

Agilent Advanced Sample Linking

A complete workflow from any laboratory information management system to the vial and analytical results



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Abstract

With the release of the Agilent Infinity III LC series, the Agilent 1260 and 1290 Infinity III Multisampler can optionally be equipped with the Agilent InfinityLab Sample ID Reader. The integration of the LC system into a client-server environment allows the use of additional software, such as Agilent Sample Linking software and Agilent Sample Scheduler for OpenLab, enabling a complete workflow that links samples from any laboratory information management system (LIMS) to the vials and HPLC analysis results. This white paper highlights the benefits of the integrated analytical workflow. In this workflow, barcodes are used to track samples from the sample list to their vial position, and the presence of the correct sample is recognized without manually entering its position. This saves time and improves ease of use, with fewer errors over the complete workflow.

Introduction

Today, analytical laboratories or departments are facing high sample loads to work more economically. High sample load and manual steps in the workflow from sample to report are likely to introduce errors and prolong workflows. To reduce errors and time, and increase ease of use, an integrated workflow from the arriving samples to the final report is highly advantageous. This can be achieved using a server-integrated solution with additional software that links every sample container with a unique, pre-barcoded vial.

The full workflow is shown in Figure 1. First, the samples to be analyzed are registered in the LIMS, then sent through Sample Scheduler for OpenLab to the Sample Linking software, where the linking of sample containers to the pre-barcoded target vial and the generation of the final sequence is managed. Here, the analyst obtaining the order is guided step-by-step to transfer the samples to pre-barcoded vials (examples of additional materials used are given in the appendix). The sample and vial IDs are linked using a benchtop barcode reader and the Sample Linking software. Both sample and vial IDs are linked to the analytical sequence, which is sent to Agilent OpenLab CDS Acquisition software through the Sample Scheduler for OpenLab. The pre-barcoded vials can randomly be placed into the sample tray in any arrangement. After placing the sample tray in the 1260 or 1290 Infinity III Multisampler, the complete content of the tray

is internally scanned from the bottom side by the optionally built-in InfinityLab Sample ID Reader; then, at the start of the sequence, the respective samples are identified and measured wherever they are positioned. After data acquisition and analysis, a report can be generated that confirms the measurement of the required samples by comparing the scanned and expected barcodes.

Workflow operation including Sample Linking software, Sample Scheduler for OpenLab, and a connection to LIMS

As a precondition, the HPLC can be started in OpenLab CDS Acquisition software to flush the tubes and capillaries, and equilibrate the column and column temperature. The acquisition method and a sequence template are present in OpenLab CDS Acquisition software. To analyze the acquired data, a data analysis method including a report is presented in Agilent OpenLab CDS Data Analysis software. The Sample Scheduler for OpenLab can be launched from the OpenLab CDS Acquisition software.

The start screen of the Sample Scheduler for OpenLab is shown in Figure 2. This screen gives a comprehensive overview about the connected instruments (under My Instruments) and their status, as well as the analysis (under My Analysis). All boxes, graphs, and numbers in this graphical overview can be clicked to guide the user directly to the respective information.

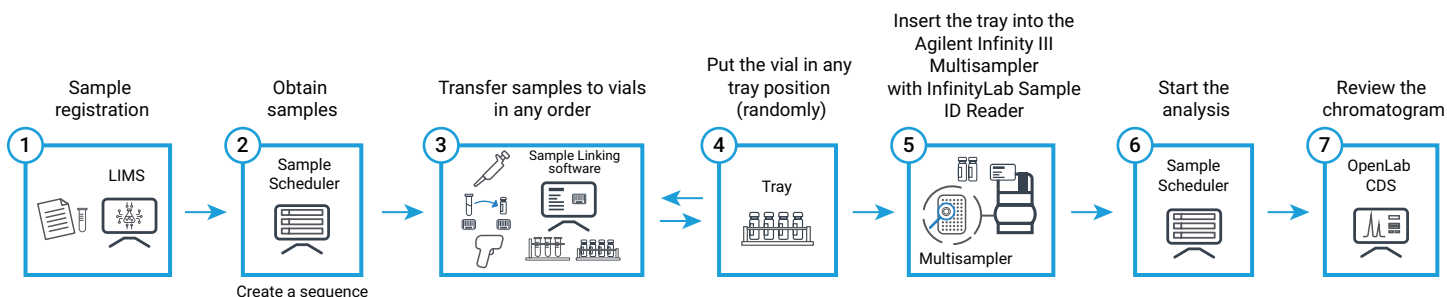


Figure 1. Integrated workflow from LIMS to results.



Figure 2. Start screen of the Agilent Sample Scheduler for OpenLab. Direct access to the respective information is available by clicking the boxes, graphics, and numbers. The menu on the left side can also be used for navigation.

After the arrival of the samples at the beginning of the workflow, the sample names and other information are directly sent from LIMS to Sample Scheduler and the unique identifier for each sample/LIMS ID is created and the task is assigned to the responsible analyst. After the operator or technician starts and logs into Sample Scheduler for

OpenLab, the samples appear in the Analyses tab as single samples or as a sequence when defined in LIMS. The sequence templates, which are predefined in the OpenLab Acquisition software, are available in the Sample Scheduler software and can be applied to the assigned samples (Figure 3).

Analyses							
<div> <div>Q</div> <div>Search</div> <div>+</div> <div>Add</div> <div>1</div> <div>Copy</div> <div>Select All</div> <div>Deselect All</div> <div>Sort:</div> <div>Merge</div> <div>Split</div> <div>Assign to</div> <div>Apply Template</div> </div>							
Name LIMS ID1	State	Project	Data file	Acq. method	Proc. method	Barcode	Instrument Vial
	Waiting	Parabens					HPLC-01 Injections: 4
Butylparaben ep0000045678	Waiting		<D>	Paraben-01.amx	Paraben-01.pmx		Vial: <input type="text"/>
Propylparaben ep0000034567	Waiting		<D>	Paraben-01.amx	Paraben-01.pmx		Vial: <input type="text"/>
Ethylparaben ep0000023456	Waiting		<D>	Paraben-01.amx	Paraben-01.pmx		Vial: <input type="text"/>
Methylparaben ep0000012345	Waiting		<D>	Paraben-01.amx	Paraben-01.pmx		Vial: <input type="text"/>
	Ended	Parabens					HPLC-01 Injections: 4

Figure 3. Agilent Sample Scheduler for OpenLab with assigned samples (shown in gray) grouped into a sequence by predefined sequence templates. The LIMS identifier can be seen together with the sample name, and acquisition and processing methods are included from the sequence template.

When this step is completed, the operator can switch to the Sample Linking software, which will link the barcoded sample containers, in single or in multiple steps, to the final barcoded target vials as follows. In the main screen of the Sample Linking software, the user's sequences will appear automatically (Figure 4A). The individual samples contained in the sequence are displayed with their name and current container ID. The sample container ID will be linked to the barcode of an empty vial by scanning of the vial's barcode,

and the sample becomes linked with the vial ID. If a sample is not part of the sequence and its barcode is scanned by accident, an error message will be displayed, and no vial will become linked to this sample. After the sample container ID and vial ID are linked, part of the sample is transferred to the vial. This procedure is repeated for all samples of the sequence. When all sample container barcodes are linked to the vial barcodes, the **Submit** button becomes active (Figure 4B).

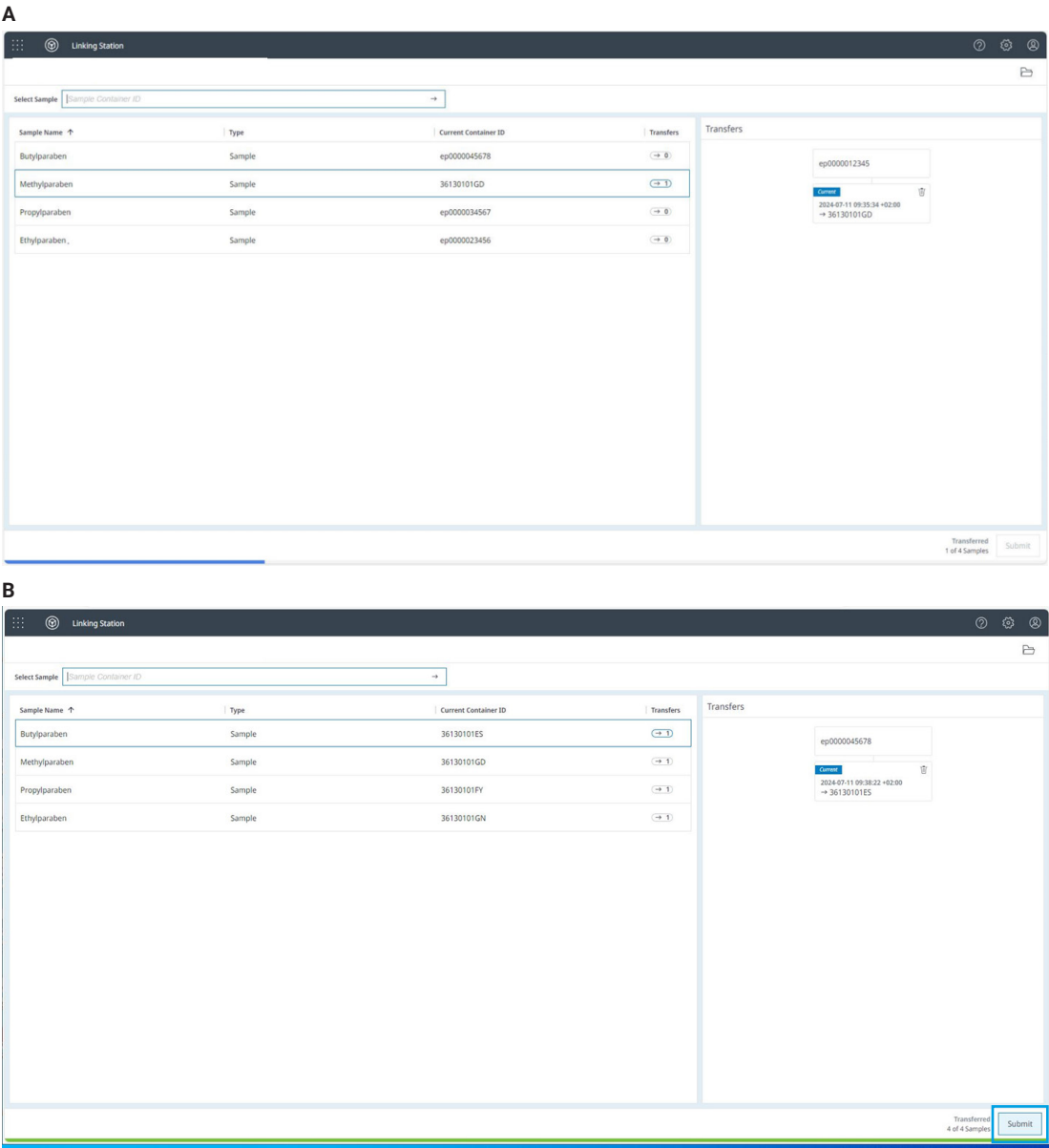


Figure 4. (A) Agilent Sample Linking software with the sample content of a selected sequence. The container ID of the highlighted sample was already updated from the LIMS ID to the vial ID. (B) Sample Linking software with the complete sample transfer from the LIMS ID to the vial ID, and the active Submit button.

After clicking **Submit** in the Sample Linking software, the sequence will be updated in the Sample Scheduler for OpenLab with the vial IDs and data file names. The sequence can be started immediately, or a starting time can be scheduled in the Sample Scheduler for OpenLab. No vial positions need to be entered into the sequence table. The 1260 or 1290 Infinity III Multisampler, which is equipped with the InfinityLab Sample ID Reader—the integrated barcode reader—will scan the new sample trays and identify the right position for injection, regardless of how the samples are arranged. For a running sequence, the status of the sequence and of the individual samples can be seen by the status bar with a representative color code on the left (Figure 5).

In the Instruments tab of the Sample Scheduler software, all connected instruments are displayed with a summary of their status. Figure 6 displays the connected instrument running the first sample of the sequence (injection 1 of 4), the analysis method, the completed samples, and the pending samples.

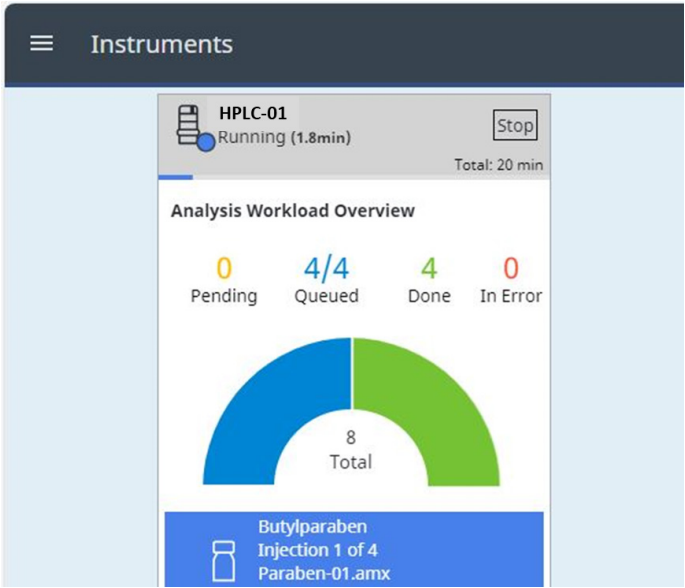


Figure 6. Status summary of the running instrument.

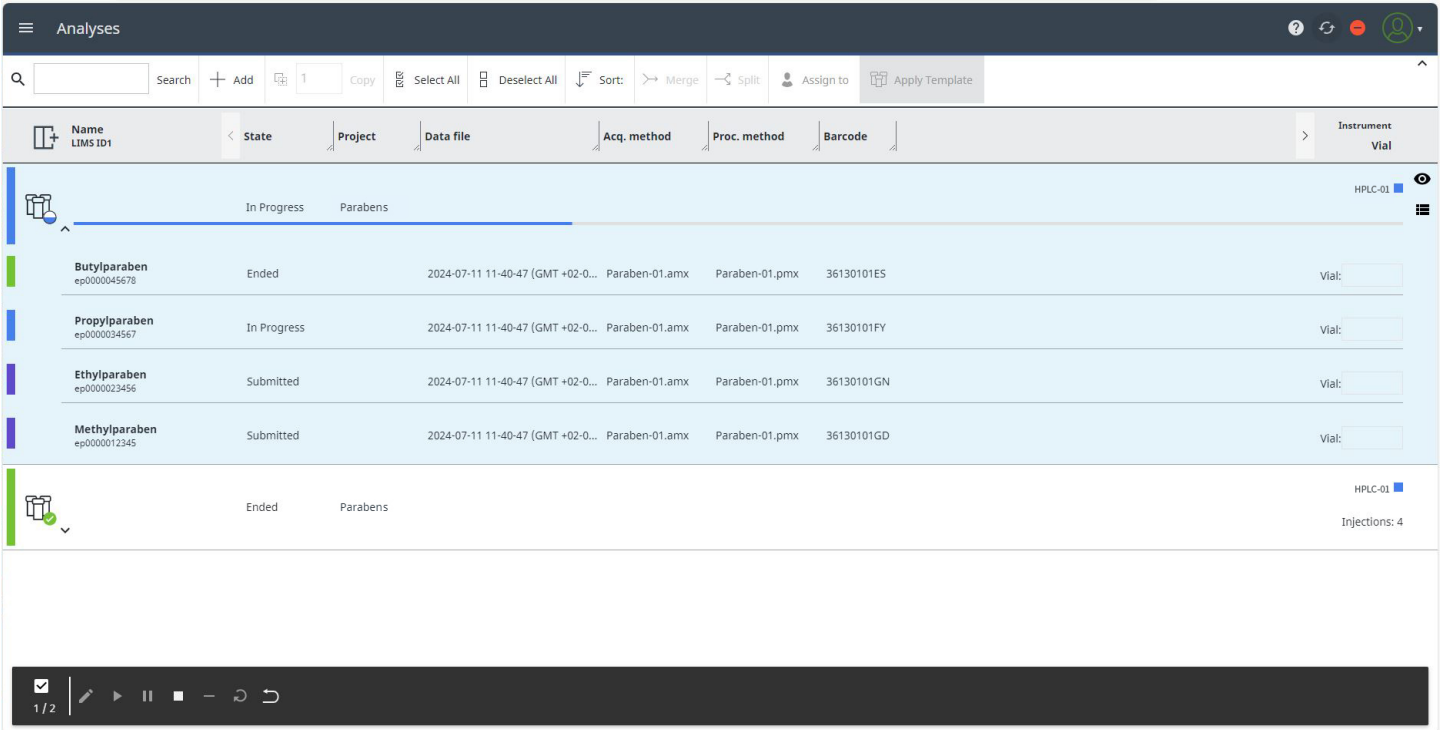


Figure 5. Agilent Sample Scheduler for OpenLab after starting a sequence. The status of the sequence and the second sample is "In Progress" (blue), the first sample is "Ended" (green), and the last two samples are "Submitted" (purple).

At the end of the sequence, all samples become marked with the status "Ended" and are color-coded in green. The data analysis that is selected in the sequence template is applied automatically, and the defined report template is filled with the calculated results (Figure 7). The data can be reviewed by a shortcut that starts OpenLab CDS Data Analysis software with the required data files.

If there is no LIMS available, a workflow for setting up the sequence, sample measurement confirmation, and flexible sample placing can be started directly from OpenLab CDS or the Sample Scheduler for OpenLab including Sample Linking software, which is detailed in other technical overviews.^{1,2}

Conclusion

This white paper describes a workflow that begins with an analytical sequence initiated by any LIMS, then links the barcodes of sample containers to the barcodes of target pre-barcoded vials. The samples are analyzed to get the final data results, and a report is transmitted back to LIMS. This closed-loop, error-free, and time-saving workflow is enabled by Agilent Sample Linking software together with the Agilent Sample Scheduler for OpenLab. Samples can be tracked through the complete workflow using barcodes to transfer them accurately from their original containers to a final barcoded vial, managed completely by the Sample Linking software. This saves time, enhances ease of use, and results in fewer errors over the complete workflow.

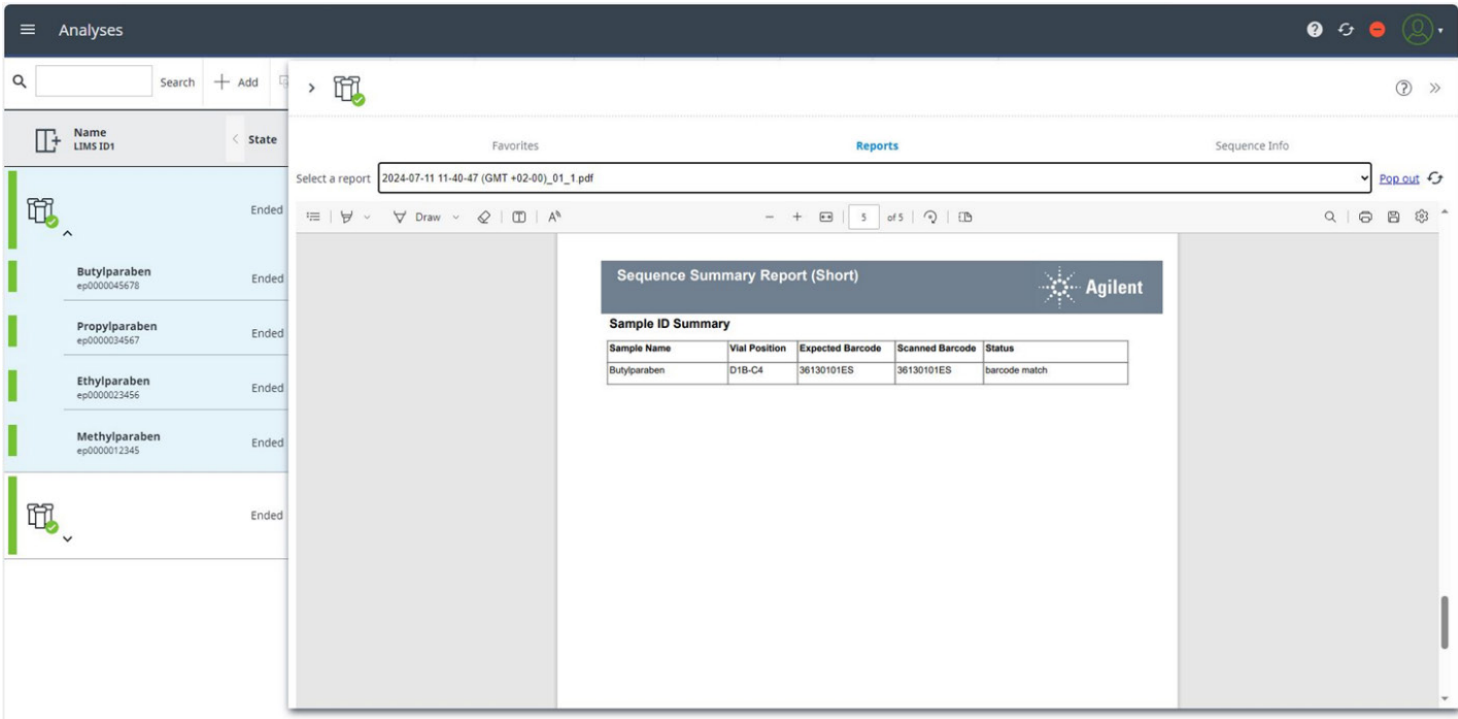


Figure 7. Agilent Sample Scheduler for OpenLab after the sequence is completed (status: "Ended", with a green color code). The selected data analysis method is applied, and a report is generated. This report shows the Sample ID Summary, which lists the expected barcode, scanned barcode, and identified vial position.

Appendix

Additional materials

- Vials with bottom barcode (part number 5181-3376-ID)
- Crimp caps, aluminum, PTFE/red rubber septa (part number 5061-3370)
- Forty-vial sample container with bottom holes for barcode reading (part number 5401-0068)
- Sample tray palette with open bottom for barcode reading (G7167-60205)
- USB handheld barcode scanner (part number 5018-0003)

References

1. Confirmation of Sample Position – Using the Agilent 1290 Infinity III Multisampler with Agilent InfinityLab Sample ID Reader – Part 1 of 2, *Agilent Technologies technical overview*, publication number 5994-7568EN, **2024**.
2. Sample Position Identification and Measurement Confirmation – Using the Agilent 1290 Infinity III Multisampler with Agilent InfinityLab Sample ID Reader – Part 2 of 2, *Agilent Technologies technical overview*, publication number 5994-7569EN, **2024**.

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