

Rethinking Routine Quality Control for Food & Beverage

Direct analysis of representative volatile quality markers in fortified wine

The Challenge

The Food & Beverage Industry is being asked to do more with less. Quality teams need to support more samples, make decisions faster, and maintain consistent product release without adding unnecessary complexity to the laboratory workflow. For many routine tests, the bottleneck is not the measurement itself, but the preparation required before the sample ever reaches the instrument.

That challenge is especially clear in products such as fortified wine. Volatile quality markers are routinely monitored to support product consistency, process control, and quality decisions. These markers are typically measured by direct-injection GC, which requires the wine to be distilled first to remove sugars and other non-volatile components that can compromise routine GC operation. That distillation step adds time and manual sample handling to an already busy QC process.

This creates a practical question for routine quality control. Can the workflow be simplified while still providing the information needed to support confident quality decisions?

A Simpler Workflow

A simpler approach begins by rethinking what routine testing needs to measure. Even established GC panels are targeted methods rather than complete characterization, so exhaustive analysis was never really the standard. What supports a release decision is a well-chosen set of representative markers, and how directly and reliably those markers can be measured. Headspace-MRR provides a direct way to do this, identifying each marker by its molecular structure rather than by retention time so it can be measured directly in the sample headspace.

In this workflow, fortified wine is analyzed directly as a neat sample. Because headspace sampling measures the volatile fraction above the sample, sugars and other non-volatile components are not introduced by direct liquid injection. The spectrAline® sampling cartridge partitions the gas phase analytes to improve sensitivity for MRR analysis. The sample moves directly to headspace measurement, with no distillation and no manual sample preparation..

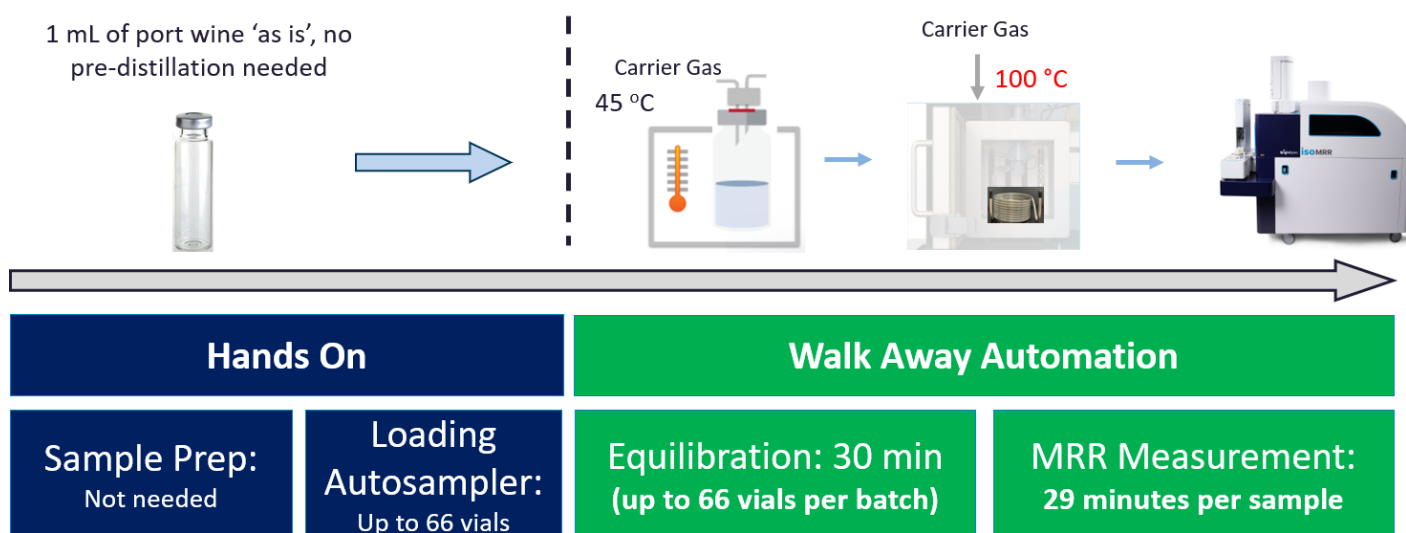


Figure 1. Automated Headspace-MRR workflow for direct analysis of fortified wine. Neat sample is equilibrated in the headspace vial, volatile analytes are transferred through the spectrAline® sampling cartridge, and structurally specific MRR detection is used for quantitation.

Application Example

To demonstrate this approach, a commercial fortified wine was analyzed using automated Headspace-MRR. The study targeted five markers, each tied to a specific quality decision: acetaldehyde for oxidation and aging, ethyl acetate for ester formation and sensory quality, methanol as a safety-relevant marker, 1-propanol and 2-butanol for the fermentation-related congener profile. The workflow quantified all five directly from neat, fortified wine, without distillation or manual sample preparation.

Quality Dimension	Representative Marker	QC Information
Oxidation / Aging	Acetaldehyde	Oxidative changes and aging-related chemistry
Flavor / Ester Profile	Ethyl acetate	Ester formation and sensory quality
Safety	Methanol	Safety-relevant volatile marker
Fermentation	1-Propanol	Higher alcohol formation during fermentation
Congener Profile	2-Butanol	Fermentation-related volatile composition

Table 1. Representative volatile quality markers selected to provide information across multiple dimensions of product quality, including oxidation, flavor profile, safety, fermentation, and congener profile.

The quantitative results are summarized in Table 2.

Analyte	Concentration in Unspiked Wine (ppm)	Estimated LOD (ppm)	Estimated LOQ (ppm)	Linear Range (ppm)	Linearity (R ²)
Acetaldehyde	28.4 ± 1.8	1.4	4.3	4-130	>0.99
Ethyl acetate	89.9 ± 0.4	0.96	2.9	3-183	0.98
Methanol	198.6 ± 6.1	8.2	24.9	25-299	>0.99
2-Butanol	<2.2 ± 0.3	3.1	9.4	9-103	>0.99
1-Propanol	80.4 ± 2.7	2.9	8.8	9-182	0.99

Table 2. Quantitation of representative volatile quality markers directly from neat fortified wine using automated Headspace-MRR.

These results support direct quantitation of representative volatile quality markers from neat fortified wine using a simplified Headspace-MRR workflow with no distillation step required.

What This Means for Food & Beverage QC

Fortified wine is one example of a broader workflow challenge across the Food & Beverage Industry. Many products are monitored through representative quality markers that support decisions on consistency, safety, flavor, fermentation, or process performance. In those workflows, the value is not only in the measurement itself, but in how efficiently the laboratory can obtain the information needed for the decision.

Automated Headspace-MRR provides a way to simplify that process for volatile quality markers. Samples can be analyzed directly, preparation steps can be reduced, and targeted quantitative information can be generated with less manual handling.

The opportunity for food and beverage laboratories is not to catalog every compound a method can detect. It is to identify the compounds that inform the decision, then measure those directly, quickly, and with confidence.