[TECHNOLOGY BRIEF]

Rapid and Reliable Targeted ToF Screening for Pesticides in Food

GOAL

To successfully carry out broad scope pesticide screening in food commodities using ToF/MS; with increased confidence in the reported results arising from the reproducibility of mass accuracy across detected peaks, even at low concentrations.

BACKGROUND

Pesticides are used to generate improved crop yields as the demands on global food production increase. The quality of the food we eat is very carefully regulated worldwide, and a key component of food safety legislation is ensuring that pesticide residues do not remain on crops sold to consumers, as this could pose a health risk.

Recently, European legislators updated the guidance for pesticide residue analysis in food and feed,[1] which now includes the recognition that accurate mass data may be used as part of the evidence for the presence or absence of analytes of interest. Consequently, data acquired on a time-of-flight (TOF) instrument can be used when reporting findings from pesticide screening analyses of food crops.

Typically, a TOF-screening approach might be used to help reduce the number of suspected positive compounds, prior to the sample being analyzed using a targeted MRM method on a tandem quadrupole instrument. However, reducing the number of false positives is essential to ensure that this approach is both robust and reliable. TOF screening also provides the ability to re-interrogate historical data for compounds not previously targeted, which offers added benefit compared with targeted MRM data.

Xevo G2 QTof acquired robust and reliable MS^E data, with exact mass RMS variation of less than 2 ppm for both precursor and product ions at a concentration less than half that of the MRL.

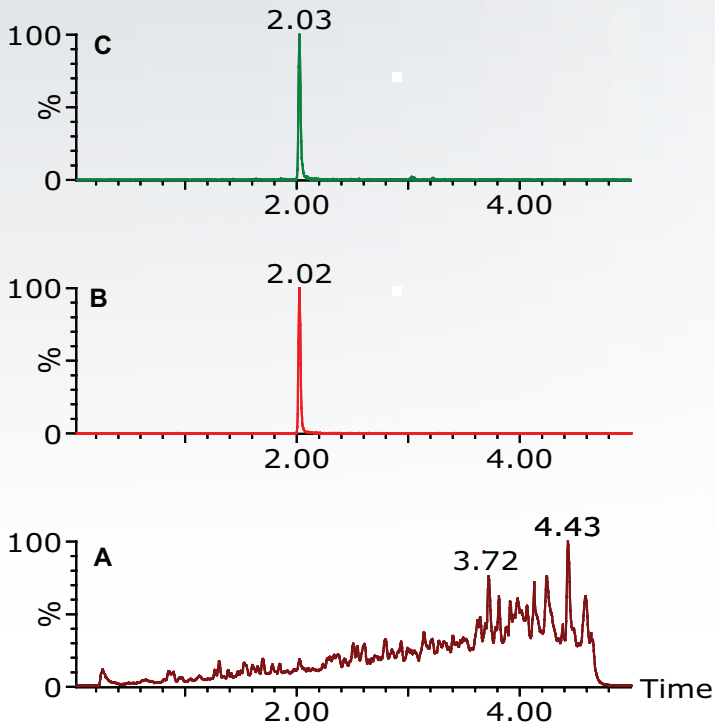

Figure 1. Thiabendazole was detected in green beans.
A: Total Ion Chromatogram for extracted green beans.
B: Extracted Ion Chromatogram for precursor ion m/z 202.0439.
C: Extracted Ion Chromatogram for fragment ion m/z 175.0330.

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THE SOLUTION

Xevo™ G2 QTof MS coupled with ACQUITY UPLC,® along with the Waters TOF Screening Pesticide Database, and POSI±IVE™ Software data processing, were used to rapidly screen extracted green bean samples. An incurred residue of the fungicide thiabendazole was detected, as illustrated in Figure 1.

The MS^E functionality of the Xevo G2 QTof Mass Spectrometer enables the acquisition of both low energy precursor ion and high energy fragment ion mass spectral data in a single run. A generic screening UPLC® gradient was used, with a total runtime of five minutes. The mobile phases used were 10 mM ammonium acetate solution in water and 10 mM ammonium acetate solution in methanol.

The extracted ion chromatograms in Figure 1 have 12 points across the low energy precursor ion peak, and 12 points across the high energy fragment ion peak, giving a total of 24 data points for thiabendazole. In addition, the Xevo G2 QTof Mass Spectrometer provides extremely accurate exact mass data for not only the precursor ions, but also the fragment ions.

Table 1 illustrates the exact mass data for thiabendazole in extracted green beans. The calculated RMS values for exact mass variation for both precursor and fragment ions were well below 2.0 ppm, even for these low mass ions.

The EU Maximum Residue Limit[2] (MRL) for thiabendazole in green beans is 0.05 mg/kg (50 µg/kg), and the data presented here is at a concentration less than half that of the MRL, demonstrating robust and reliable exact mass data at a low analyte concentration.

Scan No.	Measured Mass	ΔM (mDa)	ΔM (ppm)	Scan No.	Measured Mass	ΔM (mDa)	ΔM (ppm)
505	202.0434	-0.50	-2.47	505	175.0334	0.40	2.29
506	202.0439	0.00	0.00	506	175.0332	0.20	1.14
507	202.0436	-0.30	-1.48	507	175.0332	0.20	1.14
508	202.0442	0.30	1.48	508	175.0329	-0.10	-0.57
509	202.0437	-0.20	-0.99	509	175.0327	-0.30	-1.71
510	202.0440	0.10	0.49	510	175.0327	-0.30	-1.71
511	202.0439	0.00	0.00	511	175.0322	-0.80	-4.57
512	202.0435	-0.40	-1.98	512	175.0328	-0.20	-1.14
513	202.0441	0.20	0.99	513	175.0327	-0.30	-1.71
514	202.0435	-0.40	-1.98	514	175.0333	0.30	1.71
515	202.0433	-0.60	-2.97	515	175.0328	-0.20	-1.14
516	202.0442	0.30	1.48	516	175.0330	0.00	0.00
	RMS =	0.30	1.50		**RMS =**	0.31	1.76

Table 1. Thiabendazole in green beans @ 20 µg/kg approx. Precursor ion m/z 202.0439, fragment ion m/z 175.0330.

SUMMARY

The Xevo G2 QTof together with ACQUITY UPLC was successfully used to screen extracted green beans for pesticide residues. An incurred residue of thiabendazole was discovered at a concentration below that of the MRL but well above the Limit of Detection (LOD) of the instrument.

Use of the MS^E functionality of the Xevo G2 QTof enabled the acquisition of exact mass data for both precursor and fragment ions in one screening run, with a high level of reproducibility. This provides extra confidence in the identification of incurred residues and reduces false positives.

A reduction in false positives streamlines the workflow when transferring the samples to a tandem quadrupole instrument for confirmatory analysis, and provides valuable time-saving and efficiency benefits to the cost conscious analytical laboratory.

Waters offers a complete solution for broad scope TOF screening for food commodities, comprised of DisQuE™ sample extraction with ACQUITY UPLC separation and Xevo G2 QTof detection, followed by data processing with POSI±IVE Software.

References

1. EU Document number SANCO/10684/2009, Method Validation and Quality Control Procedures for Pesticide Residue Analysis in Food and Feed.
2. Commission Regulation (EC) number 149/2008, Annex II.

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