Technical Overview

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Smooth Migration from Single Quadrupole ICP-MS to the Agilent 9500 ICP-QQQ

Automated method transfer using the Batch Conversion Tool of Agilent OpenLab ICP-MS software

Introduction

Transitioning from a single quadrupole (SQ) ICP-MS to a triple quadrupole ICP-MS (ICP-QQQ) might appear daunting or disruptive, usually requiring the redevelopment of analytical methods and workflows. Users often wonder if they can reuse existing batches and whether routine processes will be interrupted during this switch.

Switching from SQ ICP-MS to the Agilent 9500 ICP-QQQ involves minimal disruption. Agilent provides a solution that enables smooth, automated transfer of existing SQ ICP-MS methods to the 9500 ICP-QQQ, all while preserving the current batch logic and analytical purpose.

This note explains how the Batch Conversion Tool in Agilent OpenLab ICP-MS software facilitates automated batch conversion. It allows users to seamlessly transition from SQ ICP-MS to the 9500 ICP-QQQ without needing to rebuild methods or alter their existing workflows.

Three key aspects of method migration are addressed in this document:

- The design concept and conversion behavior of the Batch Conversion Tool, detailing which batch elements are preserved or adapted during conversion.
- It also explains the rationale behind the available conversion options and how the advanced cell technologies of the 9500, such as Advanced Helium Mode (AHM) and Air cell mode, support operational continuity and potential performance improvements after migration.
- Additionally, it outlines a typical end-to-end migration workflow, including methods for reviewing the post-conversion process and assessing data quality using built-in indicators.

These points collectively show that switching from SQ ICP-MS to the 9500 ICP-QQQ can be seamless. They also illustrate how to carry out method transfer in a controlled and transparent manner, providing a practical framework for refining the method when necessary.

What is the Batch Conversion Tool?

The Batch Conversion Tool is a feature of OpenLab ICP-MS software that transforms batches created for Agilent SQ ICP-MS systems into formats compatible with the 9500 ICP-QQQ (see Figure 1).

Batches made for Agilent 7700, 7800, 7850, and 7900 ICP-MS instruments using Agilent ICP-MS MassHunter or OpenLab ICP-MS software can be imported and converted. During this process, the tool applies predefined rules to produce a batch suitable for the 9500, all while maintaining the original batch setup.

These conversion rules are based on Agilent's over 10 years of experience in ICP-QQQ development and applications. By harnessing this expertise, the Batch Conversion Tool automatically implements optimal measurement conditions and reaction strategies for each analyte, ensuring strong interference control and consistent analytical performance post-migration.

Manually recreating batch components like element selections, isotope settings, and QC configurations can be time-consuming. Alternatively, the Batch Conversion Tool automates this process, usually finishing within seconds.

The handling of individual batch components is summarized in Table 1.

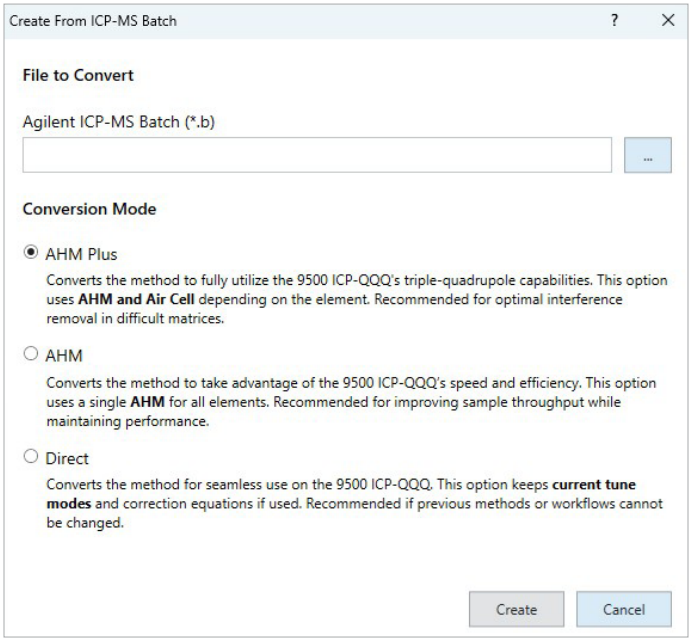
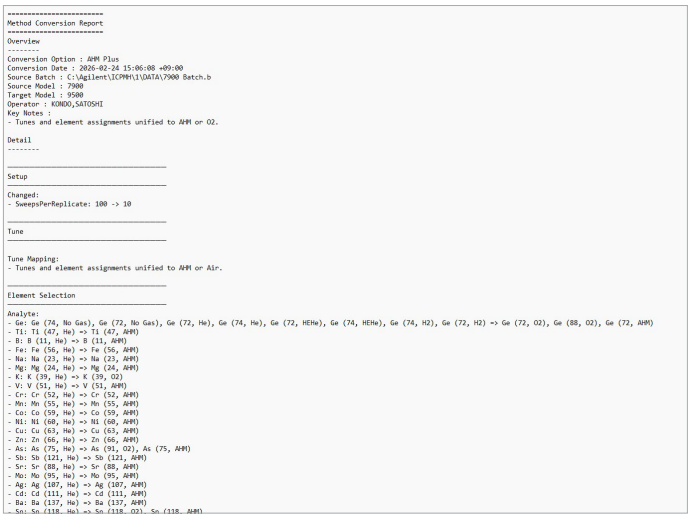


Figure 1. The user interface of the Batch Conversion Tool in Agilent OpenLab ICP-MS software.

Table 1. Handling of batch components during conversion.

Batch Component	Converted	Conversion Behavior
Setup	Yes	Spectrum mode options are updated to 9500 default settings.
Tune Modes	Yes	Converted according to the selected conversion option (see next section). Original values are retained when the "Direct" option is selected.
Tune Parameters	Yes	Converted to 9500 Auto Tune.
Element Selection	Yes	Converted according to the selected conversion option (see next section). Original values are retained when the "Direct" option is selected.
Sample Introduction	Yes/No	Original settings are retained. If the original configuration is not compatible with the 9500 hardware configuration, default settings are applied when using an Agilent autosampler.
QC Settings	No	Original settings are retained. Converted element selections are reflected.
Sample List	No	Original settings are retained.
Data Analysis Method	No	Original settings are retained. Converted element selections are reflected.

Once the conversion is complete, a report is automatically created. It offers a comprehensive overview of the conversion results and enables users to review how each batch component was processed (see Figure 2).



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Method Conversion Report
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Overview
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Conversion Option : AHM Plus
Conversion Date : 2026-02-24 15:06:08 +09:00
Source Batch : C:\Agilent\ICPMH\1\DATA\7900 Batch.b
Source Model : 7900
Target Model : 9500
Operator : KONDO,SATOSHI
Key Notes :
- Tunes and element assignments unified to AHM or O2.

Detail
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_____________________________________
Setup
_____________________________________
Changed:
- SweepsPerReplicate: 100 -> 10

_____________________________________
Tune
_____________________________________

Tune Mapping:
- Tunes and element assignments unified to AHM or Air.

_____________________________________
Element Selection
_____________________________________
Analyte:
- Ge: Ge (74, No Gas), Ge (72, No Gas), Ge (72, He), Ge (74, He), Ge (72, HEHe), Ge (74, HEHe), Ge (74, H2), Ge (72, H2) -> Ge (72, O2), Ge (88, O2), Ge (72, AHM)
- Ti: Ti (47, He) -> Ti (47, AHM)
- B: B (11, He) -> B (11, AHM)
- Fe: Fe (56, He) -> Fe (56, AHM)
- Na: Na (23, He) -> Na (23, AHM)
- Mg: Mg (24, He) -> Mg (24, AHM)
- K: K (39, He) -> K (39, O2)
- V: V (51, He) -> V (51, AHM)
- Cr: Cr (52, He) -> Cr (52, AHM)
- Mn: Mn (55, He) -> Mn (55, AHM)
- Co: Co (59, He) -> Co (59, AHM)
- Ni: Ni (60, He) -> Ni (60, AHM)
- Cu: Cu (63, He) -> Cu (63, AHM)
- Zn: Zn (66, He) -> Zn (66, AHM)
- As: As (75, He) -> As (91, O2), As (75, AHM)
- Sb: Sb (121, He) -> Sb (121, AHM)
- Sr: Sr (88, He) -> Sr (88, AHM)
- Mo: Mo (95, He) -> Mo (95, AHM)
- Ag: Ag (107, He) -> Ag (107, AHM)
- Cd: Cd (111, He) -> Cd (111, AHM)
- Ba: Ba (137, He) -> Ba (137, AHM)
- Sn: Sn (118, He) -> Sn (118, O2), Sn (118, AHM)
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Figure 2. Example of a batch conversion report.

Conversion options in the Batch Conversion Tool

When migrating SQ methods, a key concern is whether similar or improved analytical performance can be maintained without adding unnecessary complexity.

The Batch Conversion Tool offers three different conversion options, each tailored to a specific migration goal—ranging from preserving method continuity to optimizing for performance.

Option 1: AHM Plus

This option assigns AHM or Air cell mode depending on the element.

AHM is an advanced helium collision mode introduced with the 9500 ICP-QQQ. It is enabled by the 9500 ICP-QQQ system's Dual-Cell System (DCS). These technologies provide high sensitivity across the mass range while maintaining effective interference removal for routine applications. Further technical details are provided in reference 1.

Air cell mode operates as a reaction mode utilizing ambient air as the reaction gas. It minimizes interferences without requiring external gases, simplifying the operation while ensuring effective interference management. For a comprehensive explanation of Air cell mode, see reference 2.

Option 2: AHM

This option applies AHM to all elements in the batch. Using a single tune mode eliminates tune switching during analysis, significantly improving sample throughput.

Because AHM provides functional coverage comparable to that of no gas and conventional helium modes, many SQ methods can be combined into a single AHM-based workflow without compromising analytical performance. Examples of measurements conducted using AHM only are included in reference 3.

Option 3: Direct

This option retains the original tune modes and, if relevant, any correction equations. It is suitable when existing standard operating procedures or regulated workflows need to remain unchanged.

Method migration objectives and benefits

Each conversion choice corresponds to a specific migration goal while utilizing the technical benefits of the 9500 ICP-QQQ platform.

Option 1: AHM Plus is ideal for situations demanding maximum interference removal from difficult matrices. It assigns AHM or Air cell modes to individual elements, harnessing the 9500 ICP-QQQ system's full interference-mitigation capabilities during method migration.

For example, AHM has been shown to provide significantly higher sensitivity and lower background equivalent concentrations (BECs) than conventional He mode across a wide range of elements, including low-mass analytes such as Be and B, as well as mid- to high-mass elements in complex matrices.

Air cell mode effectively addresses interferences that collision processes alone cannot fully suppress, such as interferences from doubly charged rare earth elements (REE^{2+}) on As, Se, and Ge, or certain oxide-based interferences.

By combining these two modes, this option allows migrated methods to fully utilize the 9500 ICP-QQQ capabilities, leading to more robust methods that better tolerate unexpected interferences than SQ ICP-MS, especially in matrices with high salt content, carbon, or REEs.

Option 2: AHM prioritizes simplicity and speed by removing the need to switch between tune modes and leveraging its high sensitivity to reduce integration times, while still ensuring analytical robustness.

For example, many SQ ICP-MS preset methods, such as those used on the 7900 ICP-MS, involve multiple tune modes like no gas, He, and high-energy (HE) He. When measuring about 40 elements, the typical acquisition time per sample is around 50 seconds, plus extra stabilization time when switching modes. This results in a total analysis time of roughly 60 seconds.

By migrating such a method to the 9500 ICP-QQQ with a single AHM-based workflow, tune mode switching and stabilization can be avoided. Also, AHM's high sensitivity allows for shorter acquisition times without compromising performance. Consequently, total measurement time can be cut by 20% or more, boosting sample throughput without increasing method complexity.

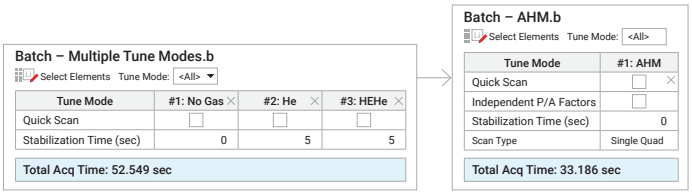

Figure 3. Comparison of analysis time before and after switching from an SQ ICP-MS preset method to a single AHM-based workflow on the Agilent 9500 ICP-QQQ. By consolidating multiple tune modes (no gas, He, HEHe) into AHM, you eliminate tune stabilization time. Combined with shorter integration times enabled by AHM's high sensitivity, this change reduces the total analysis duration.

Option 3: Direct supports strict method continuity when changes to established workflows are not permitted.

The Batch Conversion Tool turns a complicated, manual task into a straightforward process that keeps your analytical goals clear and opens opportunities to improve your methods whenever possible.

Overall migration workflow

A typical migration from SQ ICP-MS to the 9500 ICP-QQQ follows a simple three-step workflow:

1. Convert the batch copied from an existing SQ system using the Batch Conversion Tool
2. Perform measurements on the 9500 ICP-QQQ
3. Review analytical results

[1] *Note that compliance solutions such as Agilent Workstation Plus or ECM XT may require controlled transfer procedures.*

When using AHM Plus or AHM options, IntelliQuant Star Rating in OpenLab ICP-MS software aids in reviewing data quality for results obtained with AHM. The five-star rating system offers a straightforward, qualitative evaluation of overall confidence in the data, considering criteria such as spectral interferences, measurement precision, detection limits, backgrounds, and calibration quality.

Based on this assessment, selected elements can be reassigned to other modes, such as Air cell mode if needed. This workflow adds confidence during method migration, especially when updating to new cell modes. For more details on IntelliQuant and the Star Rating concept, see reference 4.

Migration from non-Agilent instruments using Method Advisor

Besides batch-based migration from Agilent SQ ICP-MS systems, methods from non-Agilent instruments can also be transferred to the 9500 ICP-QQQ by importing a target elements list (CSV file) into Method Advisor.

Method Advisor, a feature of OpenLab ICP-MS software, uses the same software-assisted logic as AHM Plus and AHM options to automatically generate most method parameters, making it easier to create methods when switching from non-Agilent or non-ICP-MS platforms.

Conclusion

The Batch Conversion Tool in Agilent OpenLab ICP-MS software allows for easy, automated transfer of existing SQ ICP-MS batches to the Agilent 9500 ICP-QQQ, without affecting current analytical workflows.

By maintaining batch structure and analytical intent, users can switch to the 9500 ICP-QQQ without needing to rebuild methods or disrupt daily operations. The tool also offers structured conversion options to help users harness the advanced features of the 9500 platform.

Additionally, migration from non-Agilent ICP-MS systems can be streamlined through element list import via the Method Advisor, providing an efficient way to create methods when transitioning to Agilent equipment. Overall, moving from SQ ICP-MS to the 9500 ICP-QQQ is a smooth, controlled process that ensures continuity and offers opportunities for method enhancement.

References

1. Dual-Cell System (DCS) and Advanced Helium Mode (AHM), Agilent publication, 5994-8985EN
2. Air Cell Mode of the Agilent 9500 ICP-QQQ with Dual-Cell System, Agilent publication, 5994-8987EN
3. Siva, S. Automated Analysis of Foods by ICP-QQQ, Agilent publication, 5994-9095EN
4. Agilent ICP-MS IntelliQuant Analysis, Agilent publication, 5994-7441EN

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