

# GC-MS/MS Pesticide Analyser Workflow Updated and Enhanced By Powerful Thermo Scientific™ Chromeleon™ 7.2 CDS Software

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## Introduction

Triple quadrupole mass spectrometers such as the Thermo Scientific™ TSQ™ 8000 Evo GC-MS/MS system have gained popularity over their single quadrupole counterparts because of their high selectivity and lower detection limits, especially in complex matrices such as those encountered in pesticide analysis in food. In this poster we present results of GC-MS/MS analysis of pesticides using timed-Selected Reaction Monitoring (t-SRM). The t-SRM optimized dwell times combined with the Enhanced Velocity Optics (EvoCell collision cell) present in the TSQ 8000 Evo enables us to monitor multiple transitions per analyte for a more confident identification without compromising quantitation sensitivity. The results we show were obtained using Thermo Scientific™ Dionex™ Chromeleon™ 7.2 CDS software, which combines powerful data analysis capability with easy pesticide analysis method creation. The Chromeleon software pesticide analyzer database contains retention times and transitions for over 1000 pesticides and other compounds of environmental interest. Historically, developing MS/MS transitions for compounds used to be arduous and time-consuming process prone to operator error, but this no longer is the case. This poster highlights the power of AutoSRM which is a tool for developing and optimizing transitions for compounds that are not yet present in the database with simple user interaction and high degree of confidence in the results.

## Method

**Hardware-** Thermo Scientific TSQ 8000 Evo GC-MS/MS with TRACE™ 1310 GC coupled with AI/AS 1310 autosampler.

**Software-** Thermo Scientific Dionex Chromeleon 7.2 CDS software

**Sample-** QuEChERS extracted lettuce matrix in 1:1 Ethyl acetate/cyclohexane spiked with Restek® GC Multiresidue Pesticide kit (Cat.# 32562) containing nine vials of standards (#1 to #9).

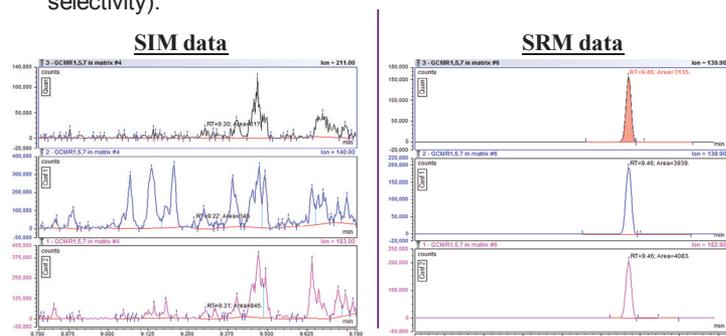
**Methodology-** The injector, column and the GC and MS run conditions are same as that recommended in the Thermo Scientific™ TSQ™ 8000 Evo Pesticide Analyzer guide. The Pesticide analyzer also contains a compound database (CDB) having 1001 compounds with expected retention time (for the given conditions) as well as fully optimized SRM transitions for at least 3 ions per compound.

**FIGURE 1. Full scan chromatogram of 10 pg/μL GC MR #1,5,7 spiked in lettuce matrix.** We see a number of extracted lettuce compounds that could possibly interfere with pesticides.



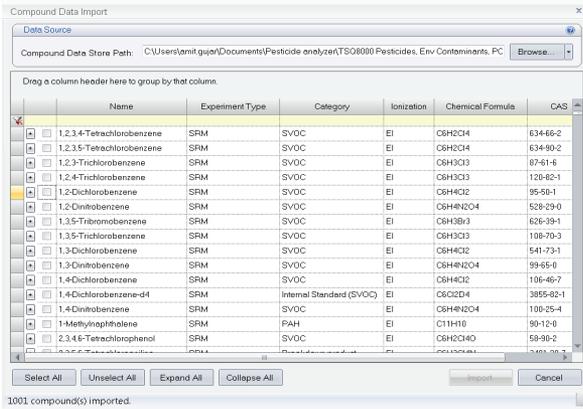
## Why Triple Quad (SRM) not Single Quad (SIM)?

Below is an example of Etridiazol (at 10 pg/μL) SIM data and SRM data. We see no matrix interferences with SRM data (high selectivity).

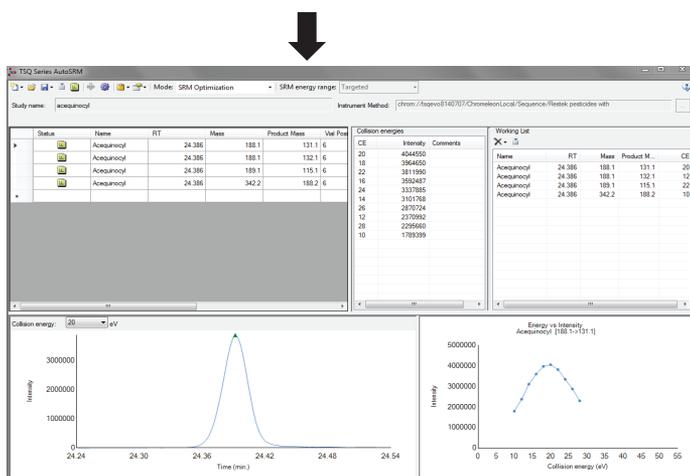


# Chromleon Pesticide Analyzer Workflow

Select compounds from the Compound Database (CDB)



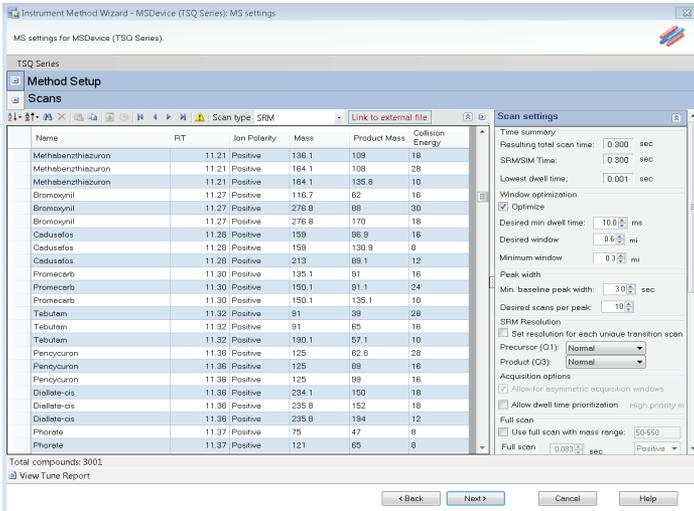
For compounds not in the CDB perform AutoSRM



AutoSRM has 3 simple one-click "Auto Process" steps -

1. Select precursor ions (or import SIM data)
2. Select product ions
3. Choose optimum collision energy

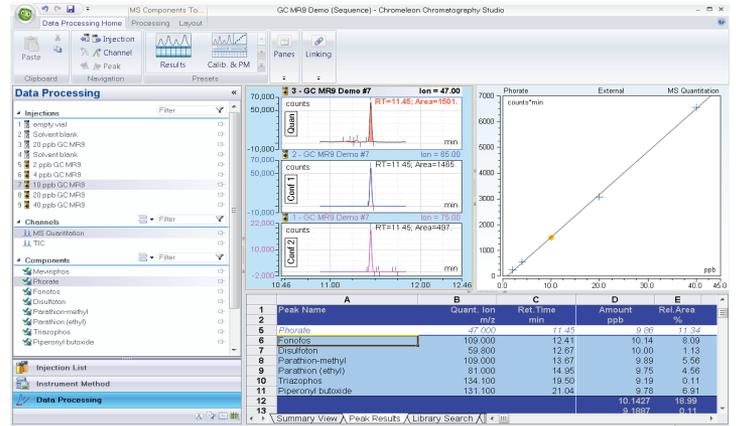
Import the compounds into MS Instrument method (the dwell times are automatically optimized (t-SRM) based on the scan settings)



Start your sequence



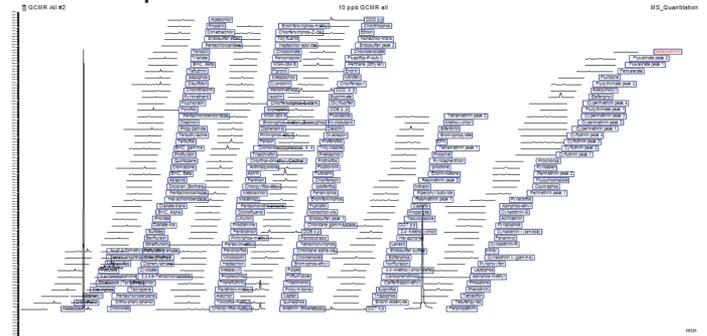
Check your results



## Results

Screening studies- Restek® GC MR #1 to #9 were spiked at 10 pg/μL levels in lettuce matrix. The whole Pesticide analyzer method for screening 1001 compounds was run on this sample. Out of the 203 compounds, 198 were detected at this trace level.

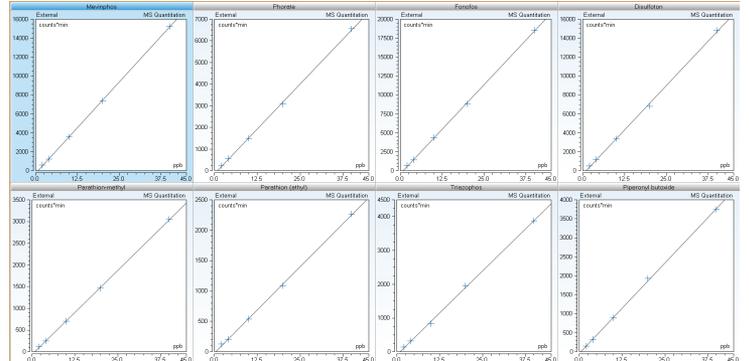
FIGURE 2. MS Quantitation chromatogram for 10 pg/μL of GC MR #1 to 9 spiked in lettuce extract.



Quantitative studies- Analytical performance of the instrument was determined by plotting the calibration curves and looking at repeatability at low concentrations for GC MR #9 mix. The limits of detection (LoD) were then determined by-

$$LoD = 2.998 \times Amount \text{ on column} \times \%RSD$$

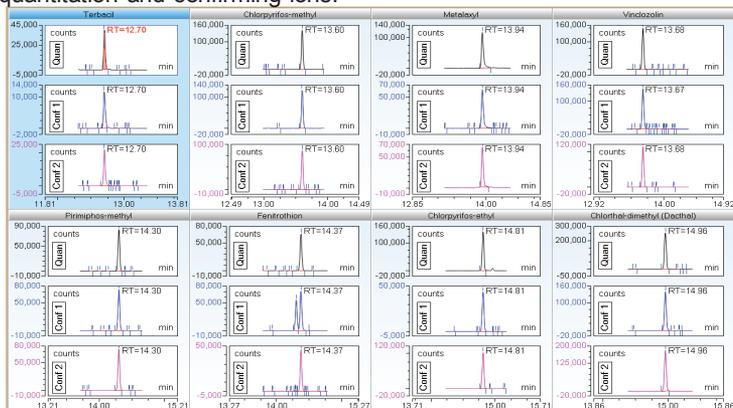
FIGURE 3. Calibration curves for Restek® GC Multiresidue Pesticide Standard #9 in lettuce matrix; 2-40 pg/μL . The average R<sup>2</sup> was 0.9994.



**Table 1. %RSDs and LoDs for Restek® GC Multi-residue Pesticide Standard #9 in lettuce matrix (8 consecutive injections of 2 pg/µL)**

Compound	%RSD	LoD, fg on-column
Mevinphos	11.4	0.68
Phorate	5.4	0.33
Fonofos	7.3	0.44
Disulfoton	8.6	0.51
Parathion-methyl	8.4	0.50
Parathion (ethyl)	10.1	0.61
Triazophos	12.4	0.74
Piperonyl butoxide	9.7	0.58

A similar study was done for a 60 pesticide mix of GC MR #1,5 and 7. Shown below are selected compounds with their quantitation and confirming ions.



## Conclusion

- The high selectivity offered by GC-MS/MS is critical in positively identifying pesticides in complex food matrices.
- Chromeleon 7.2 and AutoSRM provides an easy workflow for GC-MS/MS pesticide analysis with single platform for lab-wide instrument control.
- The TSQ 8000 Evo GC-MS/MS with timed-SRM and EvoCell provides superior detection limits, even in the most challenging samples.

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