

Improving the Analysis of Triazole Fungicides in Wheat Straw Samples using UniSpray Ionization with ACQUITY UPC² and Xevo TQ-XS

Jane Cooper¹ and Marian Twohig²

¹Waters Corporation, Wilmslow, UK, ²Waters Corporation, Milford, MA, USA



GOAL

To illustrate the improved response achieved using the UniSpray ionization source for the analysis of triazole fungicides.

BACKGROUND

When a crop protection active ingredient contains one or more stereogenic centers the enantioselective behavior must be studied as it is known that enantiomers can exhibit different bioactivities.

Analytical methods that are used to evaluate the influence of stereochemistry on degradation dynamics, environmental fate, and final residue levels, help to establish a more accurate risk assessment of crop protection products.

UniSpray is a novel ionization source with a simplified probe design that can be used for broader compound coverage. It offers greater ionization efficiency, comparable robustness and linearity to ESI, and spectra comparable with current ionization modes.

Having the ability to screen for a broader range of compounds, with increased ionization efficiency offers increased scope during method development.

Novel ionization source enables an increased range of ionization modes for atmospheric ionization MS techniques.

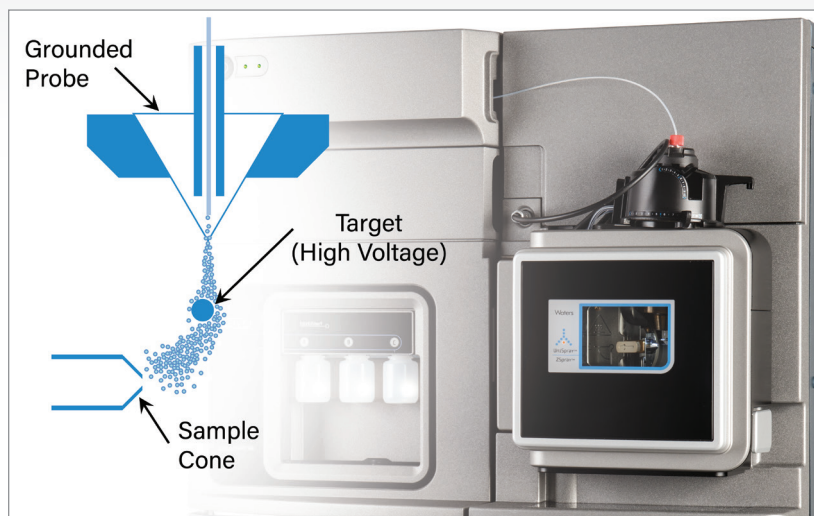


Figure 1. Xevo TQ-XS Mass Spectrometer with the UniSpray ionization source.

This technology brief, evaluates the potential of Waters® UniSpray source coupled with the ACQUITY UPC²® System and Xevo® TQ-XS Mass Spectrometer (Figure 1), versus ESI to improve peak response, repeatability and signal-to-noise (S/N), considering the analysis of triazole fungicides as a model.

THE SOLUTION

UniSpray has a grounded probe, and a stainless steel pin which is held at high voltage. The liquid stream is converted into a nebulized spray and directed at the stainless steel target (Figure 1), which creates a fine spray of charged droplets that is directed at the ion inlet orifice of the mass spectrometer. The resulting ions are sampled by the first vacuum stage of the mass spectrometer. Increased ionization efficiency, is achieved due to the enhanced desolvation and droplet evaporation.

The Xevo TQ-XS, is a high performance tandem quadrupole instrument, which offers the ultimate in reliability, reproducibility, specificity, and sensitivity, making it ideal for the determination of trace compounds in complex matrices such as field crops or soil.

UltraPerformance Convergence Chromatography™ (UPC²) is a separation technique that uses carbon dioxide as the primary mobile phase, with a co-solvent such as acetonitrile or methanol to give similar selectivity as normal phase LC.

MRM transitions, and MS parameters were optimized for the compounds considered. ACQUITY UPC² separation parameters, using the Trefoil™ AMY1, 2.5 µm Column, were optimized in order to resolve the chiral triazole fungicides with a run time of 7 minutes (Figure 2). After a QuEChERS extraction, followed by a solid phase cleanup using Oasis® MCX, sample extracts and standards were analyzed using the established MS and UPC² conditions, using either UniSpray or ESI modes.

When using UniSpray coupled with ACQUITY UPC² and Xevo TQ-XS for the analysis of triazole fungicides solvent standards, a 4.4-fold increase in peak area, 1.4-fold increase in S/N, and a 1.8-fold improvement in reproducibility were observed when compared against ESI results.

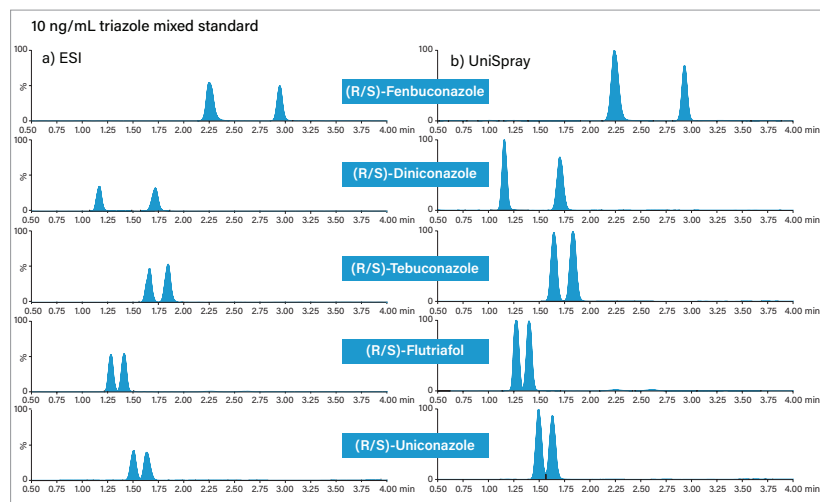


Figure 2. ACQUITY UPC² MRM chromatograms showing the enantioseparation for triazole fungicides in a 10 ng/mL wheat straw matrix matched mixed standard, using a.) UniSpray, or b.) ESI.

As illustrated in Figure 2, for the analysis of a 10 ng/mL wheat straw matrix matched triazole fungicide mixed standard, the UniSpray source produced higher signal intensities (typically 2- to 5-fold) compared to ESI under exactly the same conditions.

SUMMARY

Unispray, the novel ionization source, offers:

- Increased range of ionization modes for atmospheric ionization MS techniques.
- Increased ionization efficiency.
- Improved scope for method development.
- Improved response, repeatability and S/N using UniSpray versus ESI ionization sources for the analysis of triazole fungicides.

Waters

THE SCIENCE OF WHAT'S POSSIBLE.®

Waters, Xevo, ACQUITY UPC², UPC², Oasis, and The Science of What's Possible are registered trademarks of Waters Corporation. UltraPerformance Convergence Chromatography and Trefoil are trademarks of Waters Corporation. All other trademarks are the property of their respective owners.