the credentials you have just specified.

The OpenLab Control Panel opens with additional options in the **Navigation** pane.

- 10 Select **Users** from the **System Configuration** options.

The **Users** page is displayed.

- 11 Click **Create** in the toolbar

The **Create User** dialog box is displayed.

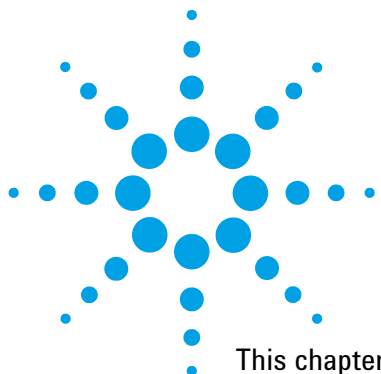
- 12 Enter a **Name** and **Description** for the new user in the upper fields.

- 13 In the **General** tab, provide a password for the new user, and mark the **User cannot change password** check box.

- 14 Switch to the **Role Membership** tab and mark the **Instrument User** and **ChemStation Operator** check boxes.

- 15 Click **OK** to create the new user.

Setup of the Operator user account is complete.



3

Checking and Editing User Privileges

This chapter describes how to view the privileges associated with a user role, and edit them if necessary.

The privileges associated with a user role are configured in the OpenLab Control Panel. You must have administrator rights to access the privileges of user roles.



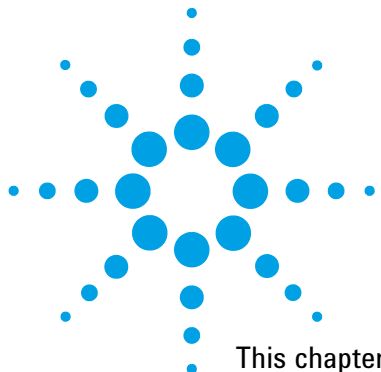
Checking User Privileges

- 1** Open the Windows **Start** menu and navigate to the **OpenLab Control Panel** item.
 - a** **Agilent Technologies > OpenLab > OpenLab Control Panel**
The **OpenLab Control Panel** opens.
- 2** In the OpenLab Control Panel **Navigation** pane, select **Administration**.
- 3** From the list of options for **Administration**, select **Roles**.
The list of user roles is displayed in the right panel.
- 4** To check the privileges associated with a user role, click **>** in the leftmost column of the list of user roles.
The list of privileges associated with the selected user role is displayed.

Editing User Privileges

- 1** In the list of user roles, select the role whose privileges you want to modify.
- 2** In the **Roles** section of the control panel toolbar, click **Edit**.
The **Edit Role** dialog box is displayed.
- 3** In the **Edit Role** dialog box, select the **Role privileges** tab.
- 4** Click **>** to the left of a privilege to open the second level of privileges.
- 5** Mark the check boxes against the privileges you want to add to the user role, and clear the check boxes against the privileges you want to remove.
- 6** Click **OK** to close the Edit Role dialog box and register the changes.

3 **Checking and Editing User Privileges** In This Book



4

Purification Data File System

This chapter describes the data structure of the Automated Purification Software and how you organize it to suit your needs.

The data structure of the Automated Purification Software can be customized to suit the working practises of your laboratory using the settings in the **Administration** dialog box. Administrators and method developers can access the administration settings from the main toolbar of the **Purification Tasks** screen, launched from the **Purification** menu of the ChemStation **Method & Run Control** view.



Default Purification Folder Structure

This section explains the default organization of the Automated Purification Software folders.

When the Automated Purification Software add-on is installed, it adds a new Purify folder into the instrument folder. Thus, if Chemstation is installed in the default location, and the add-on is configured for instrument 1, the default location for the Purification data is:

C:\Users\Public\Documents\ChemStation\1\Purify

Eight sub-folders hold all the Purification data within the Purify folder:

AnalyticalSystems	contains the different analytical systems, stored as XML files.
Calibration	contains your delay calibration runs as executed by the Purification Software.
CalibrationThreshold	contains the settings for automatic fraction collection trigger thresholds.
Exports	the default folder location for any exports made from purification software, such as liquid handler files or re-analysis sequence files.
LocationMappings	contains the different location mappings, stored as XML files.
PreparativeSystem	contains the different preparative systems, stored as XML files.
Tasks	the default root folder location for tasks. Each task comprises a folder containing the task parameters, stored as XML files, and the data and methods belonging to the task. The data is structured in different sub-folders: • AnalyticalResults contains the analytical results data • PreparativeSequence contains the preparative sequence and the corresponding methods. Also located in the Tasks folder is the preparative result set (for completed tasks). All Switch and Standby methods and results are stored in a BlankRuns folder. You can turn off the storage of blank run data in the Administration settings. (Launch the Administration dialog box from the Tasks screen). AnalyticalResults is a sub-folder of the Tasks folder in parallel with the folders of all tasks. It contains the analytical data of all tasks in the Tasks folder. This avoids unnecessary copies of analytical data when different tasks refer to the same analytical data. If sub-folders are set up in the Administration dialog box, the Tasks folder contains the sub-folders where the tasks are stored.

SST	the default location for System Suitability Test tasks, which check that the instrument is running within specifications. SST tasks are created by the method developer, and can be cloned and executed by any user. SST tasks should be executed regularly (for example, every morning) and whenever there is reason to doubt the instrument's suitability.
Templates	contains all tasks that have been saved as templates (stored as XML files).

The task subfolder has the same name as the task name within the purification software. The XML files in which the system parameters are saved also use the same name as the system name within the purification software.

NOTE

Do not use the Windows Explorer to rename any of the Purification files or folders. Rename files from within the Automated Purification Software only.

Purification Task Root Folder

You can specify the root folder for purification tasks. As you create more and more tasks, the number of tasks in the Tasks root folder increases, so, from time to time, you may want to archive old tasks to a different location to prevent their unlimited growth. The settings in the **Data Paths** page of the **Administration** dialog box help you to structure your tasks; for example, for each user, you can create a subfolder with the user name, where only tasks from that user are stored. You can create an additional folder for a time period (below the user folder), such as daily, monthly, etc. The user and time folder are created automatically and will be the default folder for each user. This structure is similar to that of the Agilent MassHunter Walkup Software.

The location of system suitability tasks is also specified in the administration settings.

Backup

After the completion of a Purification Task preparative run, the task data can be copied automatically into one or more backup locations, which must be specified in the **Backup** page of the **Administration** dialog box. All backup folders must already be established, with access for all users of the Purification Software. We recommend that these folders are network locations on dedicated backup shares on a server. The local machine with your installed OpenLab ChemStation and Automated Purification Software is used for instrument access and data processing, while your backup folders are used only to archive/back up your data.

The original path structure of your task data is maintained in the backup folder. This gives you the same browsing experience at all locations, and allows you to restore data directly to the original location. To restore data to secured locations, pay attention to the additional steps as described in “[ChemStation Secure File IO](#)” on page 19. We recommend the use of short paths for your backup locations. If your backup location paths are long, there is the risk that your backup copy of the Purification Task data exceeds the 260-character limit for data paths of the Windows file system. You can map your backup location to a single drive letter, using the **Map Network Drive** feature of the Windows **File Explorer**, which you launch from the **Easy access > Map as drive** from the **File Explorer Home** Ribbon

Enabling long paths in Windows 10

We recommend that you enable long paths (path lengths > 260 characters) on Windows 10 machines for your ChemStation and Automated Purification Software installation, as well as on the servers that should host your backups if they are Windows computers.

To enable long paths on your Windows 10 system:

- 1 Open the Windows **Local Group Policy Editor** (for example, using **Run > gpedit.msc**).
- 2 In the left pane, navigate to **Computer Configuration > Administrative Templates > All Settings**.
- 3 In the right pane, select **Enable Win32 long paths**.

4 Purification Data File System

Backup

- 4 Either double-click the item, or right-click and select **Edit** to open the settings dialog box.
- 5 Select the **Enabled** option and click **OK** to close the settings dialog box.
- 6 Close the **Local Group Policy Editor**.

NOTE

Even if you enabled long paths in Windows 10, do not use extraordinarily long paths within your tasks folder structure for your working ChemStation Purification Software instance: Some features in ChemStation may not work on long paths.

ChemStation Secure File IO

If you decide to protect the ChemStation data files with *Secure File IO* (see the ChemStation reference guides) you also want to secure the purification software data folders. Check and modify your ChemStation file security settings in the **ChemStation Administration Tool**. When using ChemStation in Secure File IO mode (that is, Secure File IO enabled, even if no directory is currently protected), then the user that is specified in the Secure File I/O account settings needs to have appropriate rights to read files from any locations required by Purification Software, such as network shares or directories (for example, analytical result set, sequence csv files, and so on).

NOTE

Backed-up data (Tasks) cannot be restored into a secured location (if the task has been removed from within Automated Purification Software).

If you want to restore data from a backup into a secured location, first *unprotect* the location in the **ChemStation Administration Tool**, then copy your task data (not forgetting to copy related analytical results). When you are finished, re-secure the unprotected location.

Glossary

Administrator	User who sets up the users of the Automated Purification Software as Operators or Method Developers in the Agilent OpenLab Control Panel.
ChemStation	OpenLab CDS ChemStation
Easy Prep mode	Automated Purification Software work mode that focuses on the key data to set up and run purification tasks. ChemStation access is blocked to prevent unintended interaction.
Expert mode	Automated Purification Software work mode that grants full access to all features and functions of the software.
Method Developer	User who provides the work environment (methods, procedures, systems, master tasks) for Operators. The Method Developer works in <i>Expert</i> mode.
Operator	User who operates an analytical and/or preparative instrument using predefined methods and procedures. The Operator works in <i>Easy Prep</i> mode.
System	A <i>system</i> within the purification software means a certain set of instrument configuration and operation parameters that describe either the analytical or preparative instrument and run. Such a parameter set provides the relevant settings in the analytical-to-preparative scale-up process.

In This Book

This manual contains information for Administrators of the Automated Purification software.

The manual describes the following:

- the role of the Administrator
- how to set up Purification users
- how to edit user privileges
- how to adjust and back up your purification data file structure

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