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Nota de aplicación

Monitoring Matrix Complexity During Ultra-Trace Level Multi-Residue Pesticide Analysis

Waters Corporation

This is an Application Brief and does not contain a detailed Experimental section.

Abstract

To analyze multiple pesticide residues in food matrices to ultra-trace concentrations while simultaneously monitoring matrix background complexity.

Introduction

One of the biggest challenges in ensuring the safety of our food supplies is the measurement of hazardous ultra-trace level components in the presence of a highly complex sample matrix. For the analysis of pesticides in food matrices, the increased use of liquid chromatography systems coupled with tandem quadrupole mass spectrometers has allowed progress in reducing the problems caused by the sample matrix. However, difficulties remain when trying to discriminate against matrix components that exhibit similar physiochemical properties. Unawareness of these difficulties in each unique sample can lead to poor quality results, and can impact a laboratory's performance and reputation.

The ability to understand the matrix challenge of each injected sample is clearly beneficial as is the ability to

monitor changes in the sample matrix between samples and batches. This capability can lead to the continuous improvement of analytical quality in the laboratory.

When operated in multiple reaction monitoring (MRM) mode, conventional LC Tandem Quadrupole Systems do not allow the direct monitoring of the sample matrix during routine high sensitivity determinations. In this technical brief, we describe the unique capability of Xevo™ TQ-S, which allows the monitoring of matrix complexity during ultra-trace multi-residue pesticide analysis.

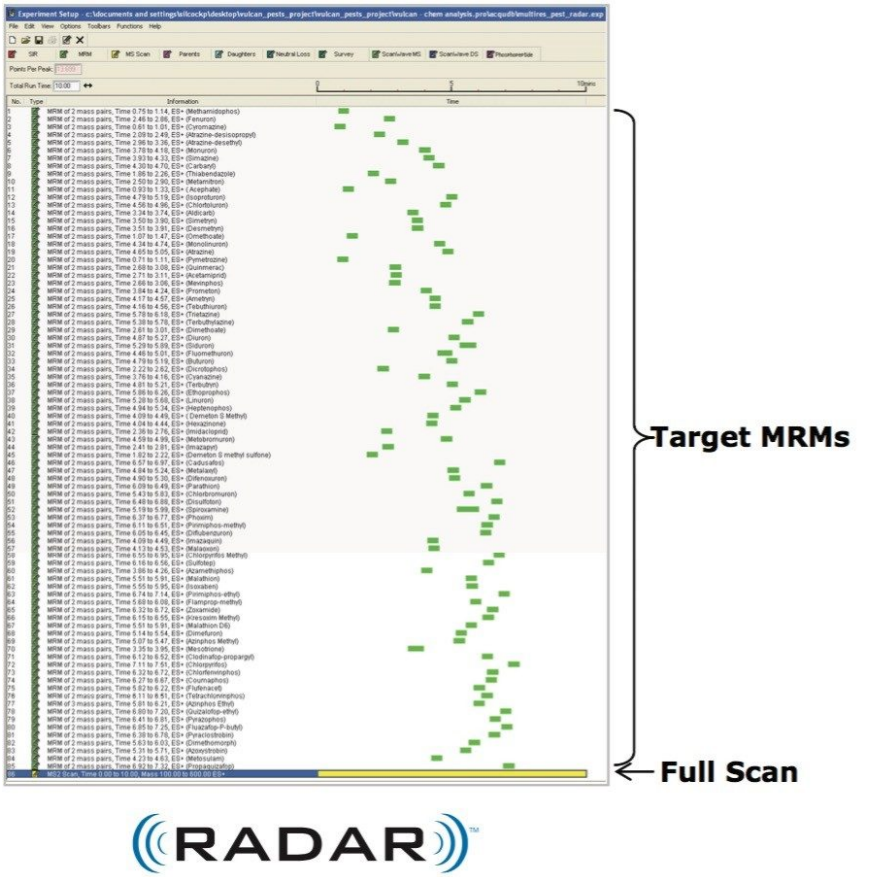

Figure 1. RADAR-enabled Xevo TQ-S method showing multiple target MRMs for pesticide residues with a continuous background monitoring full scan function.

Results and Discussion

High sensitivity determination of multiple pesticide residues in grape, avocado, marjoram, and ginger was performed using Waters™ DisQuE™ Dispersive SPE (QuEChERS) and ACQUITY UPLC™ coupled with Xevo TQ-S. Typical reversed-phase conditions were used for ACQUITY UPLC separations with formic acid-modified mobile phase to aid positive ion electrospray. Xevo TQ-S was operated with RADAR,™ as shown in Figure 1. RADAR is an information-rich acquisition approach that allows you to track your target analytes with precision in MRM mode, while simultaneously scanning the background for all other components.

Rapid acquisition rates, fast switching between MS/MS and MS, and high sensitivity are all required to accurately measure the concentrations of a large number of residues and simultaneously acquire valuable full scan data. Figure 2 shows the chromatographic data obtained during RADAR-enabled analysis of grape, avocado, marjoram, and ginger samples spiked at the lower level (0.01 mg/kg) European maximum residue limit (MRL).

The simultaneously acquired full scan data allows the observation of the matrix challenge for every individual sample injected. This information can help identify areas of potential ion suppression, as well as aid in the development of further clean-up and matrix reduction strategies. It can also help track method clean-up efficiency and any changes in sample matrix that may occur as different batches of samples are analyzed.

With simultaneous full scan capability, matrix components that co-elute with MRM target analytes can be investigated by interrogating the “always available” spectral data. In the tested grape samples, RADAR allowed a co-eluting matrix component to be observed with the pesticide dimethoate, as shown in Figure 3.

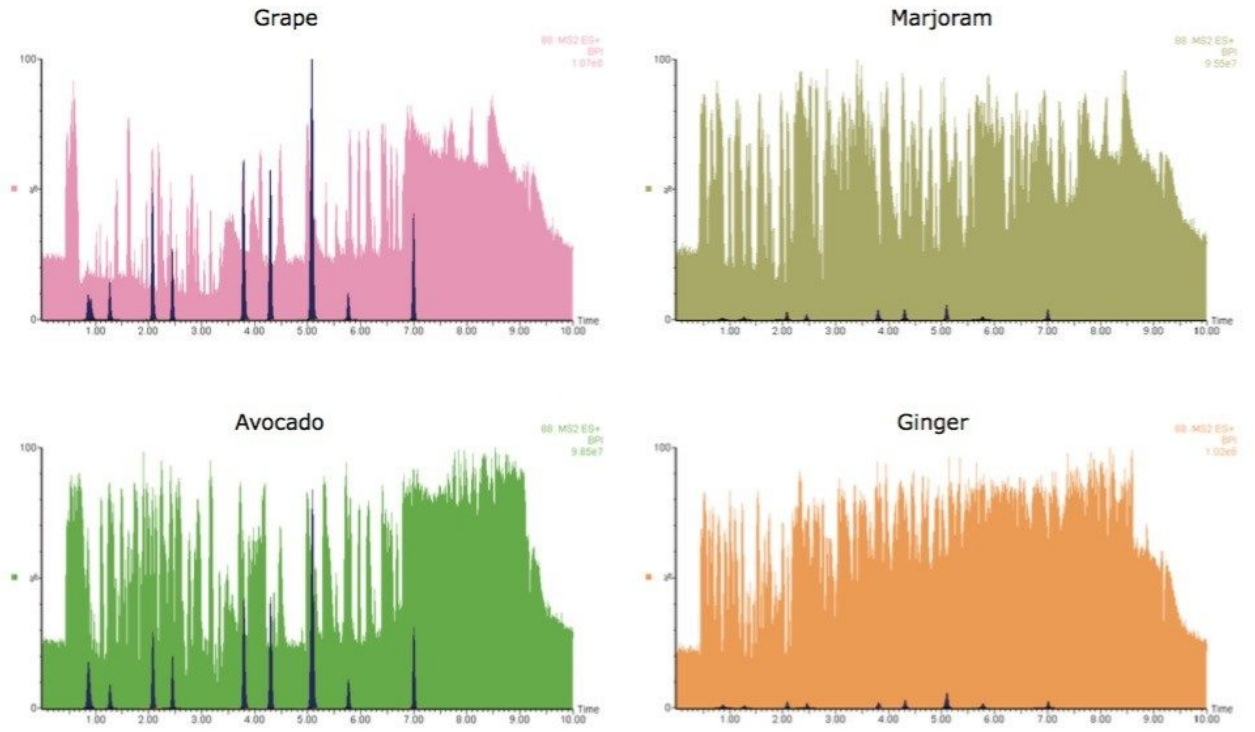

Figure 2. RADAR-enabled acquisitions of grape (matrix 1 g/mL), avocado (matrix 1 g/mL), marjoram (matrix 0.1 g/mL), and ginger (matrix 0.1 g/mL) spiked at the lower level 0.01 mg/kg European MRL. Colored chromatogram is MS2 full scan spectrum. Also shown in the overlay is a selection of simultaneously acquired pesticide MRMs.

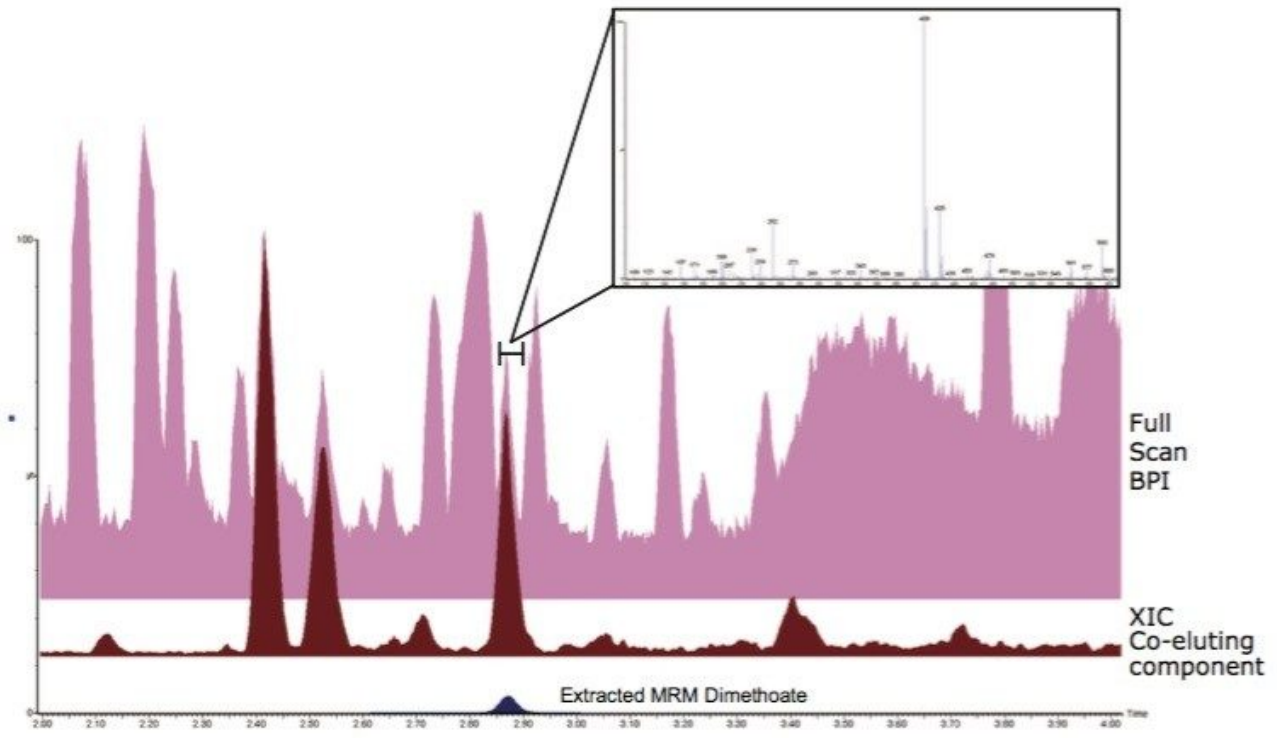

Figure 3. Extracted MRM chromatogram for dimethoate in grape (0.01 mg/kg) with overlaid simultaneous full scan and extracted mass chromatogram of co-eluting matrix component. Also shown (inset) is mass spectrum of co-eluting component.

Conclusion

The RADAR mode of acquisition enables the collection of spectral information on background components in the sample matrix while simultaneously collecting MRM data for the quantitation of target pesticides. Operating the Xevo TQ-S in the RADAR mode does not compromise the quality of the quantitative MRM data.

This mode of operation is beneficial when monitoring for the presence of ultra-trace contaminants in food. The information provided can help a laboratory develop reliable and robust methods, understand the matrix challenge of each individual sample, monitor cleanup efficiency, and observe intra- and inter- sample batch variations. This ultimately can lead to an improvement in data quality which in turn translates to more success

with business activities that are reliant on the performance of the laboratory.

Featured Products

Xevo TQ-S <https://www.waters.com/10160596>

RADAR <https://www.waters.com/waters/nav.htm?cid=134798882>

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