Multiresidue Pesticides Analysis Using Synchronous Scan/SIM Mode GC/MS

Abstract

Full scan GC/MS analysis is a commonly used data collection mode for pesticides screening, as this technique provides both qualitative and quantitative information. SIM analysis provides more sensitivity but does not provide any information regarding non-target analytes, nor does it provide any confirmation information. Combining these two analysis modes creates a more powerful analysis method that provides the best of both techniques. This application note discusses the use of the newly developed FASST (Fast Automated Scan/SIM Technique) for analysis of vegetable extracts.

Introduction

FASST GC/MS data acquisition takes advantages of both full-scan and SIM modes: high sensitivity of SIM is maintained, while qualitative confirmation of target and non-target analytes by full-scan mass spectrometry is realized. Using the FASST technique, both full-scan and SIM data are obtained in the same GCMS run by alternating at high speed between scan and SIM mode data acquisition.

Mass spectral data for over 700 agricultural chemicals has been compiled into the Compound Composer database; quantitative procedures for these chemicals have been developed providing a semi-quantitative analytical result. Screening can be conducted for a large number of agricultural chemicals in real-world samples.

Experimental Conditions

A Shimadzu GCMS-QP2010 Plus with GCMSsolution 2.5 software and an RTX-5ms (30 x 0.25 x 0.25) column were used. Conventional GC conditions using splitless, high-pressure injection were employed. The GCMS was operated in the FASST acquisition mode with a scan range of m/z 50-450. Carrot and apple extracts spiked with pesticide standards (Kanto Chemical, Japan) were analyzed using these conditions.

Results

In this study, quantitative analysis for over fifty selected pesticides was conducted using FASST data acquisition and conventional calibration procedures. Screening and semi-quantitative analysis for over 200 additional pesticides was accomplished from the same data using the Compound Composer database and software.

Target ion intensities and corresponding S/N values were compared between SIM only data and SIM data from Scan/SIM measurement. With FASST data acquisition, there was no degradation of chromatographic sensitivity in Scan/SIM using the high-speed data acquisition technology employed in the GCMS-QP2010 Plus.

Pesticides were added to carrot extract sample corresponding to 0.01ug/kg in the raw vegetable matter. Although some high-intensity matrix background peaks overlapped target compound chromatograms (see Figure 1a for TIC), all of the target compounds were easily detected. Figures 1b and 1c show chromatographic results for two target compounds.

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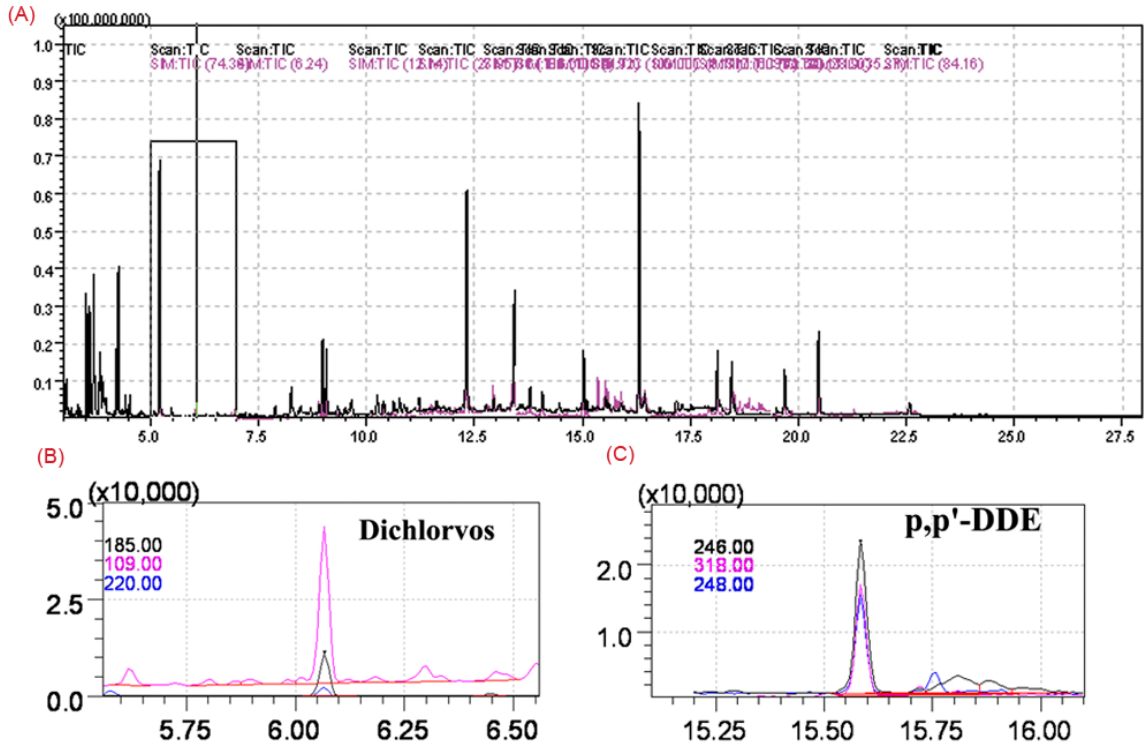

Figure 1: (a) TIC of carrot extract spiked with a mixture of 100+ pesticides. The trace in purple represents the intensities of the spiked pesticides. (b-c) SIM chromatograms of Dichlorvos and p,p'-DDE obtained using FASST

Conclusions

The GCMS-QP2010 Plus with a newly-developed synchronous Scan/SIM data acquisition mode demonstrated accurate quantitative analysis for a large number of target compounds using SIM data acquisition. High-sensitivity screening analysis for over 200 additional non-target pesticides was accomplished by using full scan data acquisition. Quantities of pesticides corresponding to 0.01 to 0.02ug/kg in raw vegetables were determined in the Scan/SIM mode. No degradation of sensitivity for the SIM data was observed for Scan/SIM compared to that acquired using the SIM-only data acquisition mode.