Rapid, Precise, and Ultra-Sensitive Detection of Pesticides in Drinking Water Using Direct Injection ACQUITY UPLC with Xevo TQ-S

GOAL

To rapidly determine ultra-trace level pesticide contamination in drinking water with high precision using direct injection onto a Waters® Xevo™ TQ-S System.

BACKGROUND

Rapid and highly sensitive analysis of drinking water is essential for protecting human health and well-being. The assurance of clean, safe drinking water has become more critical given the potential of accidental or intentional contamination, which has increased in recent years.

Highly efficient water treatment processes allow for the effective removal of the majority pesticides that have entered water sources however, drinking water regulations still require testing to ultra-trace concentrations. This requirement has led to multiple approaches for enriching samples before instrumental analysis, with solid phase extraction prior to LC/MS/MS a popular choice. In addition to this online pre-concentration and large volume injection, using specialized injection systems have been employed to introduce samples to LC/MS/MS systems. These techniques have been be very successful, but can add time, resources, and complexity to the analysis.

The ultra-high sensitivity of ACQUITY UPLC coupled with Xevo TQ-S allows direct measurement of pesticides down to parts-per-quadrillion (ppq or pg/L).
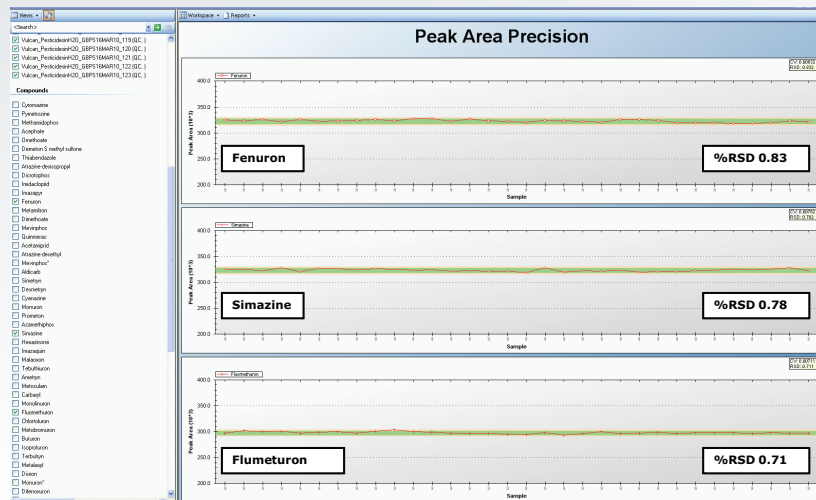

Figure 1. TrendPlot generated chart showing peak area precision of fenuron, simazine, and flumeturon for 32 injections of 100 ng/L fortified QC samples.

Cleaner, aqueous samples – such as drinking water – are highly compatible for direct injection onto a LC/MS/MS system, but large multi-analyte determinations require ultra-sensitive detection. In this technical brief, we describe the application of direct injection ACQUITY UPLC® coupled with Xevo TQ-S for the rapid, precise, and ultra-sensitive analysis of multiple pesticides in drinking water.

THE APPROACH

Drinking water samples were dechlorinated and 100 µL injected directly into a ACQUITY UPLC System 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. Multiple reaction monitoring (MRM) mass spectrometer parameters were generated by Waters Quanpedia™ Database for the determination of 81 pesticides simultaneously. The total cycle runtime of each sample was 11 min, which allows five samples to be analyzed per hour.

Typical maximum permitted concentrations of pesticides in drinking water are set at 100 ng/L for individual pesticides and 500 ng/L for total pesticides. The ability to measure with high precision at ultra-trace levels is a critical requirement to allow high quality determinations as well as observing trends in samples and sample batches. This also instills a high degree a confidence in reported results. The Xevo TQ-S allowed comfortable, high precision measurements at these extremely low contaminant concentrations without the need for any sample enrichment or complex injection systems. Figure 1 shows a Waters TrendPlot™ generated chart displaying the peak area precision for fenuron, simazine, and flumeturon over 32 injections of a drinking water QC sample fortified at 100 ng/L.
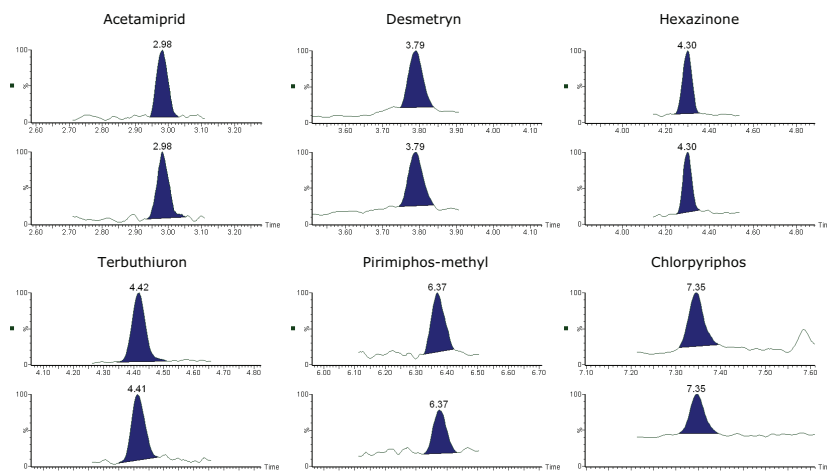

Figure 2. Ultra-sensitive detection of pesticides in water fortified at 200 pg/L (200 ppq) using direct injection on ACQUITY UPLC coupled with Xevo TQ-S.

The ultra-high sensitivity of the system allows direct measurement of pesticides down to parts-per-quadrillion (ppq or pg/L) concentrations from standard 2-mL autosampler vials using a standard ACQUITY UPLC® System. This sensitivity capability allows very comfortable measurement at the legislated levels, as well as allowing real background levels in samples to be observed. Figure 2 shows ultra-sensitive detection (with confirmatory transition) of a representative set of pesticides fortified at 200 pg/L (200 ppq and 500 times below required levels) using direct injection on ACQUITY UPLC coupled with Xevo TQ-S.

SUMMARY

The Xevo TQ-S allows ultra-sensitive detection of contaminants in drinking water, which enables real background concentrations in samples to be rapidly observed. The level of sensitivity offered helps improve laboratory quality by making measurement at legislative levels much easier with a high degree of precision and confidence.

This is all achieved with direct analysis of the water sample, which simplifies analysis, enabling a rapid time to result and a very high throughput method in the laboratory. This helps maximize laboratory efficiency and drive down costs.

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