Notices

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Safety Notices

CAUTION

A CAUTION 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 damage to the product or loss of important data. Do not proceed beyond a CAUTION notice until the indicated conditions are fully understood and met.

WARNING

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.
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 Default Purification Folder Structure

This chapter explains the default organization of the Automated Purification Software folders.
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4 Default Purification Folder Structure  13
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
1 The Role of the Administrator
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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.
2 Setting Up Purification Users

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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.
3 Checking and Editing User Privileges

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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

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## Default Purification Folder Structure

This chapter 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:

<table>
<thead>
<tr>
<th>Folder Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AnalyticalSystems</td>
<td>contains the different analytical systems, stored as XML files.</td>
</tr>
<tr>
<td>Calibration</td>
<td>contains your delay calibration runs as executed by the Purification Software.</td>
</tr>
<tr>
<td>CalibrationThreshold</td>
<td>contains the settings for automatic fraction collection trigger thresholds.</td>
</tr>
<tr>
<td>Exports</td>
<td>the default folder location for any exports made from purification software, such as liquid handler files or re-analysis sequence files.</td>
</tr>
<tr>
<td>LocationMappings</td>
<td>contains the different location mappings, stored as XML files.</td>
</tr>
<tr>
<td>PreparativeSystem</td>
<td>contains the different preparative systems, stored as XML files.</td>
</tr>
</tbody>
</table>
4 Default Purification Folder Structure

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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 are the preparative result set (for completed tasks) and all Switch and Standby methods.

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 and task parameters are saved also use the same name as the system/task 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.
Administration settings

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. The settings in 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.

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.
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).
Glossary

Administrator  User who sets up the users of the purification software as Operators or Method Developers in the Agilent OpenLab Control Panel.

ChemStation  OpenLab CDS ChemStation

Easy Prep mode  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  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 Expert mode.

Operator  User who operates an analytical and/or preparative instrument using predefined methods and procedures. The Operator works in Easy Prep mode.

System  A system 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
• a description of the Purification folder structure