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Fast and Sensitive GC-MS/MS Analysis of Trace Chemicals

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Executive Summary

The Thermo Scientific™ EvoCell collision cell technology available in the Thermo Scientific™ TSQ™ 8000 Evo triple quadrupole GC-MS increases the number of compounds that can be detected in a single chromatographic run while maintaining superior sensitivity.

Key Words

Collision cell, Contaminants, Food, Environment, Selected Reaction Monitoring, SRM, Triple Quadrupole

Introduction

A growing number of toxic chemical contaminants require detection and quantification in food and environmental samples at very low concentrations. These increased demands pose new challenges to analytical systems, such as GC-MS/MS triple quadrupole mass analyzers. Such instrumentation must accommodate a greater number of selected reaction monitoring (SRM) transitions per unit time without compromising the required target compound sensitivity.

EvoCell Collision Cell Technology

The innovative EvoCell collision cell technology (Figure 1), combined with the efficient SRM scheduling of timed-SRM (t-SRM) software[1] in the TSQ 8000 Evo GC-MS/MS, allows users to schedule several thousand unique SRM transitions in a single run, while maintaining sensitivity. This technology allows for the screening and quantification of more than 1000 compounds in a single run, while acquiring both quantitation and multiple confirming SRM transitions for each compound.

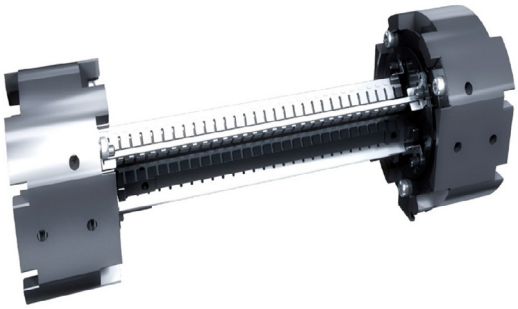

Figure 1. The EvoCell collision cell, with enhanced velocity optics, provides high SRM transition speeds, precision, and sensitivity for even the most complex methods.

A comparison of scanning speeds with the detection limit for both the TSQ 8000 GC-MS/MS (the predecessor to the TSQ 8000 Evo GC-MS/MS) and the TSQ 8000 Evo GC-MS/MS was generated for the pesticide bifenthrin. Using the EvoCell technology, bifenthrin was detected at lower levels at 200 MRM/s.

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Similar sensitivity (as measured by fg of target compound detected) is achieved when the TSQ 8000 GC-MS/MS is run at 200 MRM/s and the TSQ 8000 Evo GC-MS/MS run at 800 MRM/s acquisition speeds (Figure 2).

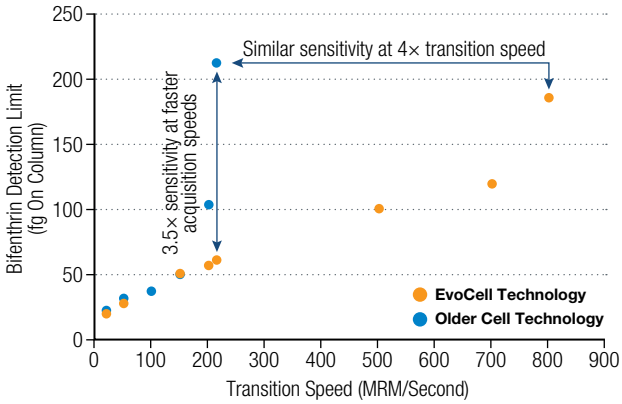


Figure 2. Equivalent sensitivity is obtained by the EvoCell technology in the TSQ 8000 Evo GC-MS/MS running at 4× the speed of its predecessor, the TSQ 8000 GC-MS/MS.

Analyzing more transitions without loss of sensitivity

An experiment was designed to test the capability of the new EvoCell. The method produced scan times of 0.5 ms for several compounds to determine the effect this would have on the sensitivity and reproducibility of the results.

Calibration standards from 1 ppb to 1000 ppb and 10 replicates of the 10 ppb standard were analyzed for more than 200 pesticides in a rice matrix, while scanning for >5000 transitions. The analytical run was 34 minutes and the data was collected using t-SRM. A total of >650 compounds were scanned with an average of eight SRM transitions per compound. With the use of t-SRM, scan times ranged from 0.5 to 124 ms for the entire run. Response curves were generated for the >200 pesticides in the calibration standards. The coefficient of determination (R^2) was >0.98 with 94% of the compounds >0.995. Figure 3 is a graphical representation of these results.

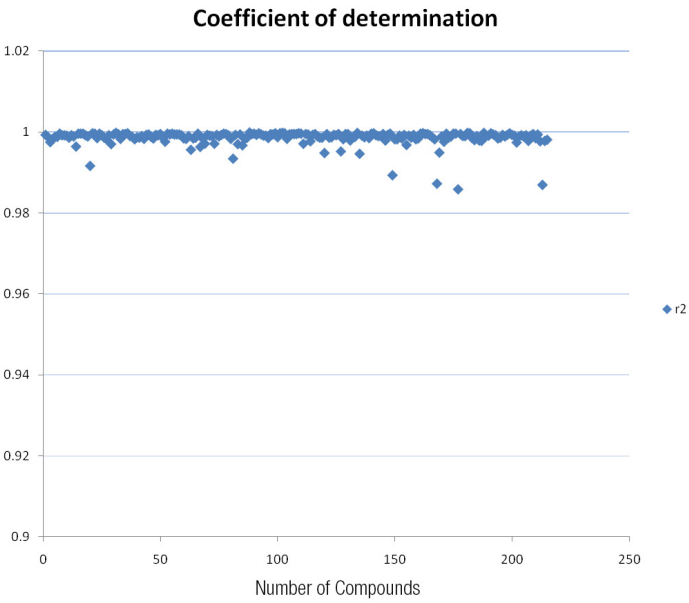


Figure 3. The coefficient of determination for ›200 pesticides, while scanning for ›5000 transitions.

Using the 10 ppb calibration standard in a rice matrix, 10 replicates were analyzed to assess the response accuracy and determine the method detection limits (MDLs) for the targeted compounds (Figure 4). This data was collected using the same instrument method to generate the response curves with the scan times for the target compounds ranging from 0.5 to 34 ms.

The results shown in Figure 5 are a selection of pesticides measured using the lowest dwell times in the acquisition method (0.5 ms). Even at the fastest scan speeds, excellent results were obtained. By acquiring data using an increased number of transitions per compound, more confirmation ions are available and the effect of matrix interference is mitigated, without the need to develop matrix-specific SRM databases.

Figure 4. The average concentration and the calculated MDL for 10 replicate analyses of a 10 ppb matrix-matched standard for >200 targeted compounds, while scanning for >5000 transitions.

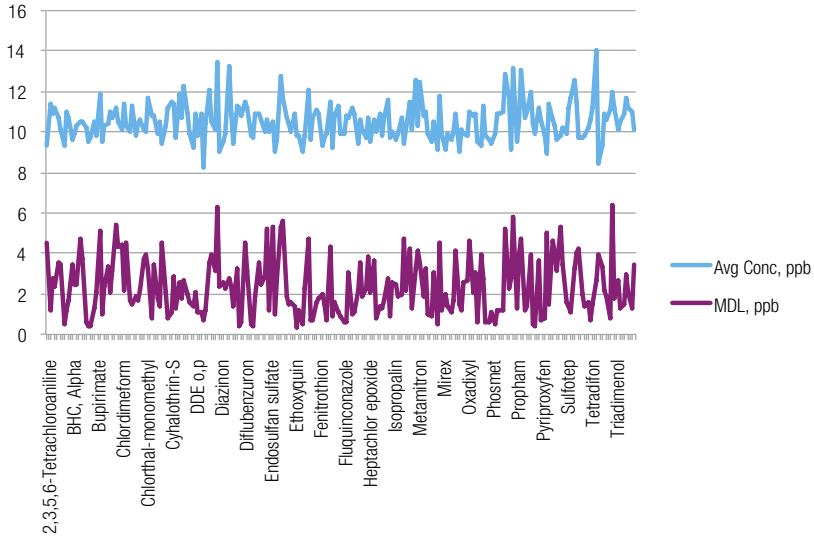


Figure 5. Analysis of pesticides in rice (10 µg/kg) with the EvoCell collision cell at 0.5 ms dwell time and 800 SRM transitions/s.

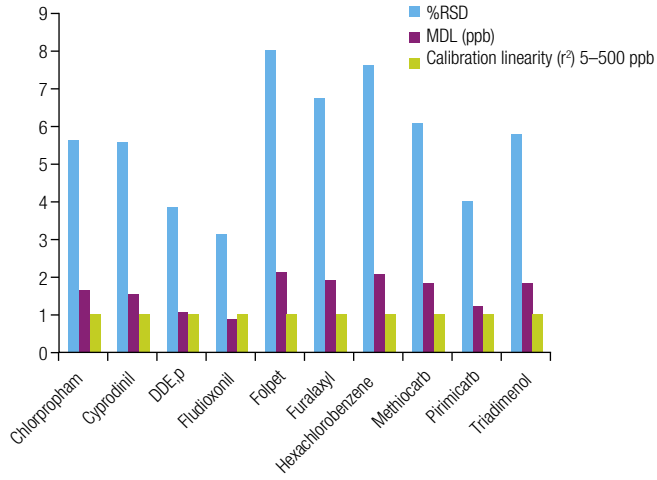


Figure 6 shows the peaks and the calibration curve for o,p-DDE at 10 ppb. The dwell time was approximately 1.5 ms/SRM transition. Results show the quantification ion and two confirming ions at this level. The area of the quantification ion is >300,000 peak area counts.

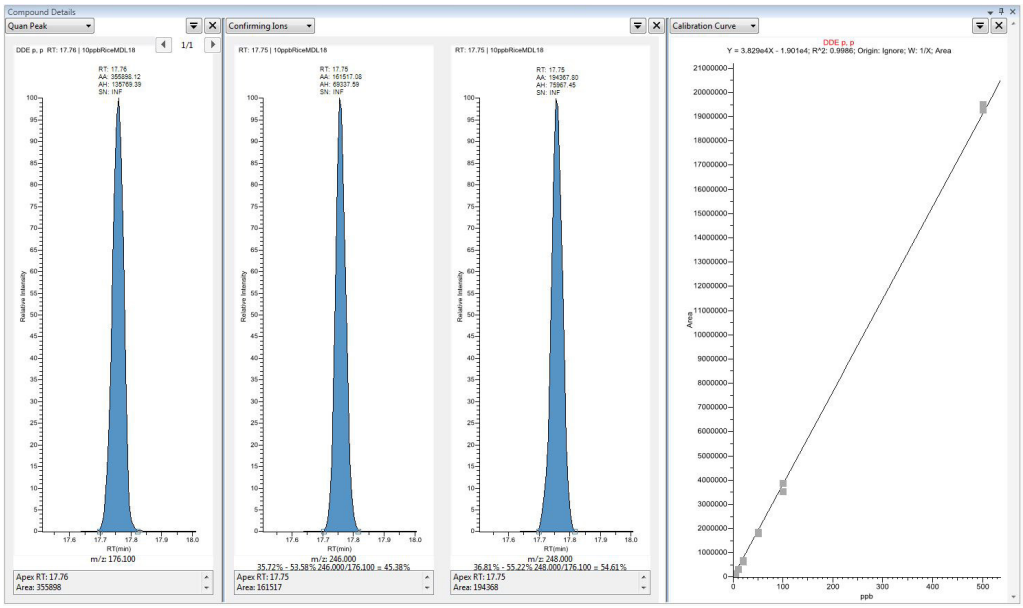


Figure 6. Quantification and confirming peaks at 10 ppb and the calibration curve for o,p-DDE, while scanning >5000 transitions.

Three-fold Sample Throughput

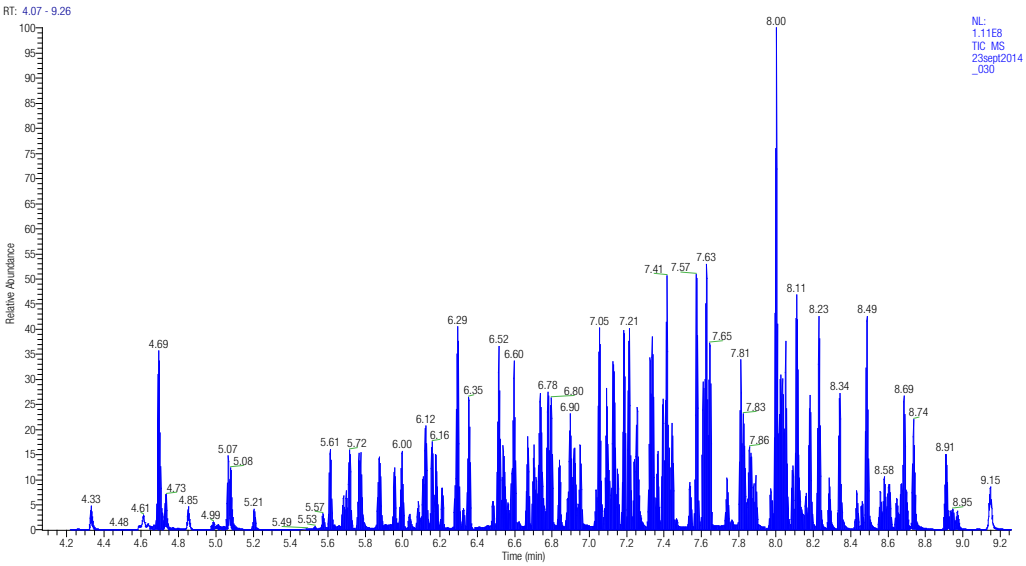
The scanning speed of the EvoCell provides the user with one of two benefits—more compounds and confirming ions or shorter run times. A method with 132 targeted pesticides can be analyzed in less than 11 minutes with the new EvoCell technology. This means more than three times the number of samples can be run with the same sensitivity and reproducibility as previously possible.

Typically, a GC analysis of 132 target pesticides is around 40 minutes, in order to obtain a sufficient number of scans per chromatographic peak, especially in time windows containing many co-eluting peaks. In order to accurately integrate the peaks of interest, at least 10–12 scans across a chromatographic peak are required. Until now, fast scan speeds compromised instrument sensitivity, especially when several SRM transitions were monitored simultaneously. Using the fast GC conditions described in Table 1, the GC run time was decreased to ~11 min with no compromise in the number of data points acquired for each chromatographic peak (Figures 7 and 8). This short run time is possible because EvoCell technology allows fast transmission of ions through the collision cell and hence faster data acquisition, without adversely affecting instrument sensitivity. Fast data acquisition leads to more information being collected in a shorter time, ultimately resulting in faster GC runs. Using this methodology allowed the sample productivity to improve by three-fold. A typical overnight batch (16 hours), which allows around 24 injections of extracts/standards, now allows injection of around 70 samples, including GC run times.

Table 1. GC and injector conditions.

TRACE 1310 GC Parameters		
Injection Volume (mL):	1.0	
Liner:	SSL single taper (P/N: 453A2342)	
Inlet (°C):	240	
Inlet Module and Mode:	Splitless	
Carrier Gas, (mL/min):	He, 1.2	
Oven Temperature Program:	Temperature 1 (°C):	60
	Hold Time (min):	1.0
	Temperature 2 (°C):	180
	Rate (°C/min)	50
	Temperature 3 (°C):	320
	Rate (°C/min)	35
	Hold Time (min):	4.0

Figure 7. Fast GC-MS chromatographic run of 132 pesticides (SRM, TIC data) at 100 ng/g and a total run time of 11 minutes. The first (dichlorvos, RT = 4.33 min) and the last (deltamethrin, RT = 9.15 min) eluting pesticides are shown.



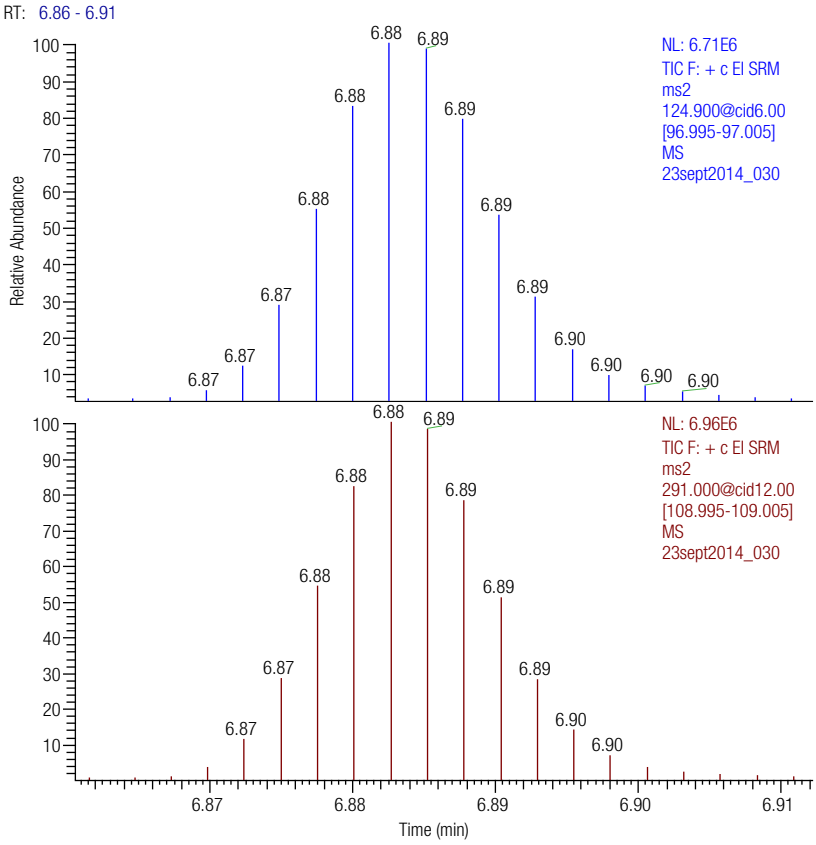


Figure 8. Parathion ethyl eluting at RT = 6.89 min showing 13 scans/peak (peak width 1.8 sec, dwell time of 1.7 ms).

Conclusion

The EvoCell collision cell technology enables:

- an increased number of SRM transitions per compound
- analysis of more compounds in a single chromatographic run
- fast data acquisition leading to more information in a shorter time
- faster GC runs without sacrificing accuracy or sensitivity

In summary, the unique technology in the EvoCell collision cell of the TSQ 8000 Evo GC-MS/MS shortens method development and allows faster turnaround time, saving time and money.

References

1. Thermo Scientific. Application Brief 52299: Thermo Scientific TSQ 8000 Triple Quadrupole GC-MS/MS Instrument Method. Sunnyvale, CA. [Online http://www.thermoscientific.com/content/dam/tfs/ATG/CMD/cmd-support/tsq-8000/scientific-resources/application-notes/Thermo-Scientific-TSQ-8000-Triple-Quadrupole-GC-MS-MS-Instrument-Method.pdf (accessed Sept. 16, 2014).]

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