Food & Environmental

Fast, Selective, and Sensitive Screening for More Than 1000 Targeted Pesticides with Identification Using Automated Library Searching

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Introduction

Recent regulations on food and environmental analysis require screening for pesticides using confirmatory techniques, such as GC/MS and LC/MS/MS. More than 1000 pesticides are used worldwide and, along with their metabolites and degradation products, are present in food and the environment. Thus, there is a demand for powerful and rapid analytical methods that can detect very low concentrations of pesticides. Alder et al. compared the use of GC/MS and LC/MS/MS for multi residue pesticide analysis and concluded "…the benefits of LC-MS/MS in terms of wider scope, increased sensitivity, and better selectivity are obvious."[1]

The big challenges for pesticide residue laboratories at the moment are the requests to test for larger number of compounds, in a wider range of commodities, in shorter time, all without sacrificing data quality.

The novel AB SCIEX QTRAP® 5500 LC/MS/MS System uses advanced eQ™ electronics, the new Qurved LINAC® collision cell, and the patented Linear Accelerator™ Trap to address the above challenges. The developed method demonstrates that the unmatched speed allows screening for more targeted pesticides using fast LC, fast MRM, and identification of detected compounds by Enhanced Product Ion scanning and library searching of the spectra.

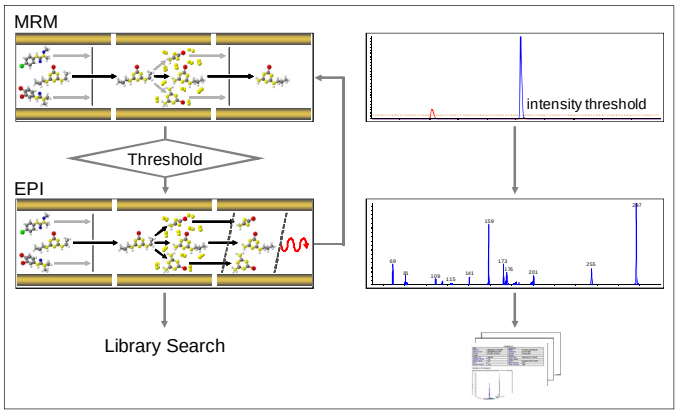

Figure 1. Setup of an Information Dependent Acquisition (IDA) experiment: A survey in Multiple Reaction Monitoring (MRM) screens for a multitude of targeted analytes with highest selectivity and sensitivity. The chromatographic signal above a specified threshold triggers automatically the Enhanced Product Ion (EPI) scanning. Acquired EPI spectra are searched against a mass spectral library for identification.

Method Details

- QuEChERS extraction of food samples and 50 times dilution to minimize possible matrix effects
- Direct injection of water samples
- Ultra High Pressure Liquid Chromatography using a Shimadzu UFLC$_{XR}$ system with a Phenomenex Synergi Fusion-RP (2.5 µm) column and a fast gradient of water and methanol with ammonium formate buffer
- Total run time of less than 10 min
- AB SCIEX QTRAP® 5500 System with Turbo V™ Source and ESI probe
- Detection of 1064 *Scheduled* MRM™ transitions and acquisition of EPI spectra to search against a library for identification in a single analysis

The analytical workflow used and an example chromatogram and corresponding EPI mass spectrum are illustrated in Figure 1.

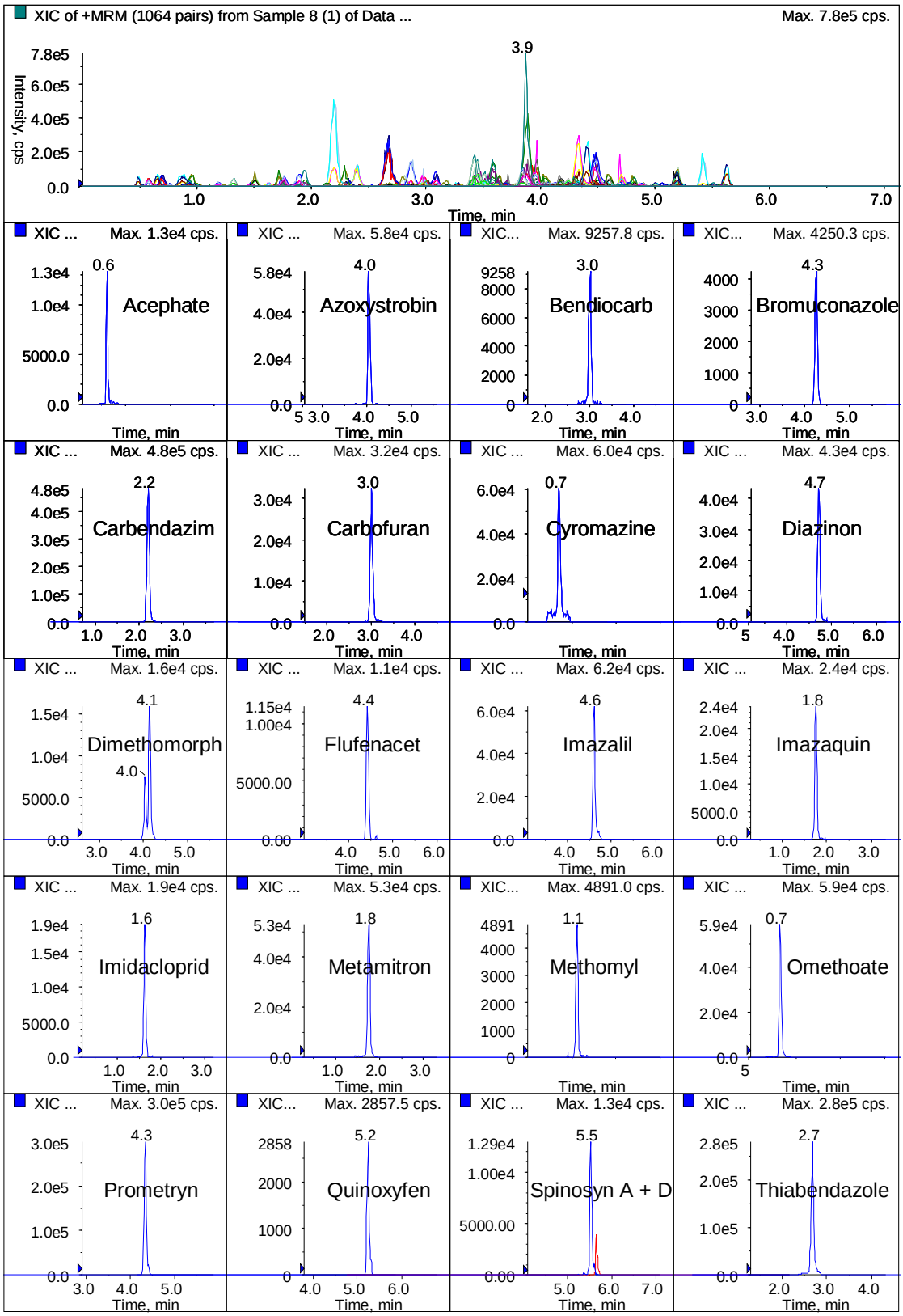

Figure 2. Pesticide Screening using 1064 *Scheduled* MRM™ Algorithm transitions in less than 10 min (top) and extracted chromatograms of individual pesticides at a concentration of 1 ng/mL (bottom).

Results

The new QTRAP® 5500 System allows the use of short MRM dwell times and pause times while maintaining highest selectivity, sensitivity and reproducibility. These short times, in combination with the *Scheduled* MRM™ Algorithm offered in Analyst® Software 1.5, make it possible to detect several hundreds — or even thousands — of MRM transitions in a single analytical run. Figure 2 shows an example of an IDA chromatogram monitoring over 1000 transitions with a run time of less than 10 min. The representative extracted chromatograms highlight the superior sensitivity allowing detection limits at sub ng/mL concentrations.

The new Linear Accelerator™ Trap of the QTRAP® 5500 System allows acquisition of EPI spectra with unparalleled sensitivity and scan speed of 20000 Da/s. The hardware and software algorithm of Dynamic Fill Time (DFT) was improved to enable a wider range of fill times starting as low as 0.05 ms. This ability to use such short fill times greatly improves quality of mass spectra by reducing space charge effects and allows acquisition of quality EPI spectra over a large dynamic range. In addition, EPI spectra generated with Collision Energy Spread (CES) are well known to contain maximum structural information for best identification.

Figures 3 and 4 show examples of using the described method to screen for pesticides in fruit samples. A number of compounds were identified and confirmed using automated library searching.

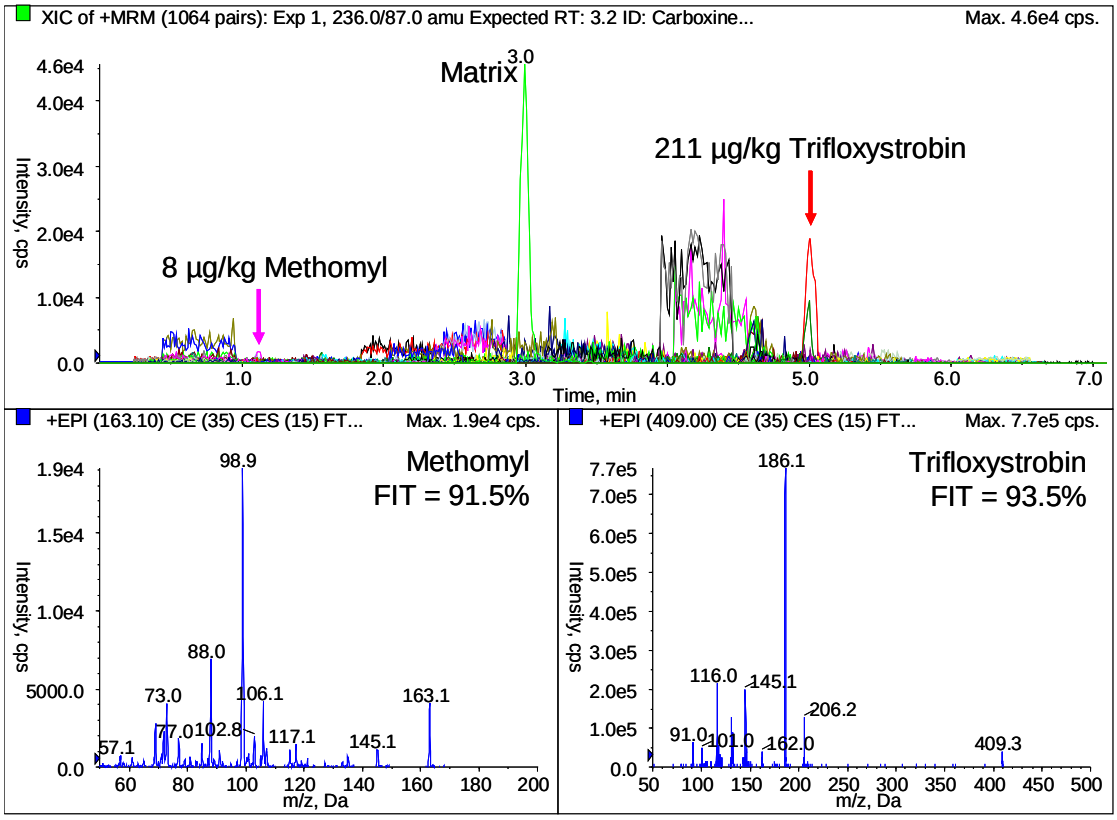

Figure 3. Detection of 8 µg/kg Methomyl and 211 µg/kg Trifloxystrobin in a grape sample and identification by library searching of Enhanced Product Ion spectra. The library match was excellent, with a FIT of >90%.

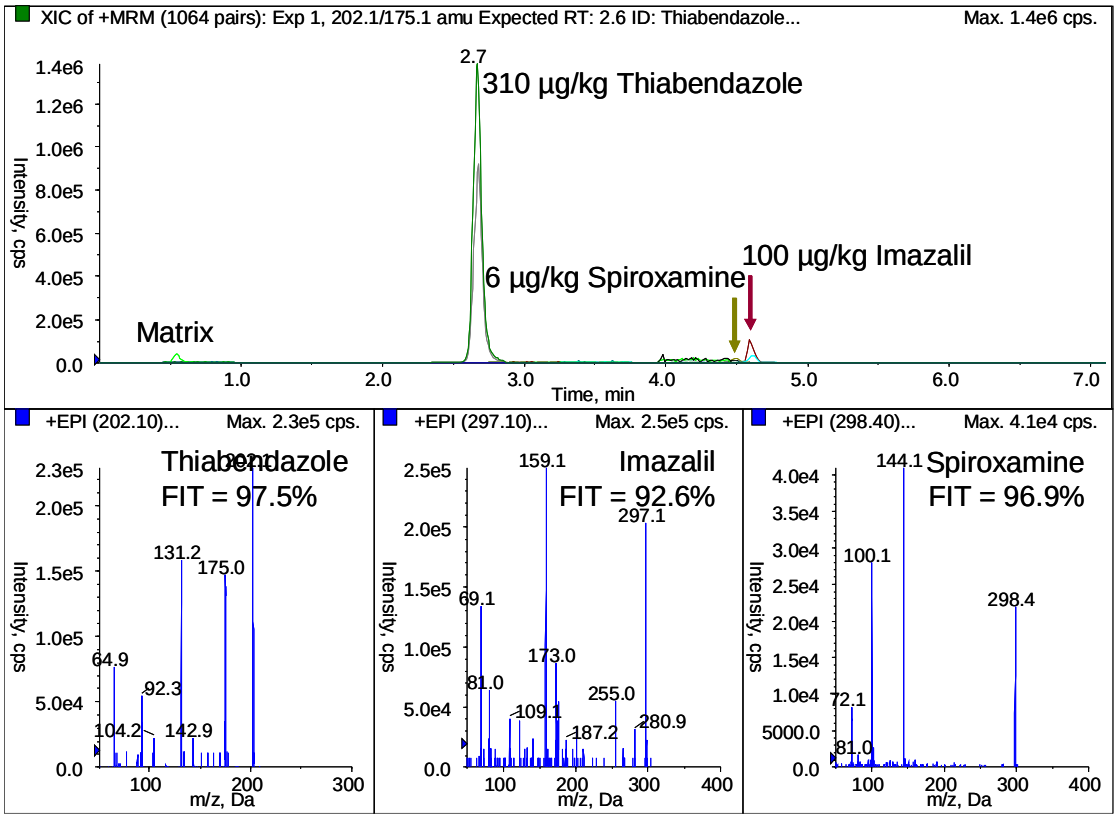

Figure 4. Detection of Detection of 6 µg/kg Spiroxamine, 100 µg/kg Imazalil, and 310 µg/kg Thiabendazole in a banana sample and identification by library searching of Enhanced Product Ion spectra. The library search results were again excellent, with FIT of >90% for all compounds

Summary

The new QTRAP® 5500 LC/MS/MS System incorporates the proven technology of the Turbo V™ source and the Curtain Gas™ interface for ultimate sensitivity and robustness. The unmatched speed of monitoring MRM transitions and acquiring EPI spectra is made possible by advanced technologies including the new Qurved LINAC® collision cell and the Linear Accelerator™ Trap. These performance criteria, together with sophisticated software algorithms such as *Scheduled* MRM™ Algorithm and Collision Energy Spread, make the QTRAP® 5500 System the ideal instrument for high throughput multi-pesticide screening at required sensitivity levels for analysis of food and drinking water. In addition, library search of EPI spectra gives highest degree of confidence in analytical results.

References

1 L. Alder, K. Greulich, G. Kempe, B. Vieth: Mass Spectrometry Reviews 25 (2006) 838-865

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