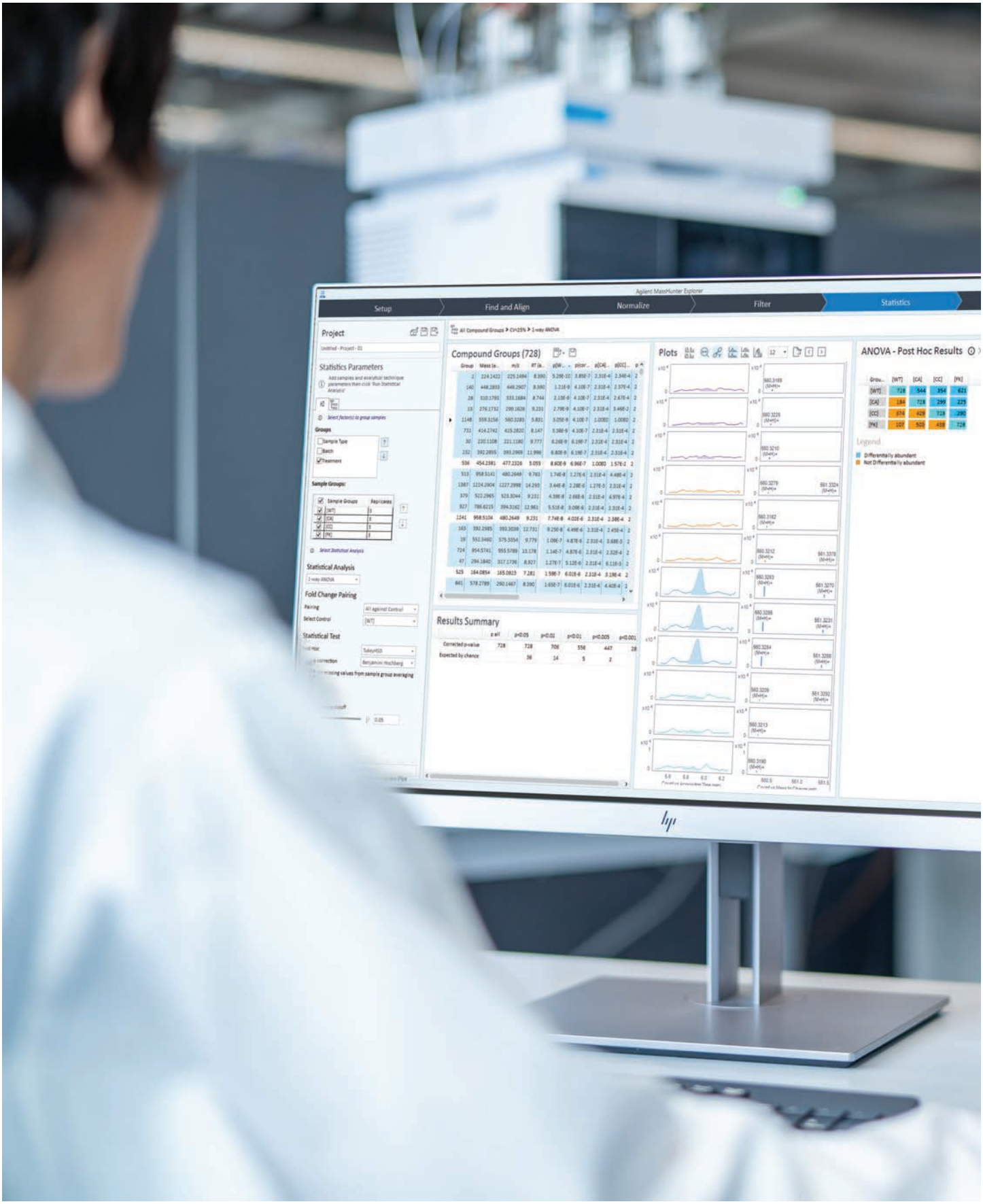
Agilent

Trusted Answers

Draw Critical Insights from Complex Data

Agilent MassHunter Explorer software for nontargeted LC/Q-TOF data


Agilent MassHunter Explorer
Setup
Find and Align
Normalize
Filter
Statistics
Project
Statistics Parameters
Compound Groups (728)
Plots
ANOVA - Post Hoc Results
Results Summary
Statistical Analysis
Fold Change Pairing
Statistical Test

Meet Your LC/Q-TOF's Best Companion for Fast, Reliable, and Simple Nontargeted Data Analysis

High-resolution Agilent LC/Q-TOF instruments deliver rich nontargeted data with excellent precision, accuracy, and dynamic range. While rich data can provide deep, comprehensive insights, it is challenging to find and identify compounds of interest.

MassHunter Explorer is designed to make nontargeted data analysis easier, faster, and smarter. The integrated user interface seamlessly combines advanced data extraction with normalization, statistical analysis, visualization, and identification procedures. Together, in a single, easy-to-use application, these tools help you confidently find insights into your data quickly, improving your research productivity.

Part of the Agilent MassHunter software suite, MassHunter Explorer is ideal for Q-TOF LC/MS nontargeted screening applications where you need to find compounds that differ between samples or groups of samples from different conditions.


Food

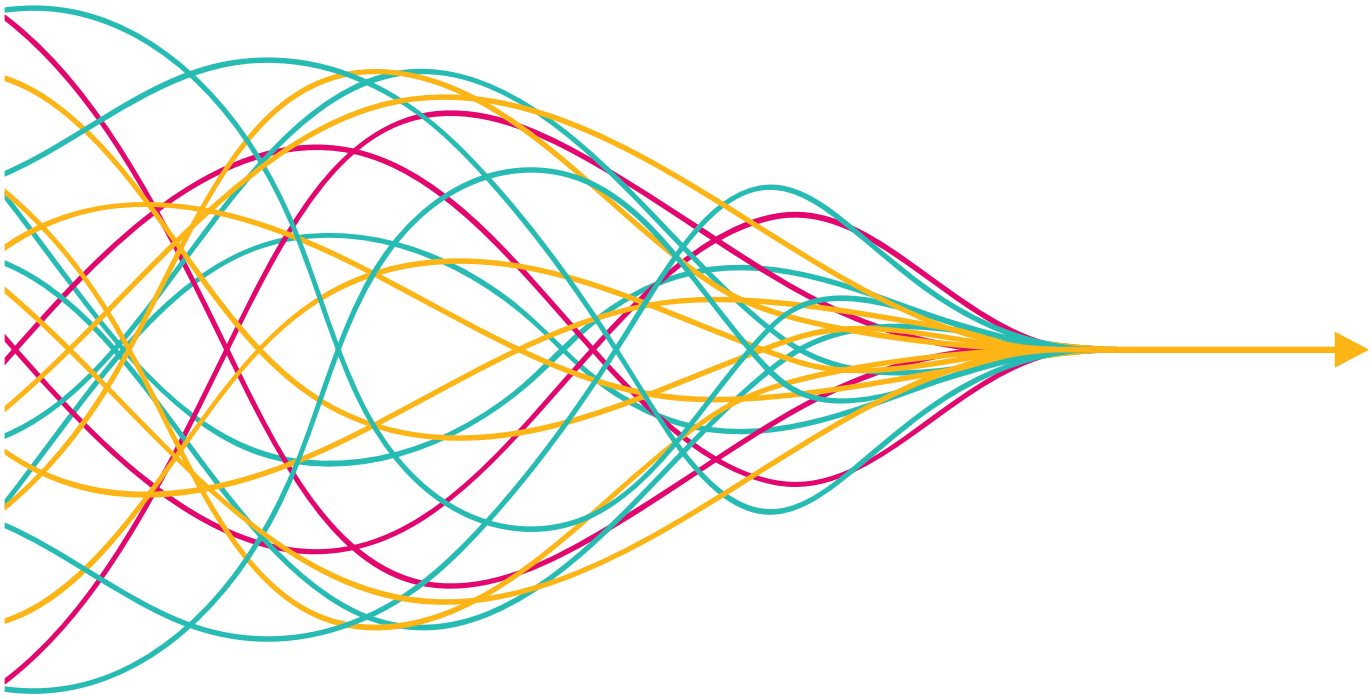

Environmental


Extractables and leachables


Forensic toxicology


Omics


Natural products



A simple, efficient path from complex data to clarity

Designed to suit both new and advanced users, MassHunter Explorer offers comprehensive analysis and visualization in one package. Its intuitive, workflow-driven interface guides you through setting up your experiment, extracting data, and using differential analyses to find and identify compounds of interest.

Substantial performance enhancements combined with the simplified presentation of analytical results make it easier to interact with and learn from the data—regardless of your prior experience with nontargeted workflows. New users can explore data with preloaded, optimized settings, while advanced users can tailor settings for less common applications.

If necessary, data can be readily exported into MassHunter Qualitative and Quantitative data analysis software, or for more advanced statistical analysis programs like Mass Profiler Professional, R, and Python.

The Agilent MassHunter Explorer: An integrated, intuitive workflow

Project-based workflows allow easy setup and transferability for beginners and experts.

Streamlined, integrated procedures simplify navigation.

Multiple statistical algorithms provide the right tools for the given data.

Preprocessing during acquisition speeds up data processing.

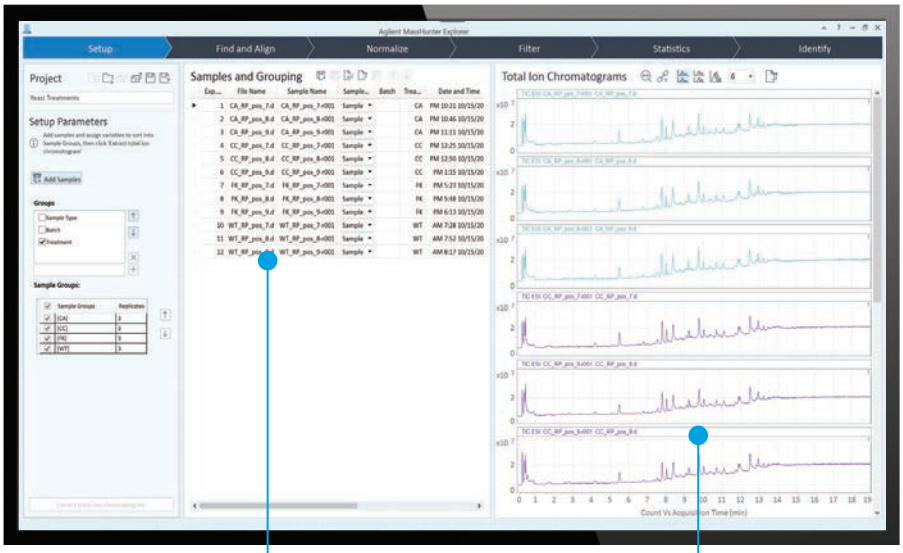
Chromatographic, spectral, and statistical data are pictured for quick review.

MassHunter Explorer guides you through setup conditions, data extraction, normalization, filtering, statistical analysis, and identification procedures required for nontargeted screening. A new user could use a processing method created by an expert, which shortens the learning curve. Methods can also be shared across your organization, ensuring consistent results and minimizing errors.

Easy steps for revealing and focusing on your underlying results

Set up your experimental design

Start by adding your acquired data and defining sample type (including a new Pooled QC option), batch, and custom grouping variables for each sample. The chromatograms are arranged, colored, and can be overlaid so that you can review reproducibility before committing to the next steps.

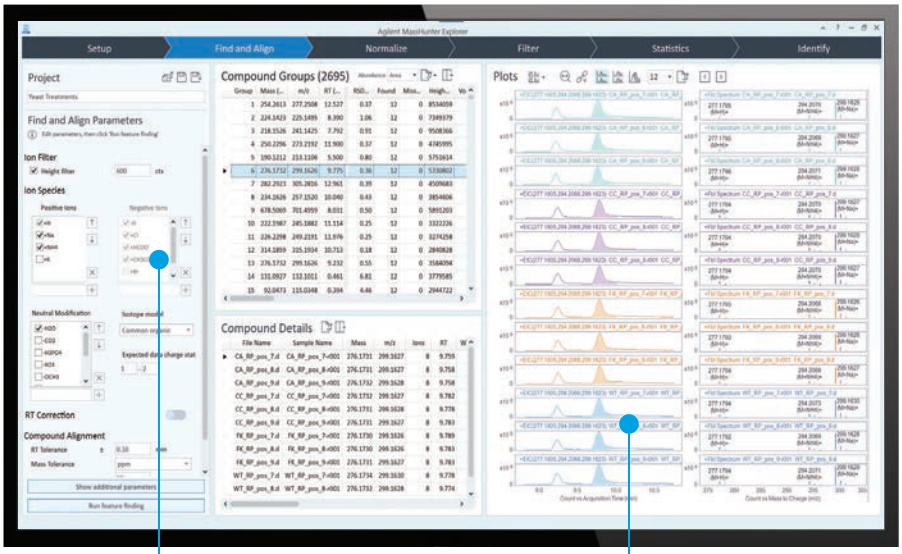


Load samples and define the groups that are associated with each sample.

Check reproducibility by reviewing chromatograms.

Find and align compounds across all samples

The Find and Align step extracts compounds from each sample using a nontargeted algorithm, then aligns the compounds across samples by mass and retention time.

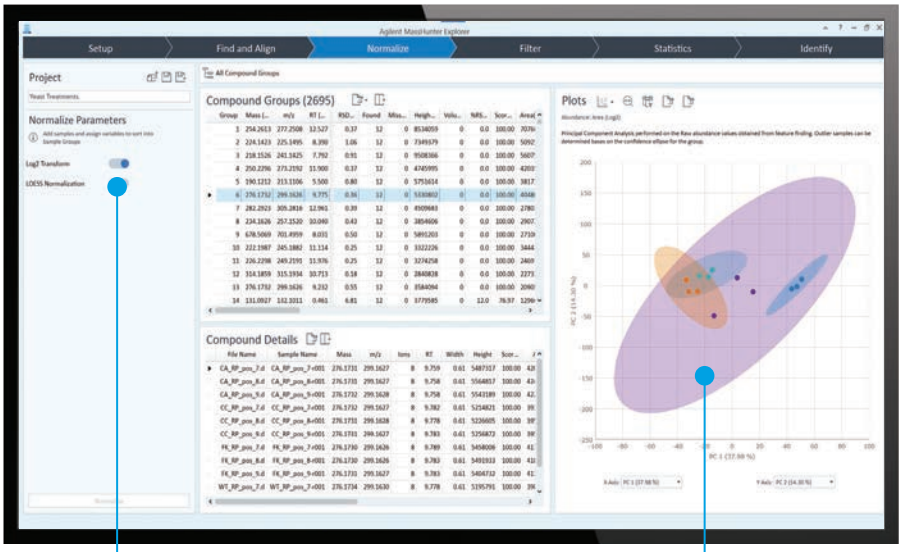


Evaluate parameters based on sample chemistry.

Review extracted ion chromatograms and spectra.

Normalize and filter data to remove unwanted variations

Unwanted systematic errors can be caused by sample preparation or instrument variation, leading to batch-to-batch variations. These errors can be moderated using locally estimated scatterplot smoothing (LOESS) normalization techniques. Filters for abundance, reproducibility, or presence in specific sample groups can help you focus on compounds of interest. Throughout these steps, a principal component analysis (PCA) lets you review data quality as normalization and filtering processes are applied.



Select normalization options.

Review sample grouping by PCA.

Focus on significant compounds

Statistical analysis techniques help you find compounds that are significantly different—or common—between groups of samples. T-tests, fold-change analyses, volcano plots, one- or two-way analysis of variance, and hierarchical cluster analysis (HCA) are all tools for finding your compounds of interest. Results from these techniques, together with the instrument data, are reviewed for immediate visualization and verification.

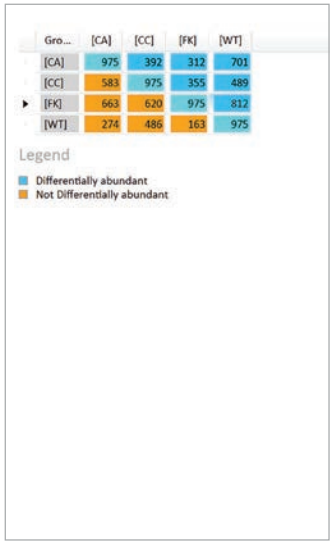
Find significant compounds of interest by selecting from a list of statistical analysis techniques.

Track how you filtered compound lists to focus on your significant compounds.

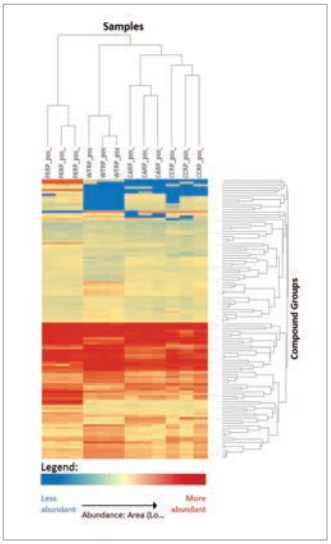
Review EIC and spectra linked with your statistical analysis results.

Linked navigation allows you to interactively select compounds either in tables or plots (like the chromatograms, spectral, or statistical plots) so that results can be easily interpreted. All plots and compound lists can be easily exported.

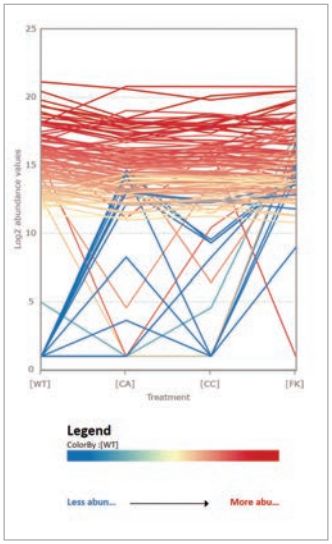
ANOVA post hoc results



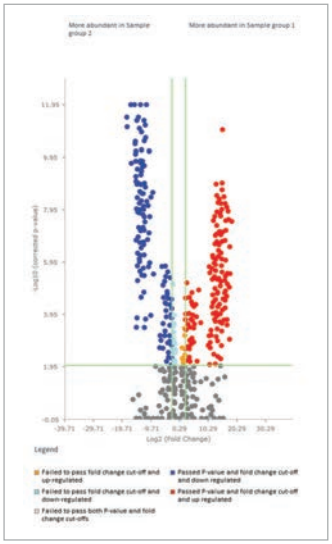
HCA plot



Fold change plot



Volcano plot

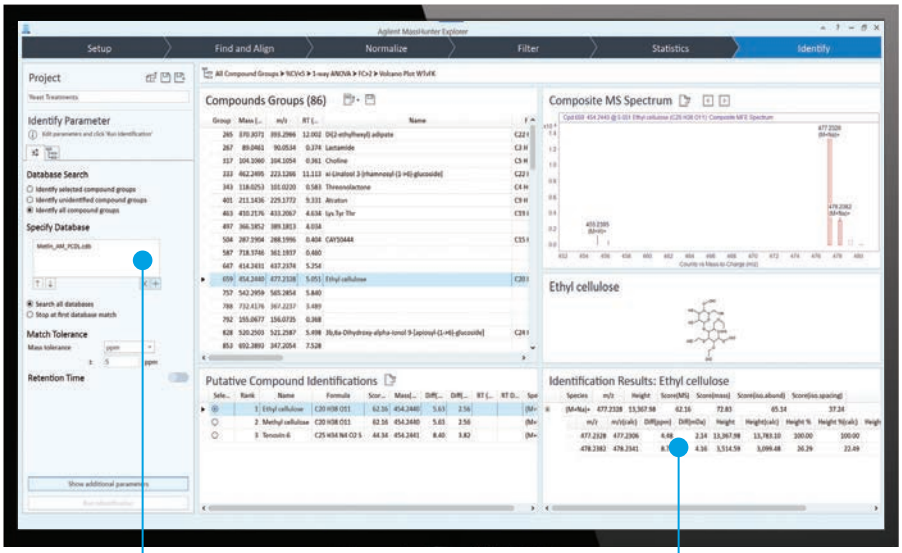


Identify your compounds of interest

Once compounds of interest are found, putative identifications are made in the Identify step. Compound identification algorithms have been optimized to match measured data with theoretical accurate masses and isotope patterns, and optionally, retention times curated into compound databases.

Highly curated Agilent compound databases can be used directly in MassHunter Explorer. These databases contain compounds of interest in industries such as food, environmental, forensics, pharmaceuticals, extractables/leachables, water screening, metabolomics, and lipidomics.

Data in open-access public libraries and databases, such as MassBank or MoNA, are available in Agilent ChemVista software.



Match analytes with compounds included in a database.

Review putative identification evidence.

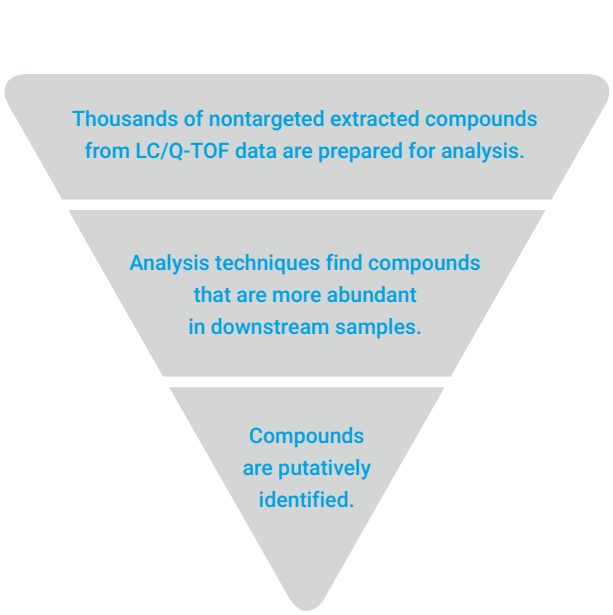
Environmental application

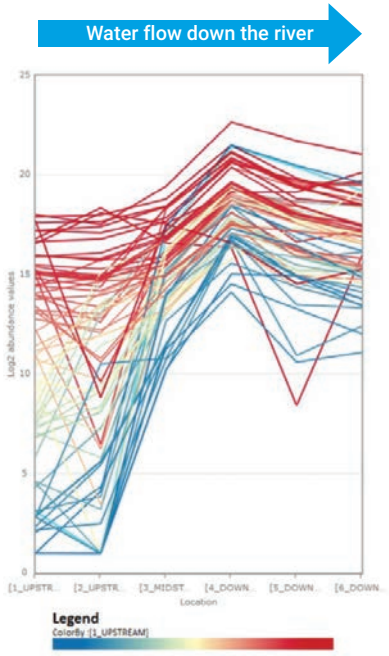
Finding and identifying emerging contaminants in river water

LC/Q-TOF systems are unmatched tools for detecting emerging contaminants, metabolites, and microbial degradation products that pollute our environment. Finding and identifying these species can be challenging, as standards are rarely available and thousands of peaks may be detected in each sample.

In this example, river water samples were collected at a pristine headwater location (control) and downstream from an urban center. The goal was to measure wastewater impact on water quality. Accurate mass analysis that combined LC/Q-TOF with MassHunter Explorer data interpretation allowed researchers to find and putatively identify environmentally significant compounds in samples collected from downstream locations.

Instead of painstakingly evaluating thousands of potential peaks, analysts were able to hone in on the significant compounds of environmental concern. The results: Fast, simple characterization of the wastewater impact, and identification of known and unknown contaminants.





Metabolomics application

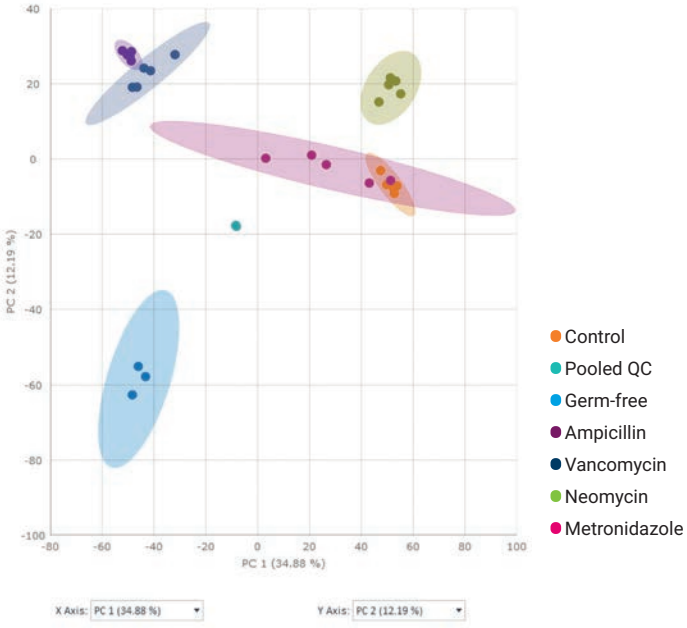
Deciphering the impact of the gut microbiome on the metabolome

With applications spanning basic, translational, and clinical research, Q-TOF LC/MS enables compound discovery by allowing researchers to profile thousands of metabolites from complex sample matrices.

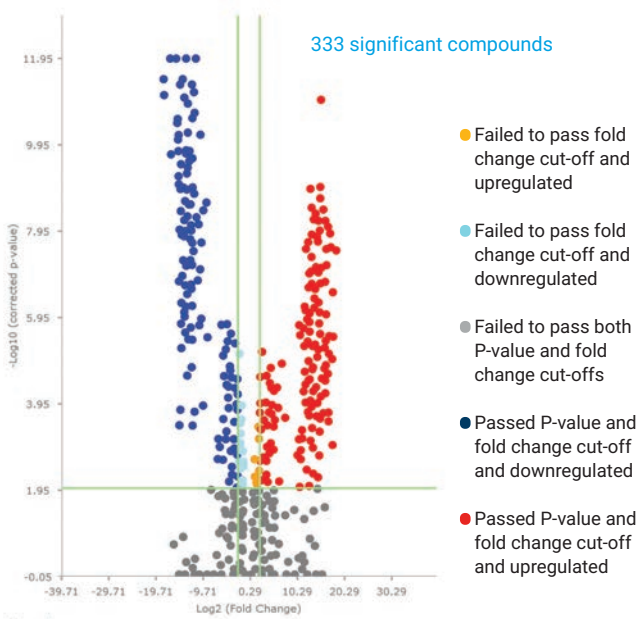
In this example, the impact of antibiotic treatment on the cecal metabolome was investigated. Cecum contents from mice treated with four different antibiotics, and from germ-free mice lacking a microbiome, were extracted and analyzed with the new Agilent Revident LC/Q-TOF.

MassHunter Explorer data interpretation demonstrated immediate sample grouping even without further filtering and statistics. To tease out 333 potential microbial-derived and/or microbial-modified metabolites, a volcano plot was used.

PCA of 35 samples representing 5,067 compounds



Volcano plot of control versus GF mice



Instead of painstakingly evaluating thousands of potential peaks, PCA analysis quickly identified the sample groups, and the volcano plot honed in on the significant species. The results include fast, simple characterization of diverse samples, and a reveal of the distinctive analytes.

Intelligence that inspires

Next-generation Agilent LC/Q-TOF instruments and software optimize your lab operations with a foundation of continuous innovation. They go beyond instrumentation to include time-saving intelligence, efficient workflows, and services provided by a trusted partner. So, you can focus on what inspires you and meet every challenge that comes your way.

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