Technical Overview

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Confirmation of Sample Position

Using the Agilent 1290 Infinity III Multisampler with Agilent InfinityLab Sample ID Reader – Part 1 of 2

Abstract

The Agilent 1290 Infinity III Multisampler can be equipped with an additional Agilent InfinityLab Sample ID Reader that offers the ability to recognize a sample position to confirm the position given in the sequence table of Agilent OpenLab Acquisition software. The use of barcodes can be integrated into the analytical workflow, saving users time through greater ease-of-use and fewer errors.

Introduction

Barcode reading plays an important role in modern laboratories by handling samples, confirming that samples were measured, and ensuring that each correct result is linked to an individual sample. This is especially important if many samples will be handled in analytical laboratories, and is applicable in a large variety of industries and organizations. This technical overview demonstrates the use of the 1290 Infinity III Multisampler with built-in Sample ID Reader for the identification of sample position and confirmation of position selected by the sequence table in OpenLab Acquisition software. Position confirmation of samples is demonstrated using paraben compounds, which are typically used as antimicrobial agents in cosmetics.[1] The use of the 1290 Infinity III Multisampler equipped with the InfinityLab Sample ID Reader for the identification of a randomly chosen sample position and a complete software-aided end-to-end workflow is shown in two other Agilent technical overviews.[2,3]

Experimental

Instrumentation

- Agilent 1290 Infinity III High-Speed Pump (G7120A)
- Agilent 1290 Infinity III Multisampler (G7167B) equipped with two vial tray drawers and an Agilent InfinityLab Sample ID Reader (G4756A or option #110 of both the Agilent 1260 Infinity III Multisampler and the 1290 Infinity III Multisampler)
- Agilent 1290 Infinity III MCT (G7116B)
- Agilent 1290 Infinity III Diode Array Detector (G7117B) equipped with a 10 mm Agilent Max-Light Flow Cell
- Agilent InfinityLab Assist Upgrade (G7178A), consisting of the Agilent InfinityLab Assist Interface (G7179A) and Agilent InfinityLab Assist Hub (G7180A)

Software

Agilent OpenLab CDS, version 2.8 or later

Column

Agilent ZORBAX Eclipse Plus C18, RRHD, 2.1 × 100 mm, 1.8 µm (part number 959758-902)

LC method

Table 1. LC method.

Parameter	Value
Solvents	A) Water B) ACN
Flow Rate	0.5 mL/min
Gradient	Time (min) %B 0 15 5 95 Stop time: 5 min Post time: 2 min
Injection Volume	1 µL
Needle Wash	3 s in Solvent B
Column Temperature	45 °C
Detection	254/4 nm, Ref. 360/16 nm, data rate 20 Hz

Additional materials

- Vials with bottom barcode (part number 5190-4032-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)

Instrument and workflow setup

The Sample ID Reader module must be inserted into the vial drawer area of the 1290 Infinity III Multisampler, replacing the bottom drawer. The upper three drawers can be used for sample vial trays. The Sample ID Reader will be recognized automatically by Agilent OpenLab CDS software and displayed as a QR-code-style icon in the OpenLab software suite user interface of the Multisampler.

In the sequence table, the vial barcode was entered in the field of expected barcodes using a handheld barcode reader connected to the acquisition PC (Figure 1). The fields for sample name and data file name can also be filled by barcode scanning. Vial position for measurement confirmation was entered manually in the vial column.

Chemicals used included methylparaben, ethylparaben, propylparaben, and butylparaben. Parabens were dissolved in acetonitrile at 100 mg/L and sealed in individual QR-coded vials. Chemicals were purchased from VWR, Germany.

Samples

- Sample 01: methylparaben
- Sample 02: ethylparaben
- Sample 03: propylparaben
- Sample 04: butylparaben

Solvents

All solvents used were LC-grade. Fresh ultrapure water was obtained from a Milli-Q Integral system equipped with a 0.22 µm membrane point-of-use cartridge (Millipak).

Results and discussion

In a typical analytical workflow, the prepared sample arrives labeled with a barcode describing sample identification details. This barcode was read into the sequence list as the sample name (Figure 1). The sample was transferred to a vial with a barcode on its bottom, and the unique vial identifier number was read into the sequence list in the expected barcode column. Vial position was entered in the vial column manually.

After generation of the complete sequence, the sample tray was inserted in the sample drawer of the 1290 Infinity III Multisampler with Sample ID Reader. When closing the drawer, all vials included in the tray were scanned automatically, and the information was stored. At the start of the sequence, the acquisition software compares the information from the scanned vials to their position with the expected barcodes from the sequence list. It analyzes them according to the order in the sequence list. Data analysis of the complete sequence shows the injection list and the expected barcode for confirmation, along with the measured information and the respective vial position (Figure 2).

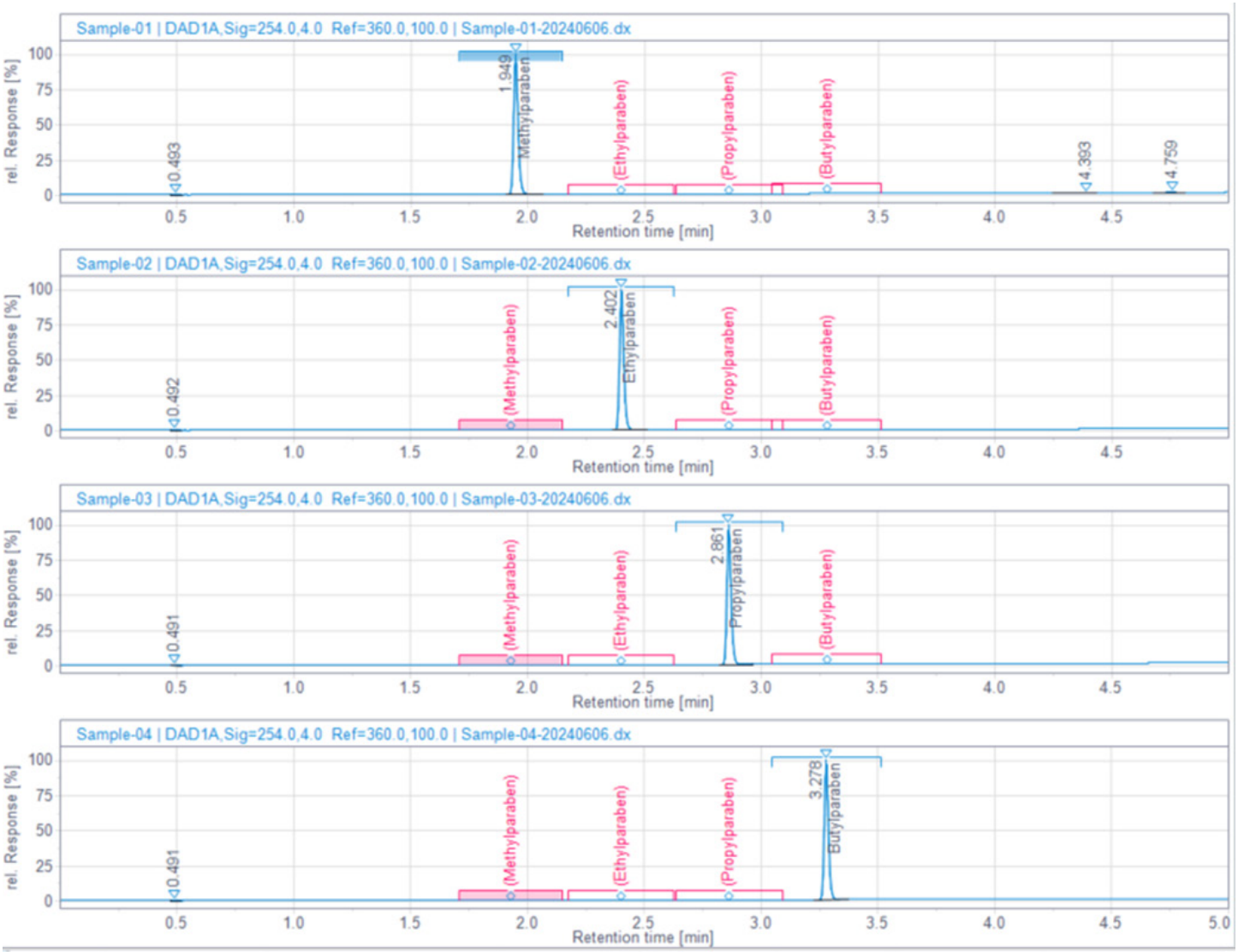
If a vial barcode is missing, or a vial was accidentally placed at a position not corresponding with the position defined in the sequence list by the respective barcode, error handling can be set in the sequence options.

There are two ways of handling misplaced vials:

1. Inject anyway: In this approach, the sample is injected, measured with the defined acquisition method, and acquired data are analyzed as defined. Both the expected and mismatching barcodes are reported in the data file.
2. Abort current injection: In this approach, the sample is skipped without injection.

		Action	Vial	Acq. method	Proc. method	Inj/Vial	Volume	Injection source	Sample name	Data file	Expected barcode
1	☑	Inject	D1F-A1	Paraben-01.amx	Paraben-01.pmx	1	Use Method	HipAls	Sample-01 >	Sample-01-20240606 >	36130101GD
2	☑	Inject	D1F-A2	Paraben-01.amx	Paraben-01.pmx	1	Use Method	HipAls	Sample-02	Sample-02-20240606	36130101GN
3	☑	Inject	D1F-A3	Paraben-01.amx	Paraben-01.pmx	1	Use Method	HipAls	Sample-03	Sample-03-20240606	36130101EI
4	☑	Inject	D1F-A4	Paraben-01.amx	Paraben-01.pmx	1	Use Method	HipAls	Sample-04	Sample-04-20240606	36130101ES

Figure 1. Sequence table used in Agilent OpenLab software suite. The expected vial barcode was scanned with an external handheld barcode reader, and the chosen vial position was entered in the vial column.



Inj. #	Sample name	Data file	Acq. method	Proc. method	Vial	Barcode	Expected barcode
1	Sample-01	Sample-01-20240606.dx	Paraben-01	Paraben-01	D1F-A1	36130101GD	36130101GD
1	Sample-02	Sample-02-20240606.dx	Paraben-01	Paraben-01	D1F-A2	36130101GN	36130101GN
1	Sample-03	Sample-03-20240606.dx	Paraben-01	Paraben-01	D1F-A3	36130101EI	36130101EI
1	Sample-04	Sample-04-20240606.dx	Paraben-01	Paraben-01	D1F-A4	36130101ES	36130101ES

Figure 2. Results of data analysis after sequence run. The injection list shows the expected barcode for confirmation with the matching barcode, as well as the respective vial position. The chromatograms show the expected compounds.

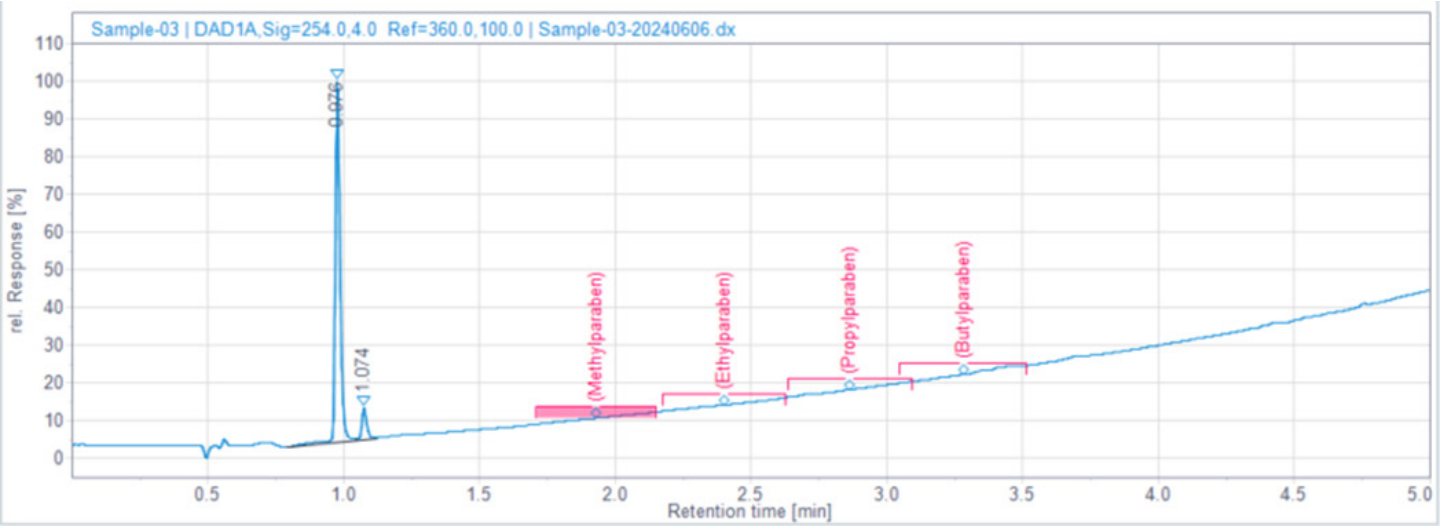
Figure 3 displays the result of an injection from a misplaced vial using the **inject anyway** option. In the injection list, there is a mismatch between the expected and observed barcode for sample 03. The resulting chromatogram shows that another compound eluted at a retention time of 0.976 minutes. This barcode confirmation prevents the accidental acceptance of a wrong measurement delivering false positive or negative data.

The scenarios of matching and mismatching barcodes, displayed in Figures 2 and 3, can be made visible in an at-a-glance sequence summary report that includes information about scanned and expected barcodes with their matching status (Figure 4).

The following scenarios can be displayed:

Table 2. Indicators of possible barcode scenarios.

Scenario	Indicator
Expected and Scanned Barcode are Identical	Not colored
Expected and Scanned Barcode Differ	Coded in red
No Scanned Barcode is Present, but Expected Barcode is Present	Coded in red
No Scanned Barcode is Present, and No Expected Barcode is Present	Not colored



Inj. #	Sample name	Data file	Acq. method	Proc. method	Vial	Barcode	Expected barcode
1	Sample-01	Sample-01-20240606.dx	Paraben-01	Paraben-01	D1F-A1	36130101GD	36130101GD
1	Sample-02	Sample-02-20240606.dx	Paraben-01	Paraben-01	D1F-A2	36130101GN	36130101GN
1	Sample-03	Sample-03-20240606.dx	Paraben-01	Paraben-01	D1F-A3	36130101E0	36130101EI
1	Sample-04	Sample-04-20240606.dx	Paraben-01	Paraben-01	D1F-A4	36130101ES	36130101ES

Figure 3. Confirmation of sample measurement at the defined position. The expected barcode reveals accidentally misplaced samples.

A

Sequence Summary Report (Short)

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Sample ID Summary

Sample Name	Vial Position	Expected Barcode	Scanned Barcode	Status
Sample-01	D1F-A1	36130101GD	36130101GD	barcode match
Sample-02	D1F-A2	36130101GN	36130101GN	barcode match
Sample-03	D1F-A3	36130101EI	36130101EI	barcode match
Sample-04	D1F-A4	36130101ES	36130101ES	barcode match

B

Sequence Summary Report (Short)

Agilent

Sample ID Summary

Sample Name	Vial Position	Expected Barcode	Scanned Barcode	Status
Sample-01	D1F-A1	36130101GD	36130101GD	barcode match
Sample-02	D1F-A2	36130101GN	36130101GN	barcode match
Sample-03	**D1F-A3**	**36130101EI**	**36130101E0**	**barcode mismatch**
Sample-04	D1F-A4	36130101ES	36130101ES	barcode match

Figure 4. Sequence summary report, including the status of barcode matching. (A) All expected barcodes match the scanned barcodes (Figure 2). (B) The scanned barcode does not match the expected barcode, and is color-coded in red (Figure 3).

Conclusion

This technical overview describes the functionality of the Agilent 1290 Infinity III Multisampler equipped with an Agilent InfinityLab Sample ID Reader for confirmation of sample positions. Vial positions and barcodes given in the sequence are checked against the barcodes identified by the Sample ID Reader in the Multisampler. The barcode confirmation and the identified position are given in the results table after data analysis for a final confirmation of sample measurement. Barcodes can be reported, highlighting misplaced samples. This saves time and enables higher ease-of-use with fewer errors for confirmation of sample analysis.

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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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