Technical Overview

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Sample Position Identification and Measurement Confirmation

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

Abstract

With the release of the Infinity III LC series, the Agilent 1290 Infinity III Multisampler can be equipped with an optional Agilent InfinityLab Sample ID Reader, which can recognize sample position without entering an exact location. Since barcodes are a part of analytical workflows, sample tracking to confirm analysis of each scheduled sample is possible. In addition to the built-in Sample ID Reader, an additional external handheld barcode reader can be connected to a PC, or sample information can be introduced by spreadsheets containing appropriate sample barcode information. This technical overview highlights the benefits of using the 1290 Infinity III Multisampler for an analytical workflow when a sample ID-reading autosampler is used. This saves time and enables higher ease-of-use with fewer errors for confirmation of sample analysis.

Introduction

Many analytical laboratories are equipped with barcode readers to introduce sample information to the analytical data software. The given information appears in the acquisition and data analysis software interface. The 1290 Infinity III Multisampler can be equipped with an internal Sample ID Reader to confirm sample identity and correct position location. This closes a gap of sample handling between barcode introduction to the acquisition software and association with the sample in the data analysis software.

This technical overview demonstrates the use of the 1290 Infinity III Multisampler with built-in Sample ID Reader for automatic sample position identification. Vials are equipped with a barcode at the bottom for reading from below the tray. Automatic identification, position location, and analysis tracking information is stored. In this demonstration, different parabens were analyzed, with the respective vials randomly inserted into the 1290 Infinity III Multisampler without giving the vial location in the sequence table.

Confirmation of the measurement of a sample by means of the internal Sample ID Reader with a given sample position and a complete software-aided end-to-end workflow is shown in two other Agilent technical overviews.[1,2]

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 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/workflow setup

The InfinityLab 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.

To switch on the barcode functionality, select **Use Barcode Reader Before Injection** in the sequence run options. In the sequence table, additional external barcodes can be read-in directly from the sample container to give a sample name and data file name. In the expected barcode field, the barcode from the respective vial can be read in with a handheld scanner for later recognition in the Multisampler (Figure 1). It is not necessary to give a vial location. After inserting the vial tray into the Multisampler vial tray drawer, the entire tray will be scanned. Vials belonging to the current sequence will be identified, and the acquisition can be started.

		Action	Vial	Acq. method	Proc. method	Inj/Vial	Volume	Injection source	Sample name	Data file	Expected barcode
1	☑	Inject		Parabene-01.amx	Paraben-01.pmx	1	Use Method	HipAls	Sample-01	Sample-01-20240528	36130101GD
2	☑	Inject		Parabene-01.amx	Paraben-01.pmx	1	Use Method	HipAls	Sample-02	Sample-02-20240528	36130101GN
3	☑	Inject		Parabene-01.amx	Paraben-01.pmx	1	Use Method	HipAls	Sample-03	Sample-03-20240528	36130101EI
4	☑	Inject		Parabene-01.amx	Paraben-01.pmx	1	Use Method	HipAls	Sample-04	Sample-04-20240528	36130101ES

Figure 1. Sequence table showing the samples contained in the run sequence. External bar codes with sample information can be read-in, for instance, in the fields for sample name and data file. The barcode of the respective vials was read-in in the expected barcode field. No positions for the vials were given.

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

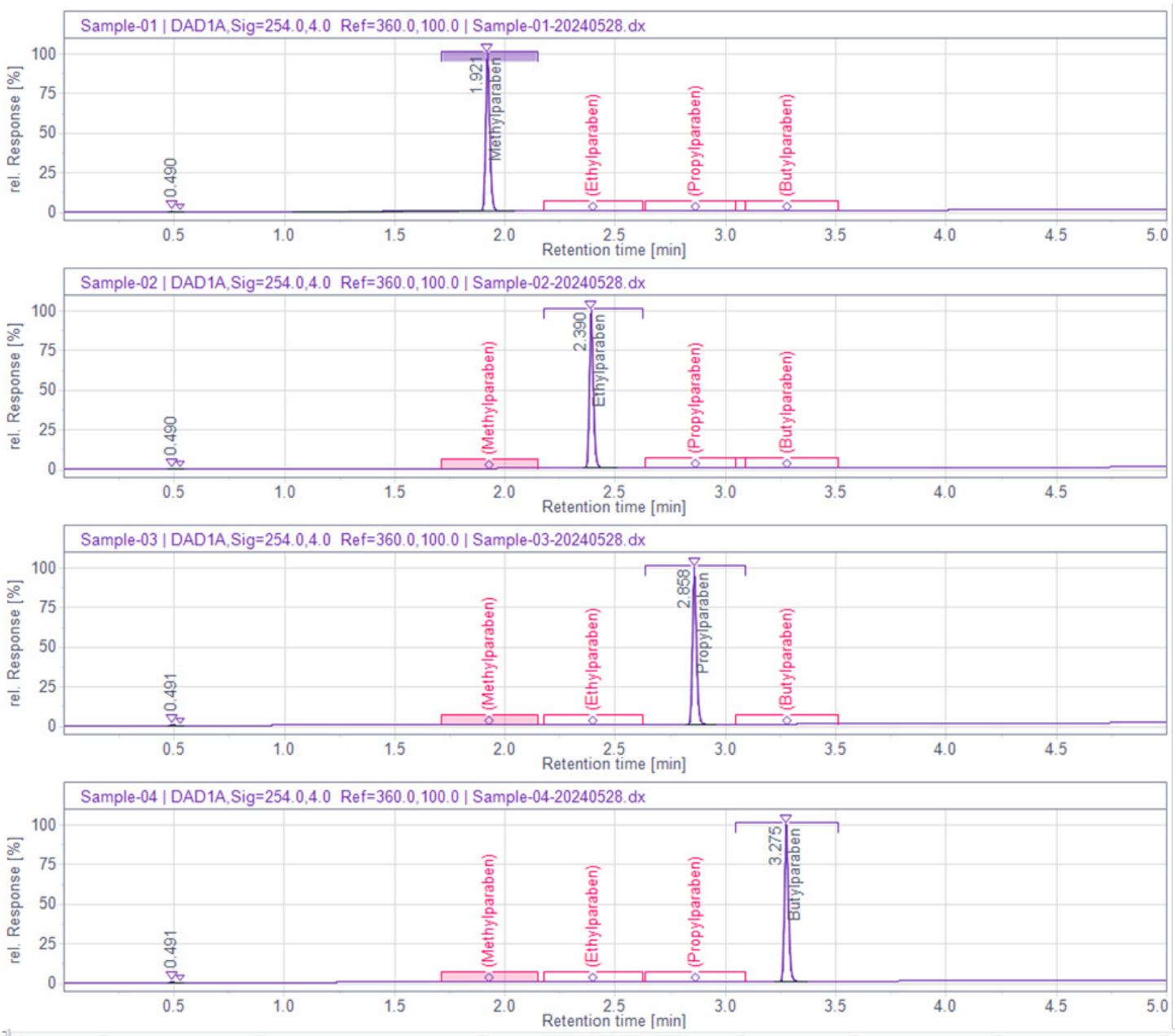
Samples:

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

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

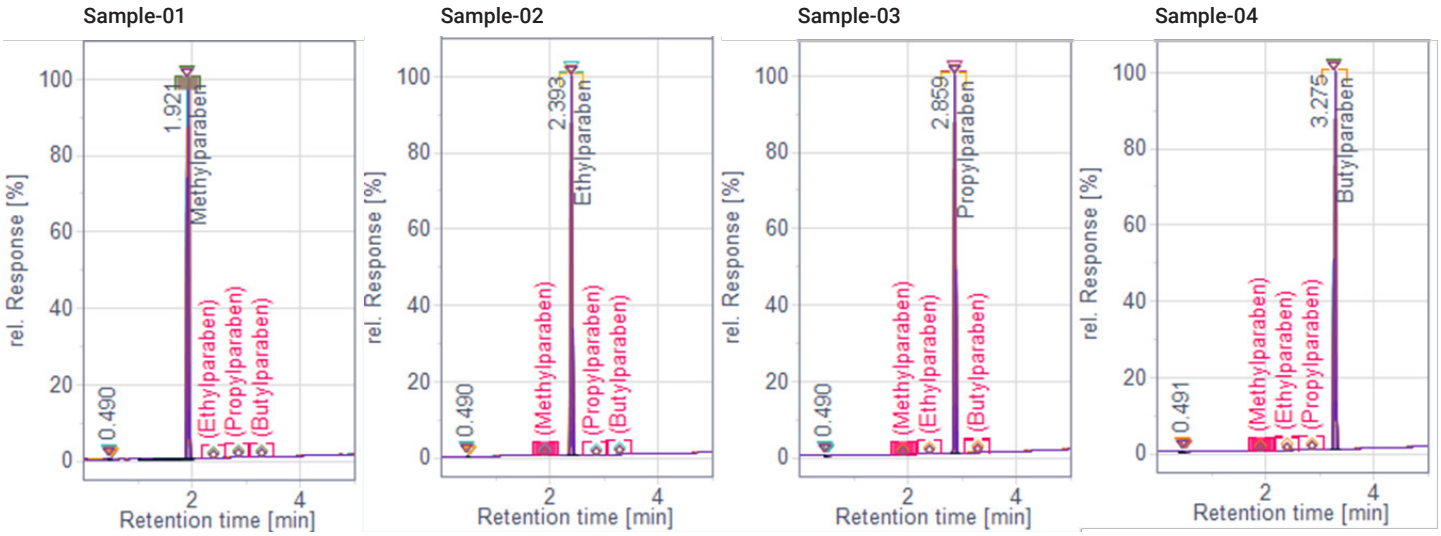
The paraben compounds used in this study were dissolved in acetonitrile (100 mg/L each) and 1 mL of each was transferred to a barcoded vial. The barcodes of the vials were manually scanned into the field for the expected barcode in the sequence table (Figure 1). Specific vial positions were not given. The vials were placed in a random order and position in a 40-vial tray for bottom barcode reading. Other positions of the tray were filled with other barcoded vials not used in this study, or left unoccupied. After placing the vial tray in the drawer of the 1290 Infinity III Multisampler, the tray was automatically taken by the Multisampler and placed above the built-in Sample ID Reader. After scanning the tray, all barcoded vial numbers were used to identify the specific vial positions at the start of the sequence. After measurement of the samples, the expected barcodes of the measured samples were confirmed and displayed in the injection list table of Agilent OpenLab Data Analysis software. The identified position was also filled in the injection table (Figure 2).
In the chromatograms, the predefined data analysis method displays the identified paraben compound. For instance, sample 01 contained methylparaben and was found in drawer one of the front tray at position D1 (D1F-D1). The expected barcode matches the one scanned from the vial by the Sample ID Reader in the Multisampler.



Inj. #	Sample name	Data file	Acq. method	Proc. method	Vial	Barcode	Expected barcode
1	Sample-01	Sample-01-20240528.dx	Parabene-01	Paraben-01	D1F-D1	36130101GD	36130101GD
1	Sample-02	Sample-02-20240528.dx	Parabene-01	Paraben-01	D1F-C8	36130101GN	36130101GN
1	Sample-03	Sample-03-20240528.dx	Parabene-01	Paraben-01	D1F-D6	36130101EI	36130101EI
1	Sample-04	Sample-04-20240528.dx	Parabene-01	Paraben-01	D1F-A1	36130101ES	36130101ES

Figure 2. Identification of randomly placed samples by expected barcode. The expected barcode was introduced with the sequence table. The vial position was assigned after confirmation of the barcode by the Multisampler (vial label example: D1F-D1: Drawer1Front, position D1).

To test this functionality in a more extensive way, the positions of the vials in the 40-vial tray were changed randomly. The following measurements were used to confirm sample identity and position (Figure 3). The scanning process was also tested for the corner positions of the tray in rows A and E at positions 1 and 8, respectively (Figure 3, table, line 4). With the following experiments, the sample vials were not placed in one vial tray, but rather were placed in front and back positions of one drawer (Figure 3, table, lines 5 and 6). Finally, the samples were placed in two vial trays in two drawers (Figure 3, table, lines 7 and 8). In both cases, the samples were placed such that one or two changes of the vial tray and drawer were necessary to measure the samples in the sequence. All identified compounds are displayed as an overlay (per vial) in Figure 3.



Line	Sample-01	Sample-02	Sample-03	Sample-04
1	D1F-D1	D1F-C8	D1F-D6	D1F-A8
2	D1F-A4	D1F-E3	D1F-C6	D1F-C2
3	D1F-C2	D1F-B5	D1F-E1	D1F-C5
4	D1F-E1	D1F-A1	D1F-A8	D1F-E8
5	D1F-B4	D2F-C3	D1F-C5	D2F-C6
6	D2F-C4	D1F-C2	D1F-E4	D1F-A6
7	D1B-D6	D1F-C1	D1F-D5	D1F-B7
8	D1B-B4	D1F-D2	D1B-D6	D1F-C6

Figure 3. Identification of randomly placed samples, including the use of multiple drawers (D1, D2 = drawer 1 and drawer 2, F, B = front, back). Chromatograms show an overlay of the respective sample.

Conclusion

This technical overview describes the functionality of the Agilent 1290 Infinity III Multisampler equipped with an Agilent InfinityLab Sample ID Reader for the identification of sample positions which have to be measured in a given sequence. The samples can be placed randomly in the 1290 Infinity III Multisampler. The barcode confirmation and identified position will be given in the results table after data analysis for a final confirmation of sample measurement. This saves time and enables higher ease-of-use with fewer errors for confirmation of sample analysis.

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. Agilent Advanced Sample Linking – A Complete Workflow from Any Laboratory Information Management System to the Vial and Analytical Results. *Agilent Technologies white paper*, publication number 5994-7570EN, **2024**.

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