Step up

productivity, confidence, and compliance
for pesticides analysis with a sample-to-result
LC-MS/MS solution

Thermo Scientific Pesticide Explorer
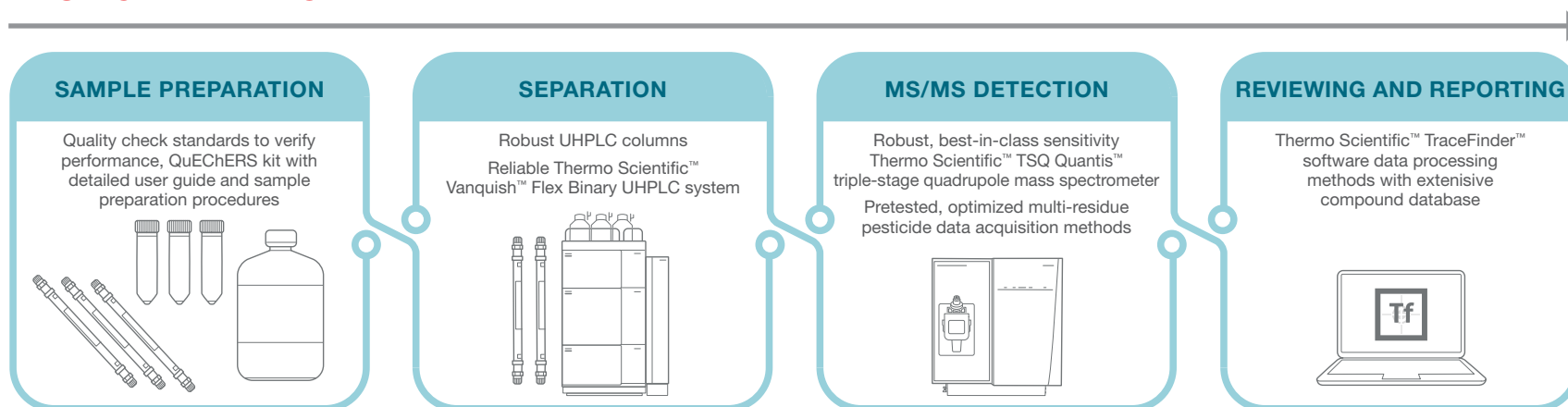
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Pesticide Explorer workflow: productivity, robustness, and regulatory compliance

The Thermo Scientific™ Pesticide Explorer workflow is an easy to implement sample-to-result, LC-MS/MS analytical workflow, tailored to deliver robust, sensitive quantitation in compliance with global regulatory requirements. With a pre-tested and validated multi-residue pesticide method for over 400 analytes in different matrices, the workflow allows food-safety monitoring and testing laboratories to step up their productivity with reduced startup time and cost, easier compliance, and robust performance. Regardless of laboratory expertise, the Pesticide Explorer workflow is designed to simplify the process of obtaining reliable, unambiguous, high-quality LC-MS/MS results.

PESTICIDE EXPLORER

SAMPLE PREPARATION	SEPARATION	MS/MS DETECTION	REVIEWING AND REPORTING
Quality check standards to verify performance, QuEChERS kit with detailed user guide and sample preparation procedures	Robust UHPLC columns Reliable Thermo Scientific™ Vanquish™ Flex Binary UHPLC system	Robust, best-in-class sensitivity Thermo Scientific™ TSQ Quantis™ triple-stage quadrupole mass spectrometer Pretested, optimized multi-residue pesticide data acquisition methods	Thermo Scientific™ TraceFinder™ software data processing methods with extensive compound database

Achieve immediate success with a comprehensive, single-provider workflow

The Pesticide Explorer workflow is an optimized single-provider solution, built by scientists for scientists working in food safety laboratories around the world. The comprehensive solution provides a reliable, high-quality LC-MS/MS workflow for analyzing hundreds of pesticide residues in a wide range of matrices.

Meet all requirements for robust multi-class pesticide residue analysis

Laboratories face numerous challenges in developing robust, sensitive quantitation workflows for multi-class pesticide residue analysis. Adding to the challenge is the difficultly of reducing cost per sample while obtaining high performance and certainty in results. The Pesticide Explorer workflow solves these challenges with a complete solution from sample to results, optimized to ensure successful analysis of pesticide residues in a variety of food matrices.

The workflow includes the TSQ Quantis triple-stage quadrupole mass spectrometer, renowned for excellent sensitivity, robustness, and speed, enabling laboratories to meet current and future regulations for multi-class pesticide residue analysis.

The immediate benefits for laboratories are:

- **Rapid start-up** with a comprehensive solution—Thermo Scientific™ HyperSep™ Dispersive SPE (QuEChERS) sample preparation kit, quality control (QC) text mix, industry-leading TSQ Quantis triple-stage quadrupole mass spectrometer, state-of-the-art Vanquish Flex Binary UHPLC system, Thermo Scientific™ Accucore™ aQ columns, TraceFinder software methods, and detailed user guide—tailored to meet the most stringent pesticide residue regulations for food safety analyses

- **Productivity** with a ready-to-run workflow that empowers users of any expertise to analyze over 400 multi-class pesticide residues in a single 15-minute analysis

- **Confidence** with robust, pre-tested, and validated multi-residue pesticide data acquisition and processing methods and extensive pesticide database of over 600 compounds with selected reaction monitoring (SRM) transitions and retention times

- **Compliance** with European Union SANTE Guidelines for pesticide residues in food for ultimate confidence in results
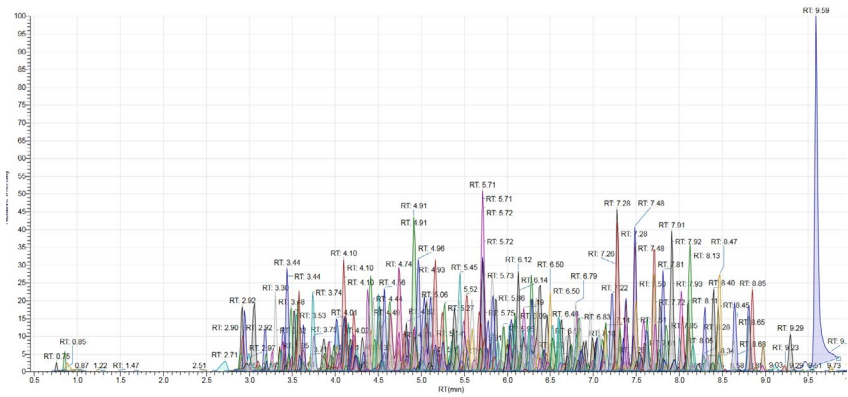
Extracted ion chromatogram of over 200 pesticide residues in baby food at 10 ng/g shown in TraceFinder software


Vanquish Flex Binary UHPLC system with TSQ Quantis triple-stage quadrupole mass spectrometer

Pesticide Explorer workflow components

- **QuEChERS** (Quick, Easy, Cheap, Effective, Rugged and Safe) sample preparation reagent slim pouch kit with full procedures

- **Quality Control (QC) standards** for performance check

- **Vanquish Flex Binary UHPLC system**

- **Accucore aQ columns**

- **TSQ Quantis triple-stage quadrupole mass spectrometer**

- **TraceFinder software** with pre-tested, validated data acquisition and processing methods, along with a comprehensive compound database

- **Detailed user guide**

Convenient, easy, and effective: QuEChERS sample preparation

The QuEChERS sample preparation kit provides a time-saving yet extremely effective approach for the extraction and cleanup of pesticide residues in food matrices. Tested sample preparation procedures are included for wine, olive oil, and baby food matrices. With the QuEChERS kit, users can easily extract and analyze samples with confidence.
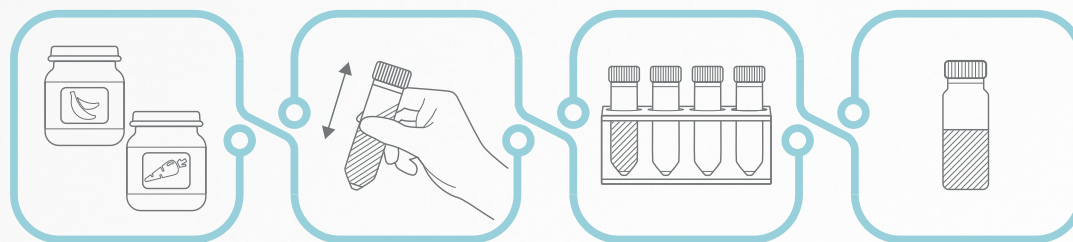
QuEChERS sample preparation method: proven, simple, and easily transferrable

Benefits of the QuEChERS sample preparation method

Characteristic	QuEChERS method
Variability	LOW: proven reproducibility for hundreds of pesticides across multiple matrices
Lab portability	HIGH: one method can be easily implemented and transferred in multiple labs and geographies
Ease of use	HIGH: easy-to-use configurations and methods allow for simple workflow implementation
Cost per sample	LOW: economical, users with varied expertise achieve similar results

Productivity and quality:
Vanquish Flex Binary UHPLC system

With excellent retention time stability and maximum pressure up to 1000 bar, the Vanquish Flex Binary UHPLC systems increase productivity without compromising quality of results. The system shares all Vanquish system values such as a design focused on uptime, robustness, and quality, enabling laboratories to address any quantitation challenge.

Speed and resolution:
Accucore aQ columns

The high-throughput, high-resolution Accucore aQ columns are ideally suited for pesticide-residue monitoring. The rugged solid-core column with polar end-capped C18 chemistry delivers excellent reproducibility for the polar and hydrophobic analytes typically found in multi-class, multi-residue pesticide analyses. When combined with the power of the Vanquish Flex Binary UHPLC system, users benefit from the extended pressure capabilities and robustness required for consistent, high-throughput separations.

Confident quantitation: TSQ Quantis mass spectrometer

With robust analysis of pesticide residues in complex matrices, the TSQ Quantis triple-stage quadrupole mass spectrometer enables food-safety testing labs to address regulatory requirements with confidence and ease. Users become productive quickly with built-in automated compound optimization and application-specific methods and reports. Outstanding scan speed permits simultaneous quantitation of hundreds of compounds at regulatory limits.
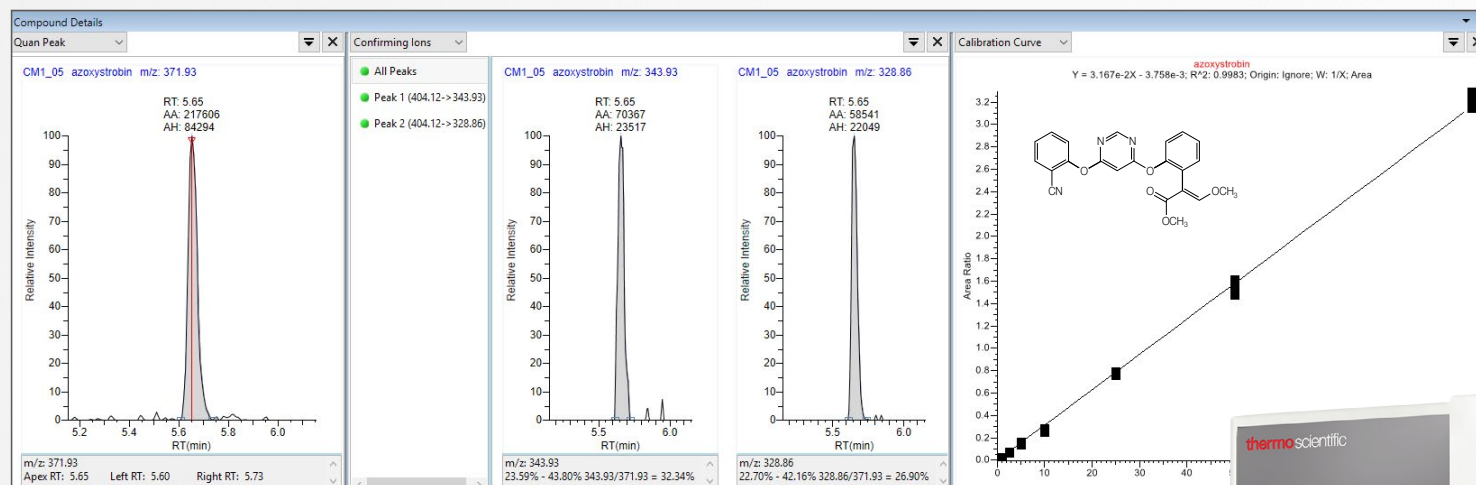
Matrix extracted standard (MES) of Azoxystrobin in wine matrix at a concentration of 1.0 ng/g, with the quantitation ion peak (left), qualitative confirming ions (middle), and calibration curve range from 0.5 to 100 ng/g (right)

Five clicks to success: TraceFinder software

TraceFinder software includes an extensive built-in compound database; the ability to screen and quantify analytes; streamlined data review; customized, editable report templates; and automatically generated reports—specifically tailored for food safety applications. From data acquisition to the final report, TraceFinder software makes workflows fast and simple.
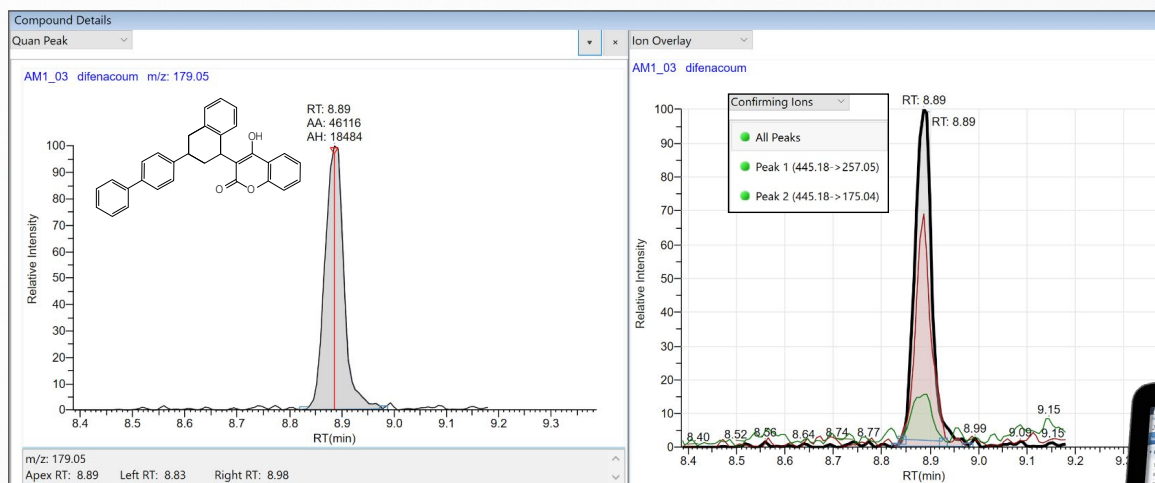
Matrix-extracted standard (MES) of difenacoum at 0.5 ng/g in wine matrix showing the quantitation ion (left) and the overlay with the qualifier ions (right) in TraceFinder software

Become more productive with a ready-to-run TraceFinder software workflow

Laboratories can substantially reduce time for high-confidence results using LC-MS/MS pesticide residue analysis methods that are included with the workflow. For ultimate ease of use, all necessary LC-MS/MS instrument parameters are specified. Users simply load and launch a method. If desired, laboratories can easily develop customized methods using the TraceFinder software compound database.

Select compounds

Choose from over 600 pesticides provided in the TraceFinder Compound Database to create a custom method, or choose one of the pre-tested, validated Master Methods for residue analysis.

Load method
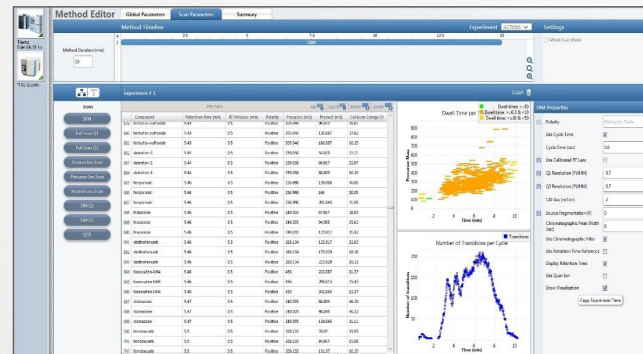
LC-MS/MS method flexibility allows users to easily edit the pre-configured methods, including the SRM transitions and retention times, if required. Visualization features in the instrument software display dwell times and SRM density throughout the entire analytical run.
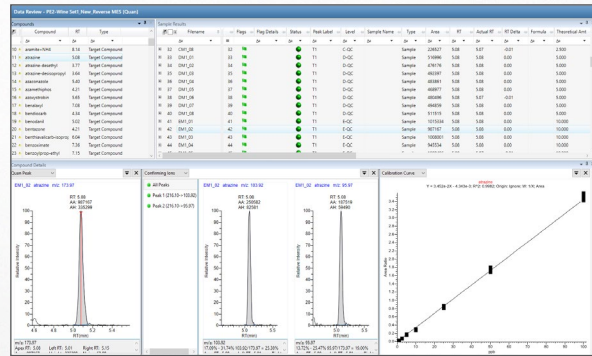
Acquire data
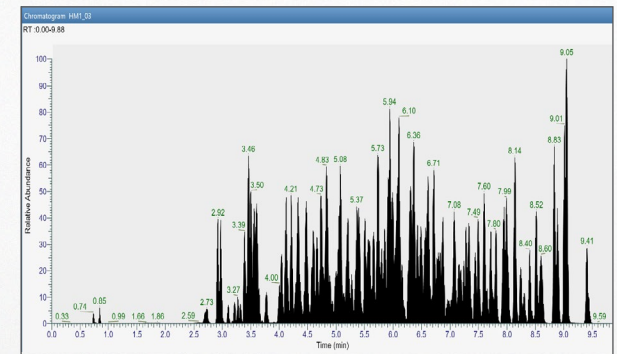
Data is acquired using optimal LC-MS/MS conditions for each multi-class, multi-residue method to deliver superb quantitative performance and sensitivity.
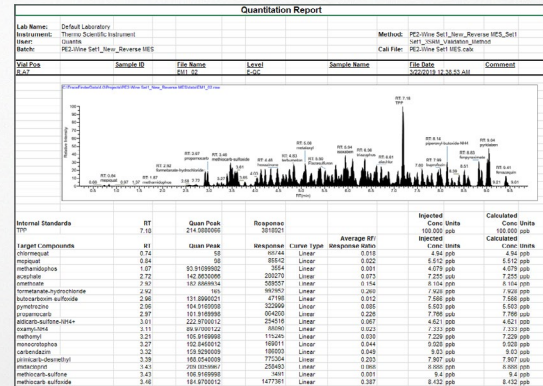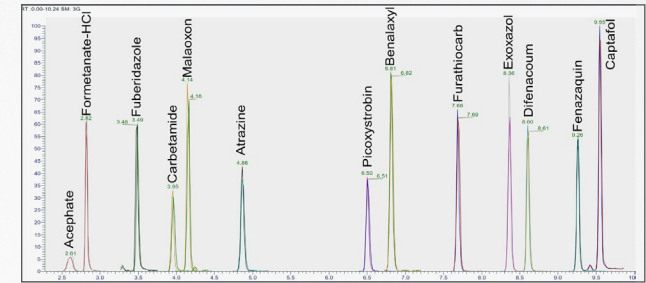
Review data

The color-flagging feature of TraceFinder software enables analysts to quickly review and confirm results.

Generate report

After data review, high-quality standard or custom reports can be used to rapidly generate useful results.

LC-MS/MS extracted ion chromatograms of white wine spiked with selected pesticides (overlay of injection #1 and injection # 300) demonstrate the robustness and reproducibility of the Vanquish Flex Binary UHPLC system and Accucore aQ column with the TSQ Quantis mass spectrometer.
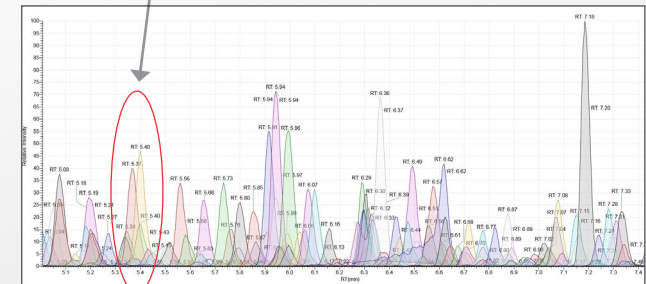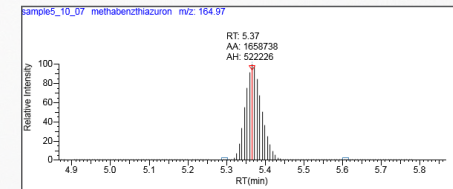
The fast scan speed with polarity switching of the TSQ Quantis mass spectrometer provides accurate quantitation of residues in large pesticide panels. Over 500 pesticides were analyzed in a wine matrix over a 15-minute run. The inset shows the scans across the target pesticide, methabenzthiazuron, at 10 ng/g.

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The most comprehensive portfolio for pesticide analysis

In addition to the Pesticide Explorer Workflow, we offer complementary technologies for the analysis of pesticide residues. While each solution has specific advantages, collectively Thermo Scientific offers the most comprehensive pesticide analysis portfolio available on the market today.

Orbitrap mass analyzer based for GC-MS, LC-MS and MS/MS

The Thermo Scientific™ Orbitrap™ mass spectrometers produce high-resolution accurate-mass (HRAM) data for confident trace-level screening and quantitation of pesticides, and identification of unknowns. Orbitrap-based instruments are renowned for high quality full-scan and MS/MS data with easy analytical set-up, efficient data processing, and retrospective data analysis.

Ion chromatography-MS/MS

For polar anionic pesticides that are challenging to analyze using conventional or hydrophilic interaction chromatography (HILIC) LC-MS/MS, the Thermo Scientific™ Dionex™ Integrion™ HPIC system coupled with the Thermo Scientific™ TSQ Altis™ triple-stage quadrupole mass spectrometer provides a powerful solution. High-pressure ion chromatography (HPIC)-MS/MS with high-capacity ion exchange columns and post-column eluent suppression, combined with high-sensitivity triple quadrupole mass spectrometer detection improves sensitivity and chromatographic separation for high-confidence analysis of polar anionic pesticides in complex food matrices.

Chromatography Data System (CDS) software

Simplified data processing and extensive multi-vendor instrument control make the Thermo Scientific™ Chromeleon™ Chromatography Data System the choice for many laboratories. The software streamlines workflows from chromatography to routine quantitative MS analysis on IC, GC, LC, GC-MS/MS and LC-MS/MS systems by delivering superior instrument control, automation, data processing, and more. Run analyses in an enterprise environment—from method creation to final reporting—to boost productivity.

Find out more at **thermofisher.com/PesticideExplorer**

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