Waters™

Application Note

Applied Benefits of Narrow Mass Windows for TOF Screening

Waters Corporation

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

Abstract

This application brief demonstrates to successfully carry out a broad scope of pesticide screening in environmental waters using TOF/MS with increased confidence in the reported results arising from the use of narrow chromatographic extraction windows.

Benefits

The stability of mass measurement on the Xevo G2 QTof enables a reduction in processing errors along with minimized false positives.

Introduction

In the environmental monitoring arena, the use of TOF screening approaches has steadily increased. This technique offers particular benefits due to the acquisition of full scan data, and the ability to re-interrogate historical data for unexpected compounds.

Screening of environmental waters is especially important because the use of pesticides and similar compounds has steadily increased in an effort to meet global food demands. When pesticides are applied to crops to increase the yield, they often end up leaching into the surrounding soil and waterways, potentially causing harm to plants and wildlife.

In response to water quality requirements and to ensure protection of the aquatic ecosystem, analysts need a complete picture of the components present in the water under investigation. A TOF/MS screening approach is ideally suited to this type of analysis; however confidence in the correct identification of contaminant compounds is vital. When analyzing data, the use of narrow mass extraction windows can reduce the possibility of peak misidentification and minimize the risk of errors.

Results and Discussion

Waters Xevo G2 QTof MS coupled with ACQUITY UPLC, along with the Waters ToF Screening Pesticide Database, and POSI±IVE Software processing, were used to rapidly screen treated sewage effluent that had been extracted using Oasis HLB SPE Cartridges. A generic screening UPLC gradient was used, with a total run time of two minutes. The mobile phases used were 10 mM ammonium acetate solution in water and 10

mM ammonium acetate in methanol.

A mix of 103 commonly used pesticides was spiked at 100 ng/L equivalent in sewage effluent. Figure 1 shows the TIC obtained from one screening run. This clearly illustrates the complexity of the sample of interest.

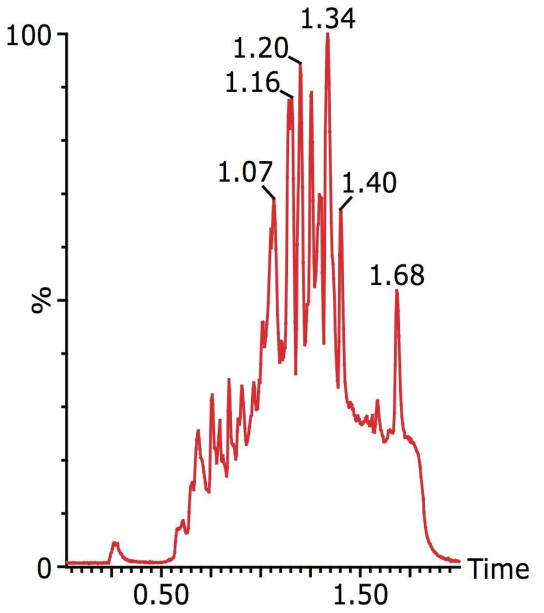

Figure 1. Mix of 103 pesticides spiked at 100 ng/L equivalent in sewage effluent.

A significant challenge when reviewing this type of data is ensuring that chromatographic peaks are correctly extracted and identified. The extracted peaks can be simplified by using very narrow chromatographic windows; however, this relies on the acquired exact mass for each compound remaining very precise across the entire peak for that compound.

Figure 2 shows the effect of using increasingly narrow mass extraction windows when reviewing Xevo G2 QTof MS data. This demonstrates that narrowing the chromatogram window provides unequivocal identification of the peak of interest and removes any additional peaks that have masses close to that of fenuron, due to the additional selectivity afforded by this approach.

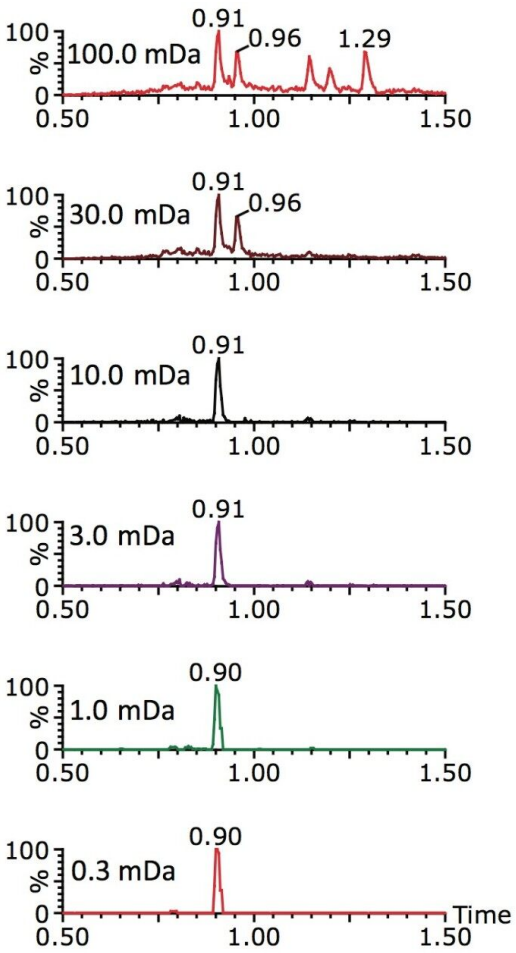

Figure 2. The effect of narrowing the XIC for Fenuron m/z 165.1028.

Conclusion

Oasis HLB SPE extraction with rapid ACQUITY UPLC separation and detection by Xevo G2 QTof, followed by data processing using POSI±IVE Software, were successfully used to screen extracted sewage effluent for pesticide contaminants at ultra-trace levels. The compound fenuron, which is widely used as a herbicide, was discovered in this very challenging matrix.

Confidence in identifying this peak as fenuron was enhanced by the ability to apply very narrow mass extraction windows, which removed any additional peaks that were close to the exact mass of fenuron. This

demonstrates the stability of mass measurement on the Xevo G2 QTof, and enables a reduction in processing errors along with minimized false positives.

Featured Products

ACQUITY UPLC System <https://www.waters.com/514207>

POSI±IVE <https://www.waters.com/10145280>

720003423, April 2010