



Rapid and Sensitive Targeted ToF Screening for Pesticides in Environmental Waters

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

Abstract

In this application brief, we describe broad scope pesticide screening in environmental waters using TOF/MS. This method provides increased confidence in the reported results arising from the ability to maintain excellent exact mass accuracy, even in the presence of many high-intensity background ions.

Benefits

Xevo G2 QTof was able to maintain the exact mass accuracy of the malaoxon ions in an extremely complex sample matrix during a screening run with a total turn-around time of only two minutes.

Introduction

In recent times, the use of pesticides, herbicides, and fungicides has steadily increased, in an effort to meet global food demands. A percentage of such chemicals applied to crops will, inevitably, end up leaching into the surrounding soil and waterways. Strict environmental monitoring is mandated, which endeavors to safeguard the environment and protect plants and wildlife from harm as a result of exposure to these types of chemicals.

To ensure protection of the aquatic ecosystem, analysts require a complete picture of the components present in the water under investigation. A TOF/MS screening approach is ideally suited to this due to the acquisition of full scan data and the ability to re-interrogate historical data for unexpected compounds.

Many key compounds of interest are likely to be present at ultra-trace levels at the same time as other naturally occurring compounds at very high concentrations, such as humic and fulvic acids, which are formed from plant material decomposition. This means that the TOF instrumentation must be sufficiently sensitive and accurate to ensure that hazardous materials are correctly detected and identified, while at the same time maintaining exact mass accuracy for components at very low concentrations.

Results and Discussion

Waters Xevo G2 QTof coupled with ACQUITY UPLC, along with the Waters TOF Screening Pesticide Database, and POSITIVE Software data 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 runtime of two minutes. The mobile phases used were 10 mM ammonium acetate solution in water and 10 mM ammonium acetate in methanol. Several pesticide residues were detected, including malaoxon – a degradation product of malathion, as illustrated in Figure 1.

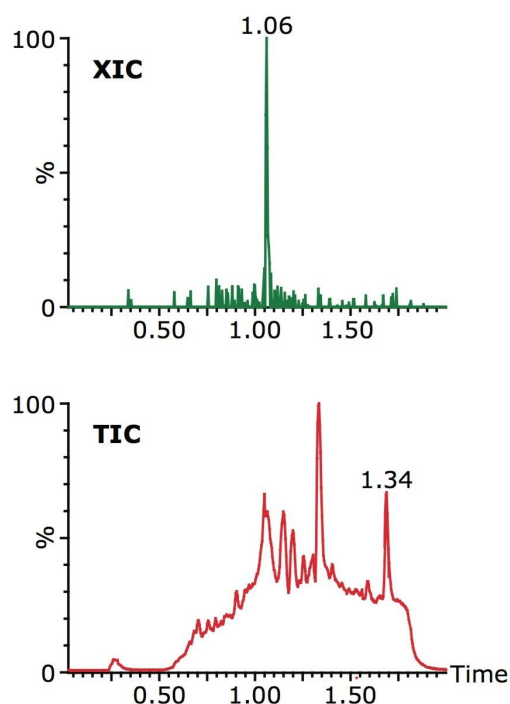


Figure 1. TIC and XIC for malaoxon @ 200 ng/L in extracted sewage effluent: m/z 337.0487.

Chromatogram extraction window: 20 mDa

The compound of interest eluted at a point in the chromatogram where a large number of background matrix components also elute, as seen from the high intensity of the TIC around 1 minute in Figure 1. To ensure the integrity of the data, it is essential that the TOF instrument is capable of maintaining excellent exact mass accuracy for the compound of interest under these circumstances.

Figure 2 shows the full scan spectrum at 1.06 minutes, which illustrates the intensities of all the ions present. The magnification of this spectrum around the mass of the compound of interest, malaoxon, indicates the clear presence of malaoxon with an excellent exact mass accuracy maintained.

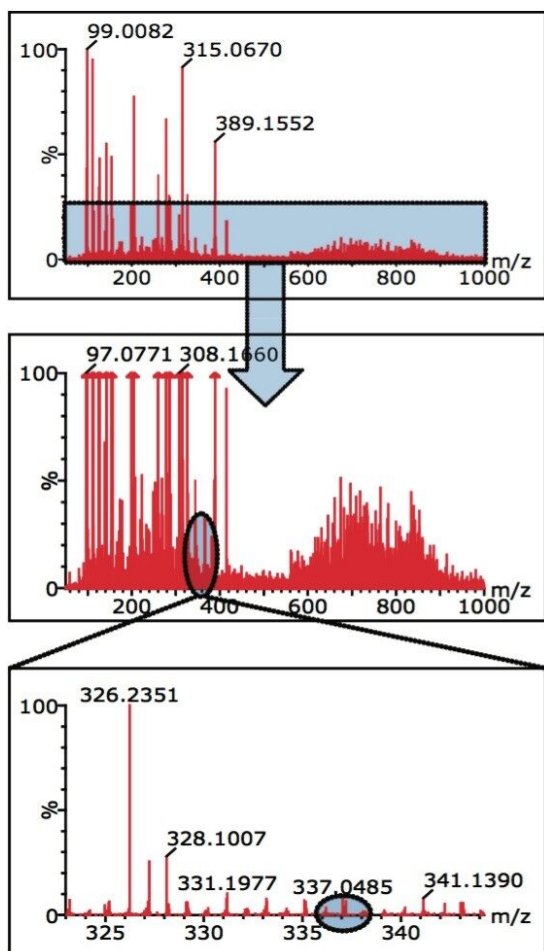


Figure 2. Malaoxon in sewage effluent @ 200 ng/L: m/z

337.0487

Mass error: 0.6 ppm (0.2 mDa).

Conclusion

Oasis HLB SPE with rapid ACQUITY UPLC separation and detection by Xevo G2 QTof, followed by data processing using POSITIVE Software, were successfully used to screen extracted sewage effluent for pesticide contaminants at ultra-trace levels. The compound malaoxon, a degradation product of malathion, was discovered in this very challenging matrix.

Xevo G2 QTof was able to maintain the exact mass accuracy of the malaoxon ions in an extremely complex

mixture during a screening run with a total turn-around time of only two minutes. This offers rapid sample throughput with increased confidence in the detection and identification of compounds present, as result of the accurate and precise exact mass data acquired.

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