Application Note

Improve Product Ion Confirmation Scanning with Xevo TQ-GC

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

Abstract

Use product ion information simultaneously with MRM acquisition to provide additional compound information and aid in verification of results.

Benefits

Add confidence in results using product ion confirmation scanning.

Introduction

When analyzing pesticides in complex food matrices it is important to be certain that the results are correct. If the results are questionable, then the analysis has to be repeated which takes extra time and delays sample turnaround. Reporting a false positive could cause a shipment of food to be delayed or destroyed, impacting revenue for food companies. Reporting a false negative could result in contaminated foods reaching consumers, which could be catastrophic for the reputation of the food manufacturer and the testing laboratory. In order to meet the requirements for identification of pesticide residues, at least two MRM transitions are monitored and their ion ratios and retention times must match that of the reference for the compound of interest. Waters™ Xevo™ TQ-GC can perform MRM analysis as well as a product ion confirmation scanning (PICS) in a single acquisition, providing added confidence in the results.

Results and Discussion

PIC scanning is activated by a single check box in the method editor and automatically triggers a product ion scan or full scan when a peak is detected by MRM, following the apex of the peak. This results in a spectrum that can be used to further verify the presence of a compound by looking at other product ions that are associated with the compound of interest. In the example shown in Figure 2, a full scan PICS acquisition was performed. As the Xevo TQ-GC is an electron ionization (EI) based system the full scan data offers a 70 eV NIST searchable spectra. In this example, the PICS spectrum was submitted for a search against the NIST 2017 library to further confirm the presence of PCB 18. The PICS spectra can also be incorporated into TargetLynx™ Application Manager processing which automates the identification of compounds detected by MRM.

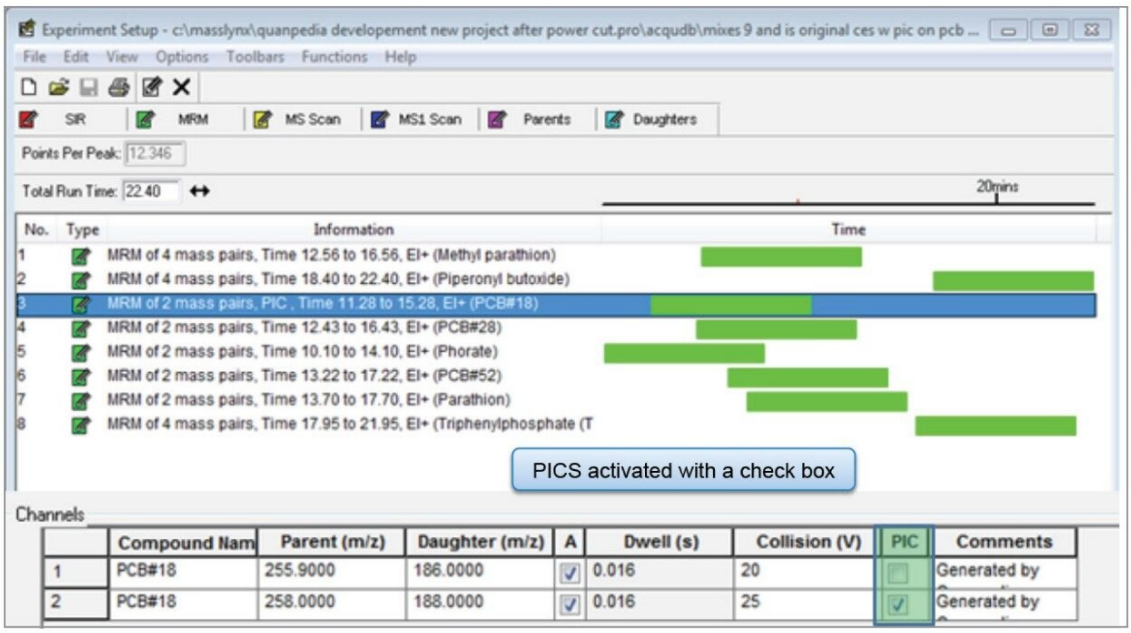

Figure 1. MS editor enables PIC scan with a single click.

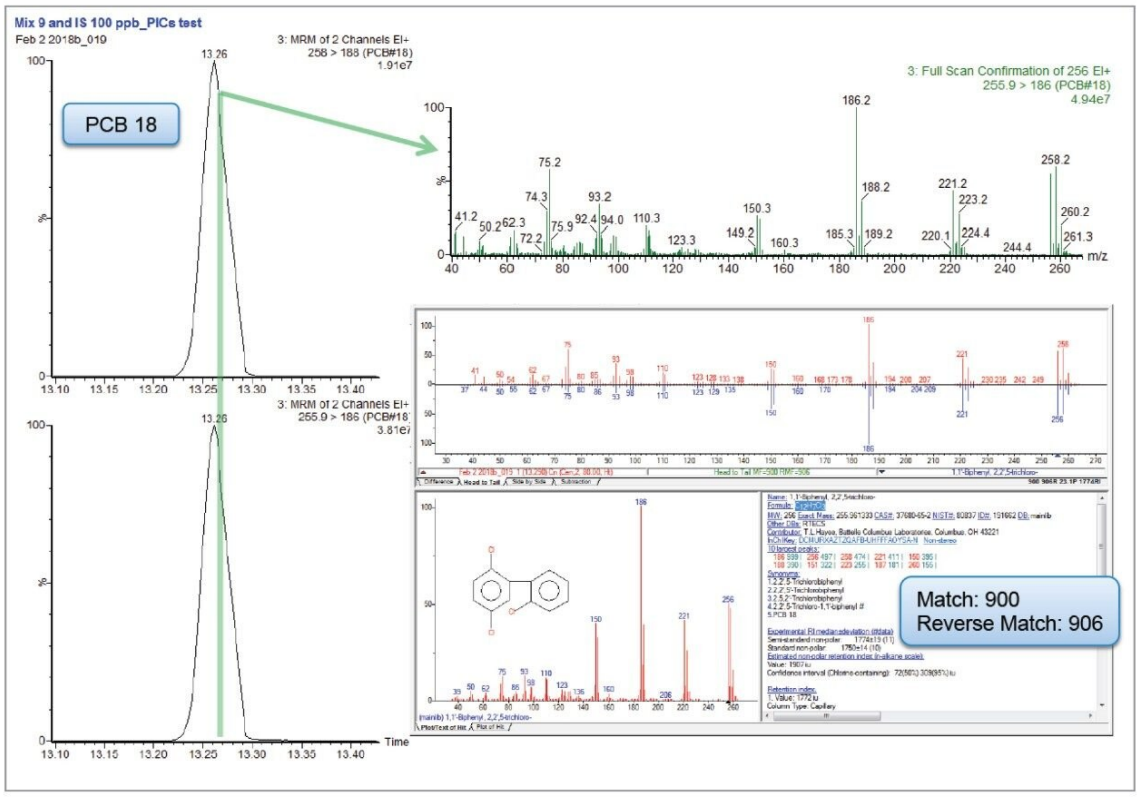

Figure 2. PICS of PCB 18 confirmed with NIST library search.

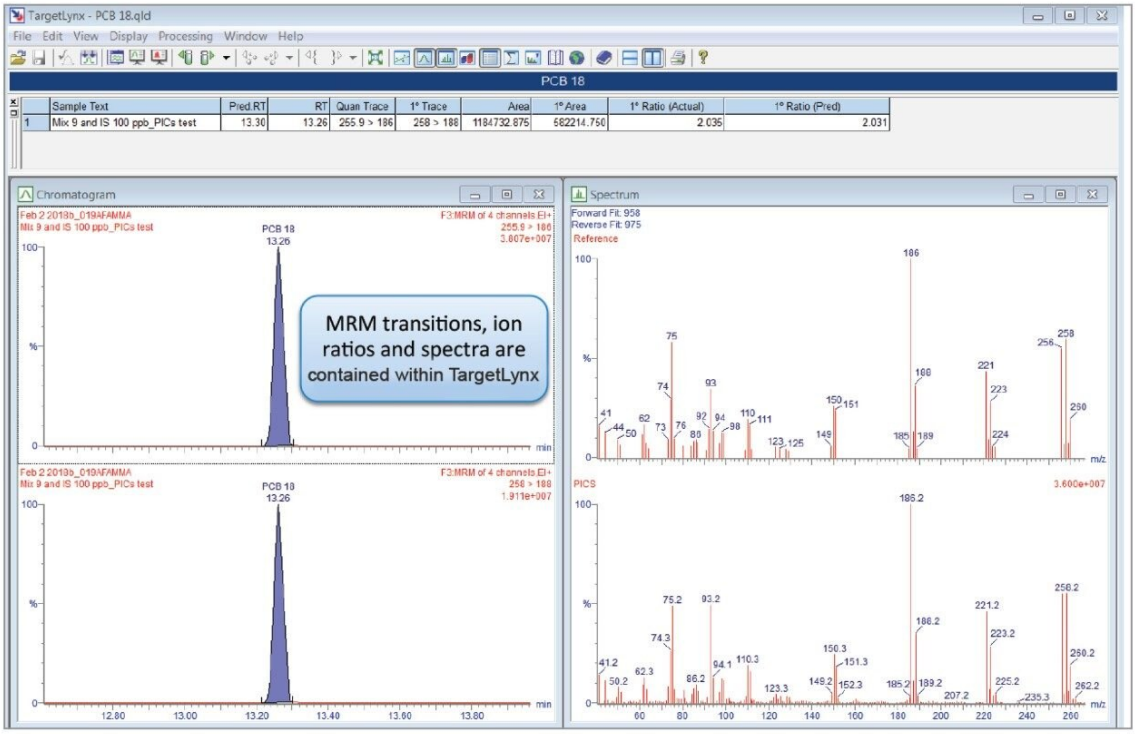

Figure 3. Incorporation of PICS spectrum in TargetLynx Application Manager.

Conclusion

The Xevo TQ-GC equipped with PICS allows users to have full confidence in the results produced from the system. Having full scan or product ion data concurrent with MRM acquisitions provides useful compound information, which can aid in identification and clarification of the results.

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Xevo TQ-GC Mass Spectrometry System <https://www.waters.com/waters/nav.htm?cid=134977323>

TargetLynx <https://www.waters.com/waters/nav.htm?cid=513791>

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