

# Agilent InfinityLab Purification Solutions

Operator's  
Quick Reference Guide



**Agilent Technologies**

# Notices

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## In This Book

This manual contains instructions for Operators on how to use the Automated Purification software.

### **1 The Role of the Operator**

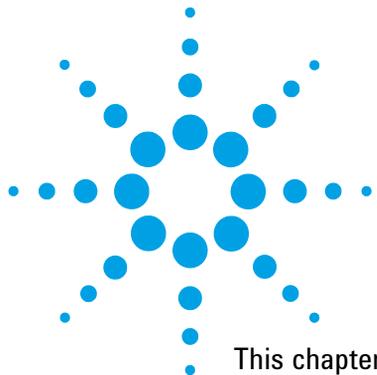
This chapter describes the role of the user of the Automated Purification Software in Easy Prep mode.

### **2 Executing a Purification Task**

This chapter gives instructions for users with Easy Prep user rights on how to execute a Purification Task.

# Contents

<b>1</b>	<b>The Role of the Operator</b>	<b>5</b>
<b>2</b>	<b>Executing a Purification Task</b>	<b>7</b>
	Configuring a new task	9
	Running a task	10
	Processing partial data and cloning tasks	11
	Reviewing the analytical results	13
	Reviewing the purification results	14
	Forcing the Purification Task to Close	16



# 1 The Role of the Operator

This chapter describes the role of the user of the Automated Purification Software in Easy Prep mode.

Operators of the Automated Purification Software work in *Easy Prep* mode to perform purification runs. If the samples have not been analyzed on a separate analytical instrument, the purification runs include the analytical runs. Typically, the Operators have been trained by a Method Developer on the work environment and operating procedures.

The Operators:

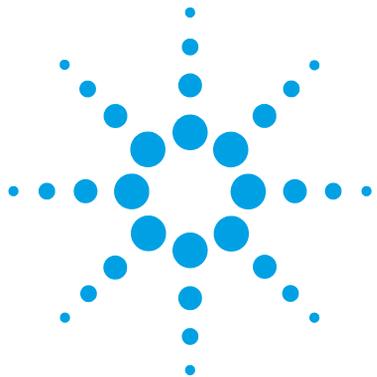
- provide the samples for use in the purification run
- know the analytical and preparative instrument and operating system settings that apply to their samples. These have been set up in the purification software by a Method Developer.
- set up a purification run in the purification software by creating a *purification task* based on a matching task template prepared by a Method Developer. Operators can also create a new task as a clone of an existing task, for example, to re-run a stopped task, to run samples of the original task that have not yet been run, or to repeat a system suitability task.
- complete the missing information (analytical data source, analytical-to-preparative vial mapping, and injection volume) to run the task.
- run the purification task and review the results.

For Operators, access to the Automated Purification Software is limited to the main purification workflow user interface (the purification task screen) and its key settings (system definition, analytical and preparative run). While in the purification task screen, ChemStation functionality is inaccessible to avoid unintended interference. The ChemStation screen reports are thus not suitable for Operators.

If Operators get stuck or need help, they should contact a Method Developer.



**1** **The Role of the Operator**  
In This Book



## 2 Executing a Purification Task

Configuring a new task	9
Running a task	10
Processing partial data and cloning tasks	11
Reviewing the analytical results	13
Reviewing the purification results	14
Forcing the Purification Task to Close	16

This chapter gives instructions for users with Easy Prep user rights on how to execute a Purification Task.

A *purification task* in the Automated Purification Software describes all settings of a purification experiment, including its results, once the experiment is complete.

Purification tasks are managed in the purification task screen, which is thus the center for the execution of all purification work:

- configuration of the purification job (samples and operating setup)
- submission of the analytical and preparative runs (including progress indication and stop)
- review and modification of the target identification from the analytical run
- review and export of the purification results (collected fractions)

**1** In the ChemStation **Method and Run Control** view, open the **Purification** menu and select **Tasks**.

The purification task screen is shown, displaying in its upper region a list of all tasks in the selected task folder. Details of the selected task (setup and result info) are displayed in the lower region. By default, the configuration tab with the **Select System** page of the selected task is displayed.

After launching the **Tasks** screen or logging in, you are in the **User task** view by default. This view displays the tasks in your default user tasks root folder. You



## 2 Executing a Purification Task

### In This Book

can choose a different root folder or navigate to another user's folder in the **Purification task parameters root folder** text-box at the top of the tasks list. As a Method Developer you can modify and submit other users' tasks. As an Operator, you can modify and submit only your own tasks.

## Configuring a new task

- 1 Click **Add Task** to select a task template or choose to clone the currently selected task and create a new purification task.
- 2 Verify that the **Analytical System** matches the system providing the analytical run, and the **Preparative System** that corresponds to the current preparative instrument configuration.

The current instrument configuration of the preparative system is displayed in the table.

If one of the systems does not match, choose another template to create your task. If there is no matching template, ask the Method Developer to create one.

- 3 Select the **Analytical Run** page and specify the source of the analytical run:
  - To run an analytical scouting sequence on a combined analytical and preparative system, select an existing ChemStation sequence or prepare a sequence from scratch. Select the path and name of an existing ChemStation sequence in the text input field or click **Edit sequence** to start editing a sequence from scratch or modifying a selected sequence. You can also import a sequence as a text (CSV or TXT) file.
  - To use analytical results that have already been acquired on a stand-alone system, specify the location of the source files (result set or single sample results) in the text input field.  
Select data files using the **Process?** check box in the sequence table.
- 4 Select the **Preparative Run** page and specify a **Preparative base method**.
- 5 Set the preparative vial locations and injection volumes. You may want to apply a location mapping for vial locations. Specify the injection volume for the first sample and use the fill-down option to apply the same volume for other samples.

## Running a task

- 1 Click  **Run** in the top toolbar of the **Task** dialog box to start the purification run.

If the analytical sequence has not yet been run, it will be submitted to the ChemStation run queue.

If the analytical run is already available, the process will start with the evaluation of the analytical results.

The buttons in the top toolbar also allow you to stop a run in progress or unschedule a scheduled run that has not yet started. If the run queue is

paused (for example, after a stop) you can resume it using the  **Resume** item in the **Task** toolbar. Note that the / items can be helpful if the run gets stuck or lost for any reason.

The run progress is displayed in the bottom line of the **Task** screen. Run state events and important processing events are displayed in the **Logbook** tab.

If you stopped your run, or your run was aborted (by the instrument), call your method developer. He can create a clone of your aborted task to enable you to process the missed samples.

You can log off while the run is proceeding and you or another user can log in and create and/or submit other tasks. While no user is logged in, the Purification Software is locked (in sync with ChemStation) and switched to the **Scheduled Tasks** view, which lists the running and all scheduled tasks from all users with their remaining times. At any time while you are logged in, you can switch to the **Scheduled Tasks** view to see the purification tasks run queue.

## Processing partial data and cloning tasks

You are dealing with partial data under the following conditions:

- You stopped your analytical or preparative run, or your run was stopped due to an instrument error (such as solvent bottles running empty). In such a case, some of the planned samples were executed but others were missed.
- You have a large set of analytical data from a separate analytical instrument, but you want only a subset of it to be purified in one task. For example, your preparative plate does not have the capacity to hold all samples.

Task cloning (or copying) means creating a new task with the same settings and analytical data as another task. The preparative results are not cloned.

- 1 Select the task to be cloned in the task list of your purification task dialog box.
- 2 create a new task as a clone of the selected task by choosing **Add clone of currently selected task** in the **Add Purification Task** dialog box.

If you want to repeat a (previous) system suitability test run, you can clone the system suitability test task and let it run in **SST Tasks** view.

If your analytical run was stopped or aborted, the successfully processed samples remain as analytical result data with the task. Purification proceeds with those samples only.

- 1 If you want to process the remaining/missed samples from such a task, create a clone of the incomplete task.
- 2 In the new cloned task, go to the **Analytical Run** page of the **Task Configuration** and click **Revert to sequence**.

This restores your original sequence.

- 3 Click **Edit Sequence** and remove the samples that already ran successfully.
- 4 Click **Accept changes** to save your modified sequence with the task.

If your preparative run was stopped or aborted, the successfully processed samples are saved with the task, which is now in a *completed* state, and no further modifications can be made. You can proceed to reviewing your purification results and export fractions as described in “[Reviewing the purification results](#)” on page 14.

## 2 Executing a Purification Task

### Processing partial data and cloning tasks

- 1 To process the missed samples of the purification run, create a clone of the partially processed task.
- 2 In the new cloned task, go to the **Analytical Results** tab and select the samples to be purified by marking the check boxes in the **Purify?** column.
- 3 Re-submit the purification run for the selected (missed) samples.

If you want to process only a subset of the samples from your available analytical data, select the analytical data (result set folder or folder of your single sample results) in the **Analytical Run** page of **Task Configuration** of a new task.

- 1 Select those samples that you would like to be evaluated and purified in the **Process?** column of your analytical samples table.
- 2 Create a new task as a clone of your previous task to run another subset of samples from your analytical data and select the next subset of samples.

Make sure that all tasks that refer to the same analytical data are stored in the same root folder, because the analytical results are copied into the same root folder.

This avoids unnecessary copies of your analytical data. For example, the default root folder is C:\Users\Public\Documents\ChemStation\1\Purify\Tasks. The analytical results are then stored in C:\Users\Public\Documents\ChemStation\1\Purify\Tasks\AnalyticalResults.

If your tasks are organized in user name and time-specific sub-folders, the analytical results will be copied into each such folder, where needed.

## Reviewing the analytical results

- 1 If the master task has been set up to review the analytical results before starting the preparative run, select the **Analytical Results** tab to review the results once the evaluation of analytical results has completed.

You can review and change the target for purification before continuing with the purification step.

In the **Analytical Results** tab, the identified target compound and the calculated gradient profile are visualized. Spectral data of each peak is displayed within the spectra tab. Target masses or formulas can be corrected.

### NOTE

All changes in the **Analytical Results** tab apply to the selected sample, so you must step through all samples that you want to review or for which you want to change settings. If settings have to be adjusted for all samples, return to the **Task Configuration** tab to change the global settings, then restart the evaluation of the analytical results.

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- 2 When you are satisfied with the results, click  **Run** in the top toolbar of the **Task** dialog box to start the preparative run.

## Reviewing the purification results

- 1 To display the purification results, click the **Preparative Results** tab.

OR

Open the **Purification** menu in the Chemstation **Data Analysis** view and select **Results**.

The purification results are shown in a window with four sections:

- Upper left: the samples list. You can choose to view the samples either as a tabular display or as a graphical representation of the autosampler tray.
- Upper right: the fractions collected. You can choose to view the fractions either as a tabular display or as a graphical representation of the fraction collector.
- Lower left: the signals display, which shows all collected chromatograms from the selected sample. The peaks are annotated with start and end ticks and retention times, and the collected fractions are denoted by colored bands.
- Lower right: the spectra display, which shows the spectra for the selected fraction.

The **Preparative Results** tab displays the location of the injected samples in the autosampler and the location of the collected fractions in the fraction collector. It indicates the collected fractions in the chromatograms and the corresponding spectral data that have been acquired. The display of spectral data is an interactive process: clicking on a peak of the chromatogram displays the spectral data, or clicking on a collected fraction displays the spectral data and the chromatographic information. Select fractions to export by CTRL-clicking fractions in the graphics or the table. Selected fractions can be exported as a re-analysis sequence file or a liquid

handler pooling file by clicking  in the Purification Task toolbar.

The fraction locations and containers/trays/plates might not match the sampler containers/trays/plates for a re-analysis sequence. In this case, you may want to choose the **Convert fractions to parking lot locations** option in the **Export Selected Fractions** dialog box, which converts your fraction locations to the PLOT format. This allows you to re-configure your containers in the

sampler using the parking lot of the **Sampler Entry** tab of the ChemStation **Method And Run Control** view.

## Forcing the Purification Task to Close

If you get into a situation where you need to exit the Purification Task screen but you cannot exit because of a pending run issue, such as **Waiting for Standby**, you can use the following procedure:

- 1 Unschedule any scheduled tasks.
  - Click  **Unschedule** in the top toolbar.
- 2 Resume the run queue.
  - Click  **Resume** in the top toolbar.

The Automated Purification Software waits for a few seconds, then tries to resume the run. If the run cannot resume, it is aborted, and reported as **Dropped** in the purification **Logbook**. This releases the task from its Pending status, and you can safely exit the Purification Task screen.

- 3 Fix the issues in the ChemStation before rescheduling the purification tasks.

# 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.
Purification task	Entity in the purification software that describes all settings of a purification experiment, including its results once the experiment has completed.
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.
System suitability test	Specific preparative-only workflow task, used to purge the auto-sampler, flush the instrument and verify that the compounds in a standard sample are separated as expected. Regular purification tasks can be submitted to run only if the last system suitability test was <i>passed</i> or <i>accepted</i> by a method developer.
Tasks root folder	Folder on disk where the Purification tasks are saved. Default folder for instrument 1: <b>C:\Users\Public\Documents\ChemStation\1\Purify\Tasks</b> Different tasks root folders can be defined in the <b>Purify</b> folder; for example, if a default tasks root folder with user's name or time stamp is defined in the <b>Administration</b> dialog box. A valid tasks root folder must be selected in the <b>Purification Tasks</b> dialog box to create and submit Purification tasks. When the <b>Purification Tasks</b> page is opened, the <b>User tasks</b> view is shown and the default tasks root folder is displayed and is editable. The SST tasks root folder is a tasks root folder containing System Suitability Test tasks only. It is editable in the <b>Administration</b> dialog box only by an advanced user. Default folder for instrument 1: <b>C:\Users\Public\Documents\ChemStation\1\Purify\SST</b>
Template	Template created from an already defined Purification task, used for creating a new Purification task. A template includes all settings of a task (such as analytical and preparative system settings, ion species, gradient and scale-up parameters, fraction collection settings) but does not contain any run data (result set, chromatograms, spectra). A template does not include analytical or preparative sequence. However, analytical and preparative sequence fields are pre-populated according to the task used to create the template.

## Glossary

Templates can be created and modified by Method Developers only.



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## In This Book

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

The manual describes the following:

- the role of the Operator
- how to execute a Purification Run

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