Applications Note

AccuTOF-GC Series

375 Pesticides x 5 Ions Exact Mass Database for Multi-residue Pesticide Analysis

Introduction

The AccuTOF GCx has high sensitivity, high mass resolution, high mass accuracy, a wide dynamic range and a high speed acquisition rate, all simultaneously (Figure 1).

Additionally, JEOL has developed a pesticides exact mass database that consists of 5 ions each for 375 different compounds which means that there are 1,875 total exact masses for multi-residue pesticide analysis. And because the TOF continuously collects the complete *m/z* region for each mass spectrum, we do not need to setup any SIM or SRM conditions, as is done for QMS and QqQMS systems. Therefore, the TOFMS can be used for both quantitative and qualitative analysis, simultaneously. In this application note, we show a portion of the pesticide database and the advantages of the GC/HR-TOFMS system for the multi-residue pesticide analysis.

Sample and Instrument

Commercially-available pesticide standards PL2005 Pesticide GC-MS Mix I, II, III, IV, V, VI, and VII (Hayashi Pure Chemical Ind.,Ltd.) were measured using GC/EI. After the measurement, a one-point drift compensation with *m/z* 207.03235 ($C_5H_{15}O_3Si_3^+$, column background) was used to calibrate the exact mass information for all pesticides.

Result and Discussion

As a starting point, we checked the high selectivity extracted ion chromatograms (EICs) effects using an actual food sample. To do this, we prepared a pesticides solution, a pre-treated ginger sample solution and a pretreated, pesticides-spiked ginger sample solution. Next, both ginger samples were tested and showed a large background signal in their GC/EI TIC. The enlarged EI mass spectrum for the pesticides spiked ginger sample for Atrazine is shown in Figure 2. We can clearly see the Atrazine fragment ion at *m/z* 158.027, but an impurity component from the ginger at *m/z* 158.109 was also detected which was very similar in mass to the targeted Atrazine fragment ion. In this case, low-resolution mass spectrometry would not be able separate these ions from each other, which would in turn result in an incorrect quantitative value. To show this, we made low-selectivity EICs using +/- 0.5 Da window at *m/z* 158 for each of the three samples as shown on the right side of Figure 3 (same Y-axis scale). These results showed a large chromatographic peak in both the ginger sample and the

Figure 1. 4th generation of the JEOL GC/HR-TOFMS system JMS-T200GC "AccuTOF GCx"

pesticides-spiked ginger sample. Their peak intensities and area values were actually higher than the Atrazine peak intensity and area of the pesticides-only data.

On the other hand, a high-resolution mass spectrometer can easily separate these similar *m/z* values from each other. As an example of this, high selectivity EICs with narrow mass window (+/- 0.05 Da) were created using the AccuTOF GCx data (Figure3, left side). In the unspiked ginger sample data (Figure 3, left-middle), there was no chromatographic signal. However, the Atrazine peaks in both the pesticide sample and the pesticides-spiked ginger sample showed very similar peak intensities. These results show that the chromatographic interference effects can be reduced for real world samples using the high resolution/high selectivity EIC technique on the AccuTOF GCx.

In order to make these high selectivity EICs, it is important to use the correct exact masses for all pesticides components. All of the 375 pesticide exact masses were stored in an Excel spreadsheet database and were then copied and pasted into to the quantitative table of the JEOL multi-component quantitative analysis software (Figure4). Afterwards, the pesticides standard solutions can be measured and then examined using the exact mass information for each of the 375 pesticides (5 ions each).

Conclusions

This high selectivity technique is necessary for getting the correct quantitative analysis results from actual real world samples, and these results show that only high-resolution mass spectrometry can provide this information.

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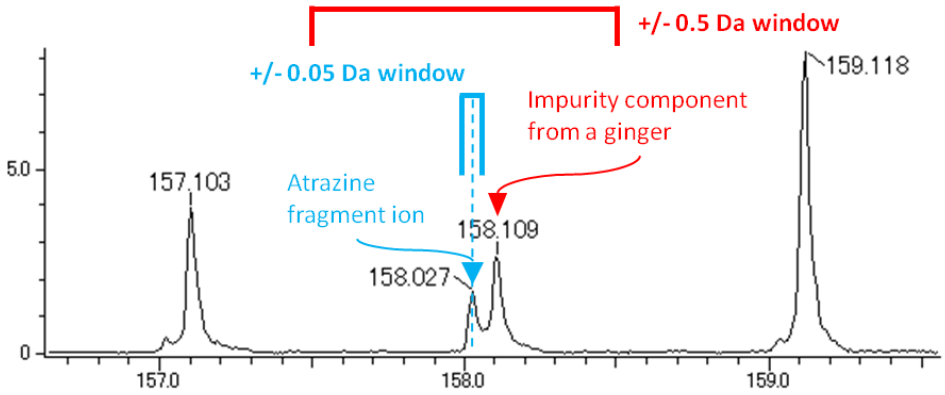

Figure.2 The enlarged EI mass spectrum of the pesticides-spiked ginger sample for Atrazine.

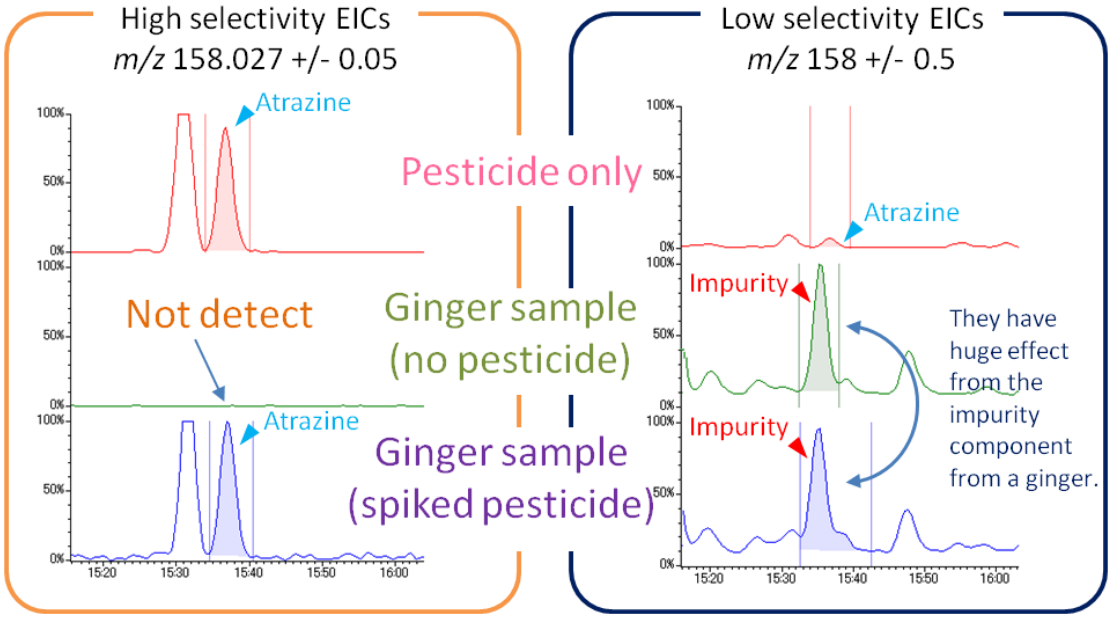

Figure 3. High and low selectivity EICs for Atrazine (same y scale).

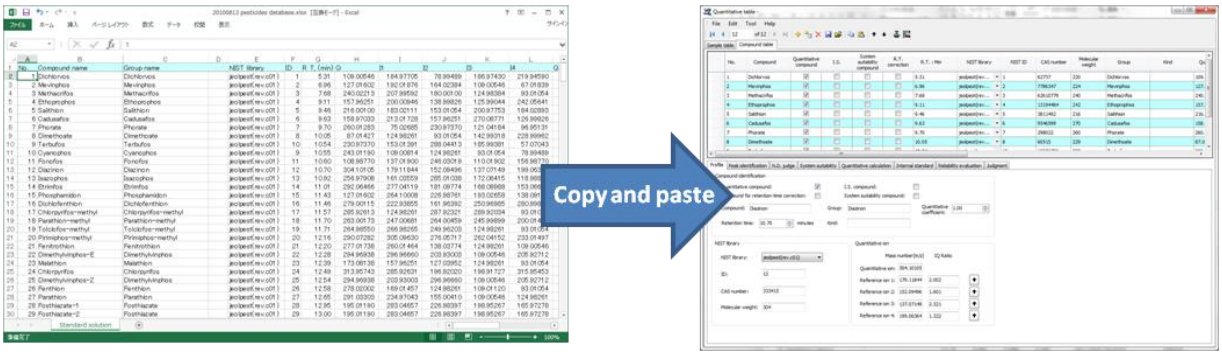

Figure 4. The pesticides database (left) and the quantitative table (right).

