# MS Data Processing With Full Flexibility Of Universal Processing Software.

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## Overview

Liquid Chromatography (LC) in combination with triple quadrupole Mass Spectrometry (MS) is more and more a common analysis technique in routine laboratories. Especially when using MS/MS selected reaction monitoring (SRM) for a large number of components data handling can be a bottle neck. This poster will show MS data processing of pesticides in water samples using an already established chromatography data system which is now also capable of processing large quantities of MS data.

## Introduction

In routine practice, screening of pesticide residues in a large variety of fruit and vegetable samples is carried out by a number of different analytical techniques, LC-MS/MS being one of the routine approach. When considering the throughput of the lab, data processing is an important part of the total workflow of any multi-method covering up to hundreds of compounds.

Traditional data analysis with triple quadrupole MS/MS analysis is based on evaluation of multiple SRM experiments whereby a number of known contaminants is measured and quantified using available standards. With increasing number of compounds to be screened, samples to be measured, and data to be reported as fast as possible, data analysis can be optimized and automated.

## Methods

Blanks, calibration standards, QC standards and unknown samples are injected via conventional reversed phase chromatography with a gradient elution, coupled to the latest state of the art Triple Quadrupole MS.

### Liquid Chromatography

Thermo Scientific™ Dionex™ UltiMate™ 3000 RSLC system.

**FIGURE 1. UltiMate 3000 RSLC System and TSQ Quantiva Triple Quadrupole MS.**

### Mass Spectrometry

MS analysis was performed with a Thermo Scientific™ TSQ Quantiva™ Triple Quadrupole MS with AIM Technology.

**FIGURE 2. Schematic Overview of Triple Quadrupole LC-MS/MS.**

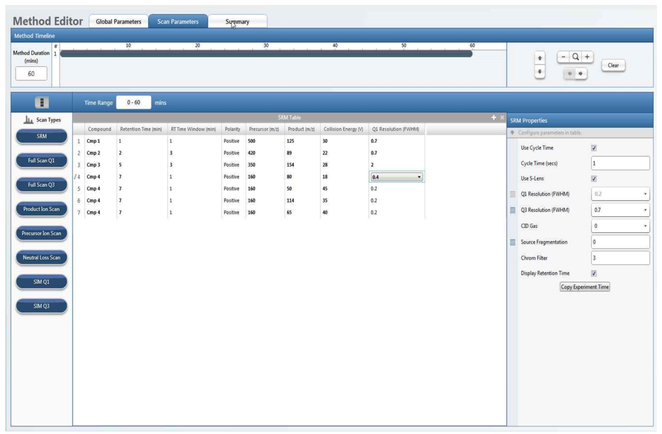

*Parameters*

| | |
|---|---|
| Source | HESI |
| Polarity | Positive |
| ISV | 3500V |
| Sheath gas | 40 arb units |
| Aux | 15 arb units |
| Vaporizer | 280 °C |
| Transfer | 350 °C |

*Experiment*

| | |
|---|---|
| SRM transitions | Quantitation and Confirmation |
| Resolution Q1 and Q3 | unit mass resolution |
| Cycle time | 0.4 sec |

**FIGURE 3. SRM Acquisition Table.**




### Data Analysis

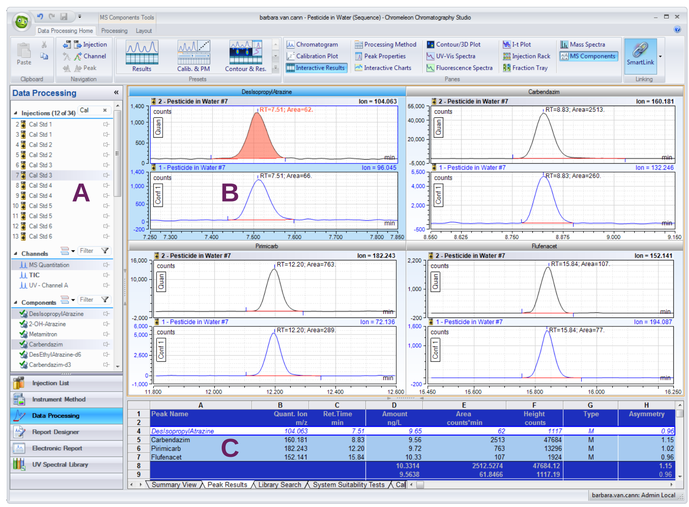
Data analysis was performed with Thermo Scientific™ Dionex™ Chromeleon™ Chromatography Data System (CDS) software.

## Results

### Data Evaluation

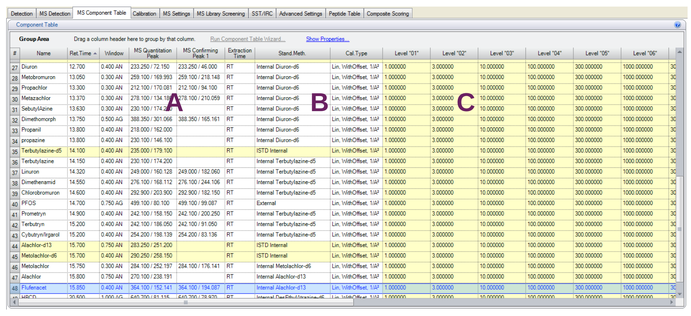
All data evaluation is performed in the Chromatography Studio (Figure 4). Chromeleon CDS operates with the principle of Dynamic Data Processing. This ensures the selections and changes made are instantly reflected in the data and results. For example, when selecting one or more components and/or injections in the navigation pane (Figure 4A), the component traces (Figure 4B) and corresponding results (Figure 4C) are shown. All changes are automatically applied to all injections in the sequence.

**FIGURE 4. Chromatography Studio showing Navigation Pane (A), MS Component Traces (B) and Interactive Results Tables (C).**




Detection parameters and component settings (Figure 5) in the Processing Method are applied to all component traces.

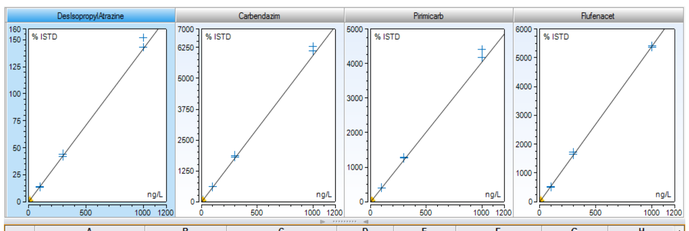
**FIGURE 5. Comprehensive Component Table, including Quantitation and Confirming peaks (A), Calibration settings (B) and Calibration levels (C)**




### Quantitation

After injection of calibration standards, curves were calculated as defined in the processing Method (Figure 5B and C), using the Chromeleon CDS algorithm (Figure 6). Peaks (quantitation and confirming), representing the components in the SRM trace were integrated automatically, using the Cobra™ peak detection algorithm.

**FIGURE 6. Calibration plots of selected components, including calibration curve parameters.**




| | A | B | C | D | E | F | G | H |
|---|---|---|---|---|---|---|---|---|
| 1 | Peak Name | Ret.Time min | Cal.Type | Number of Points | Rel.Std.Dev. % | R-Square | C0 (Intercept) | C1 (Slope) |
| 2 | | | | | | | | |
| 4 | *Desisopropylatrazine* | *7.51* | *Lin, WithOffset, 1/A²* | *12* | *5.2754* | *0.9982* | *0.0542* | *0.1416* |
| 5 | Carbendazim | 8.83 | Lin, WithOffset, 1/A² | 12 | 10.1079 | 0.9950 | 1.0858 | 5.9230 |
| 6 | Pirimicarb | 12.20 | Lin, WithOffset, 1/A² | 12 | 11.1309 | 0.9948 | 0.3174 | 4.0423 |
| 7 | Flufenacet | 15.84 | Lin, WithOffset, 1/A² | 12 | 8.4784 | 0.9973 | -0.0303 | 5.4060 |
| 8 | | | | | 11.1309 | 0.9982 | | |
| 9 | | | | | 5.2754 | 0.9948 | | |

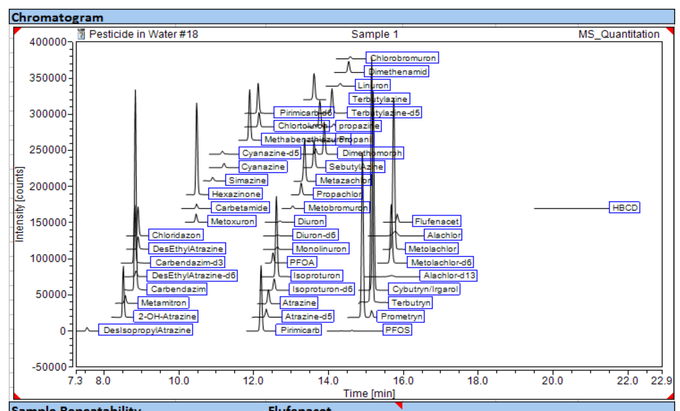
Summary View | Peak Results | Library Search | System Suitability Test

The amounts in all standards and samples were calculated based on the calibration results. The recovery of the standards compared to the theoretical amount (Figure 7).

**FIGURE 7. Overview of confirmation ratios and actual and theoretical amounts of flufenacet in all calibration and QC standards.**

| Standard Recovery | Flufenacet | | | | |
|---|---|---|---|---|---|
| No. | Injection Name | Conf. Ratio % | Amount ng/L | Theoretical Amount ng/L | Deviation % |
| 2 | Cal Std 1 | 0.83 | 0.94 | 1.00 | -5.91 |
| 3 | Cal Std 1 | 0.78 | 1.07 | 1.00 | 6.86 |
| 4 | Cal Std 2 | 0.84 | 2.80 | 3.00 | -6.74 |
| 5 | Cal Std 2 | 0.74 | 3.10 | 3.00 | 3.48 |
| 6 | Cal Std 3 | 0.74 | 9.85 | 10.00 | -1.49 |
| 7 | Cal Std 3 | 0.72 | 10.33 | 10.00 | 3.31 |
| 8 | Cal Std 4 | 0.80 | 98.22 | 100.00 | -1.78 |
| 9 | Cal Std 4 | 0.81 | 95.12 | 100.00 | -4.88 |
| 10 | Cal Std 5 | 0.79 | 318.86 | 300.00 | 6.29 |
| 11 | Cal Std 5 | 0.80 | 304.52 | 300.00 | 1.51 |
| 12 | Cal Std 6 | 0.78 | 992.79 | 1000.00 | -0.72 |
| 13 | Cal Std 6 | 0.78 | 1000.75 | 1000.00 | 0.07 |
| 14 | QC | 0.81 | 28.75 | 30.00 | -4.17 |
| 15 | QC | 0.80 | 29.93 | 30.00 | -0.22 |
| 16 | QC | 0.81 | 30.91 | 30.00 | 3.05 |

**FIGURE 8. Calculated ion ratios, amounts and repeatability in Sample 1.**




| Sample Repeatability | Flufenacet | | | | |
|---|---|---|---|---|---|
| Name | Conf. Ratio % Flufenacet | Retention Time min Flufenacet | Area counts*min Flufenacet | Height counts Flufenacet | Amount ng/L Flufenacet |
| Sample 1 | 0.81 | 15.84 | 616.9 | 11350 | 51.45 |
| Sample 1 | 0.81 | 15.84 | 618.1 | 10964 | 51.96 |
| Sample 1 | 0.79 | 15.84 | 621.1 | 11228 | 53.54 |
| Sample 1 | 0.80 | 15.84 | 646.8 | 11408 | 53.01 |
| **Average** | **0.80** | **15.84** | **625.7** | **11237** | **52.49** |
| **Standard Deviation** | **0.01** | **0.00** | **14.17** | **197.13** | **0.95** |
| **Relative Standard Deviation** | **0.93** | **0.00** | **2.26** | **1.75** | **1.82** |

## Conclusion

To process the data with MS detection several parameters have to be entered depending on the experiment and settings. Here we demonstrated that by selecting the appropriate SRM transition data can be quantified on one of the SRM transitions, usually the most intense fragment. The other fragment can be used to confirm the compound detected. Calculation of concentration is as simple as with other detection techniques, where the area is compared to concentration with or without an internal standard.

The objective of the work was to demonstrate the use of Chromeleon CDS with the latest triple quadrupole. The processing of MS data in Chromeleon CDS is handled the same as conventional chromatography data. Dynamic Data Processing ensures the selections and changes made are instantly reflected in the data and results, saving huge amounts of data processing time. Data processing was complete and fast in an intuitive environment.



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