# Intelligence That Inspires Insight

Agilent Revident LC/Q-TOF system

# Revident

## **Revolutionize** Your **Identification** with Rock Solid Evidence

Meet your future challenges with Revident LC/Q-TOF

# Start Building Your Lab of the Future Today

To stay competitive and adjust to changing industry requirements, you need evolved instrumentation at the core of your complete workflow solution for meeting current and future challenges. You must also be certain that your lab can respond to emerging and unexpected contaminants through broader screening and retrospective analysis.
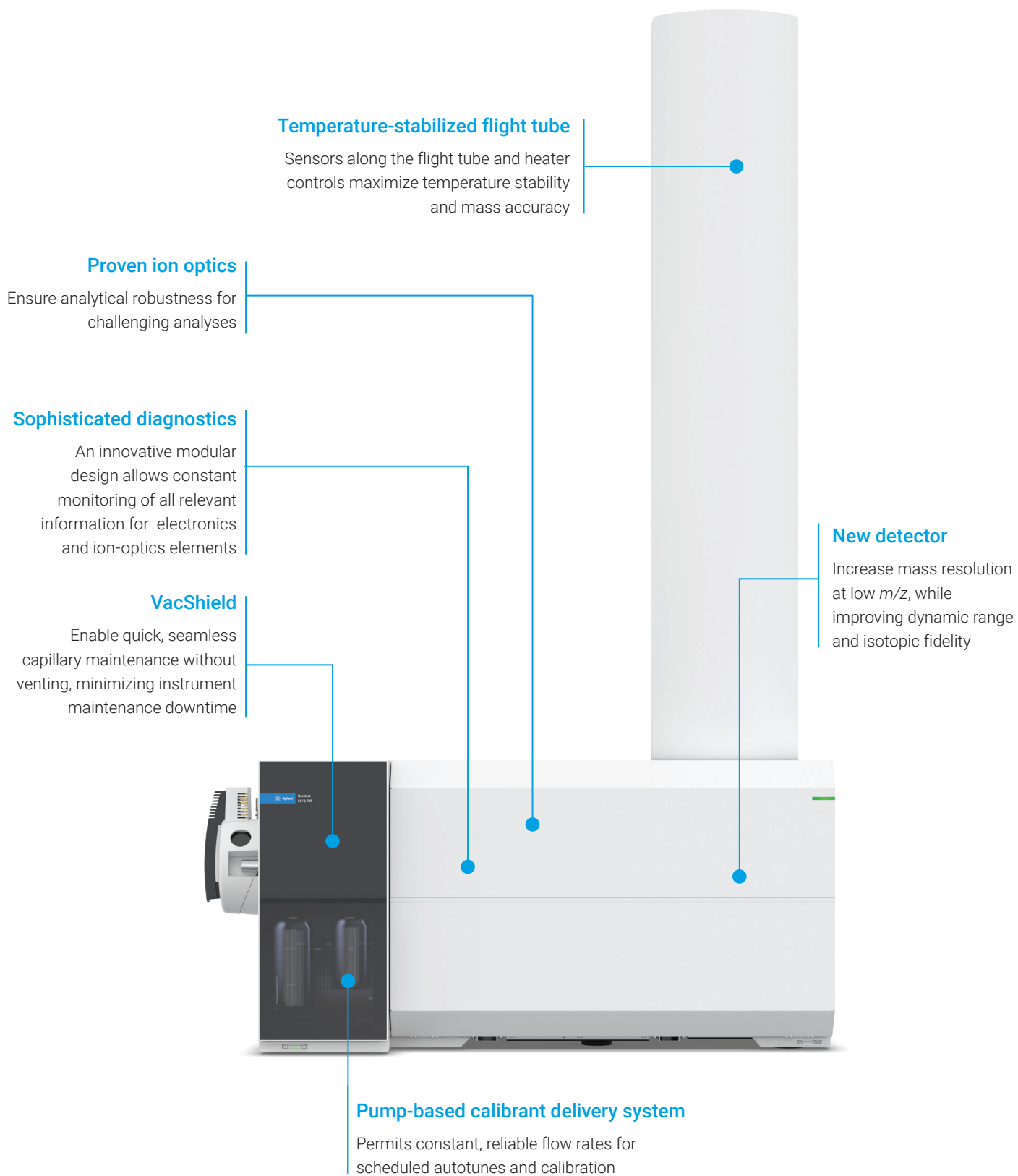
## The Agilent Revident LC/Q-TOF system

The Revident quadrupole time-of-flight LC/MS system (LC/Q-TOF) answers these challenges by maximizing operation time and productivity with sophisticated instrument intelligence.

Enhanced with multiple workflow capabilities, the Revident LC/Q-TOF lets you identify—and quickly assess—compounds in question. Its combination of isotope fidelity, mass accuracy, and dynamic range produce outstanding spectral quality that builds a foundation of data you can rely on. And it forms the core of workflows that let you look at more compounds, and retrospectively check samples without having to rerun, ensuring that you comply with regulations and maintain credibility.

# Innovation that expands your lab's potential

With its high performance and robustness, the Revident LC/Q-TOF mass spectrometer helps you achieve your most challenging throughput and data quality goals—without compromise.

### Temperature-stabilized flight tube
Sensors along the flight tube and heater controls maximize temperature stability and mass accuracy

### Proven ion optics
Ensure analytical robustness for challenging analyses

### Sophisticated diagnostics
An innovative modular design allows constant monitoring of all relevant information for electronics and ion-optics elements

### VacShield
Enable quick, seamless capillary maintenance without venting, minimizing instrument maintenance downtime

### New detector
Increase mass resolution at low $m/z$, while improving dynamic range and isotopic fidelity

### Pump-based calibrant delivery system
Permits constant, reliable flow rates for scheduled autotunes and calibration

# Intelligence that powers ultimate productivity

The Agilent Revident LC/Q-TOF includes multiple innovations that empower your lab to meet increasing sample throughput and productivity demands. Sophisticated, yet easy-to-use onboard intelligence provides immediate validation of results, improves analytical speed, and reduces downtime by predicting when maintenance is needed. Time-saving automation software lets you schedule autotunes and calibrations in advance, so the instrument will be ready to run samples when you walk into the lab.

What's more, the identical user experience between the Agilent triple quadrupole LC/MS (LC/TQ) and Q-TOF LC/MS systems harmonizes operation in labs that need multiple platforms.

Smart tuning

- Peak instrument performance
- Greater instrument consistency
- Faster startup time
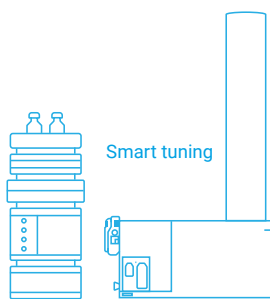
## Exceed your productivity goals with smart features

Developed to help labs meet their ongoing at-capacity challenges, the onboard innovations in the Revident LC/Q-TOF provide a pathway to increased throughput and efficiency. All without having to add more instruments and personnel, or extend lab hours.

## Peak performance, no guesswork

Tuning a high-resolution mass spectrometry instrument for specific applications is time consuming. The Revident LC/Q-TOF features an innovative tuning algorithm that takes the guesswork out of achieving peak performance. Smart procedures use machine learning techniques to evaluate many parameters simultaneously, resulting in faster startup time and greater consistency.

Smart monitoring

- Early maintenance feedback
- Real-time vitals
- Key operations tracking
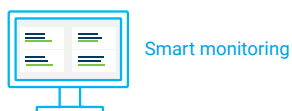
## Maximize uptime, anticipate downtime

Unexpected instrument issues and the resulting downtime are disruptive, especially if you don't know the source of the problem. The Revident LC/Q-TOF monitors its own vitals, giving you a real-time overview of the system's health. Key operational areas are tracked and monitored as part of early maintenance feedback, helping you pinpoint where and when issues may arise.

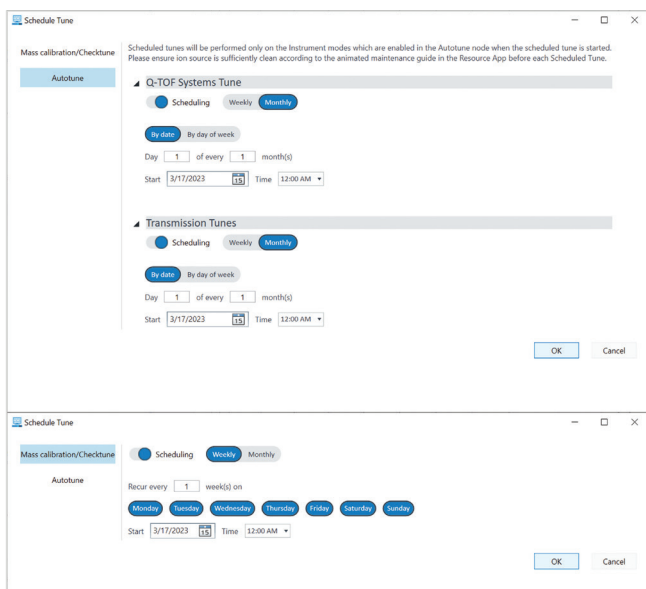### Maximize your most valuable resource: Time

Intelligent Reflex workflows minimize downtime by keeping the Revident LC/Q-TOF running, even during data evaluation. From carry-over to saturation, fast screening to suspect screening confirmation and iterative MS/MS, the instrument will continue acquiring data, letting you focus on your results.

# Ensure maximum instrument uptime



## Reduce maintenance time by 92% with Agilent VacShield

Maintaining your LC/Q-TOF has never been so easy. VacShield lets you remove the capillary and run the cleaning cycle in as little as 30 minutes, compared to six hours or more with venting and disassembly. So, you can spend more valuable lab time focusing on sample analysis—like large scientific population studies.

## Make sure your instrument is ready when you are

Start your day on a productive note with a scheduled autotune. You can automatically set your LC/Q-TOF to tune and calibrate before you arrive in the lab, or instruct the instrument to produce periodic checktune reports.

## Monitor system health in real time

Early maintenance feedback actively monitors instrument metrices and reports the results to you. Each component has its own built-in monitor, so you can quickly and easily review status and know the health of your instrument.
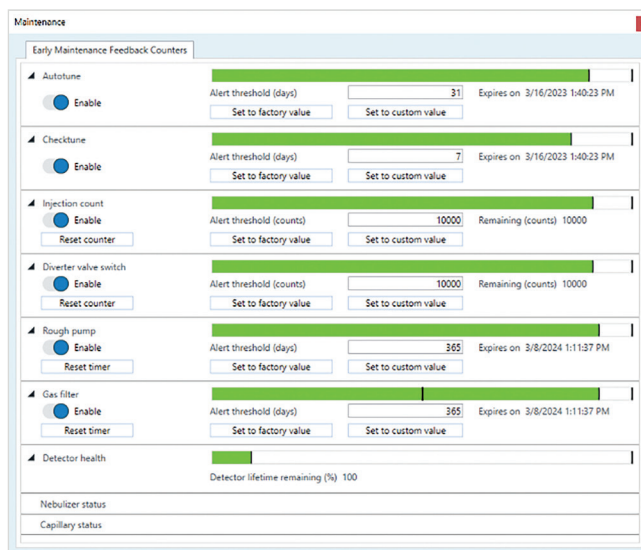
# Instrument detection limit and spectral quality

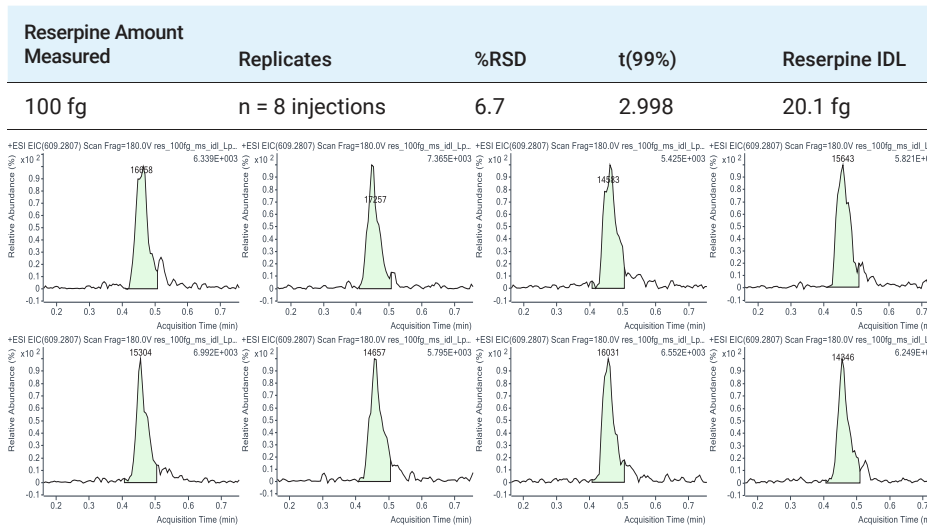## Demand a more meaningful measure of analytical sensitivity

Today's low-noise mass spectrometry systems require a statistical standard that measures true analytical sensitivity: specification proportional to ion count. Agilent is leading the way by measuring performance using instrument detection limit (IDL), which is characterized by:

– A rigorous metric based on statistical analysis of response precision (%RSD)

– Measurements at or close to the instrument detection limit (IDL)

– Accurate assessments of the system's true detection limit and LLOQ

– A uniform, practical means of evaluating analytical sensitivity



Using the isotope fidelity of the Revident LC/Q-TOF ensures unambiguous identification.
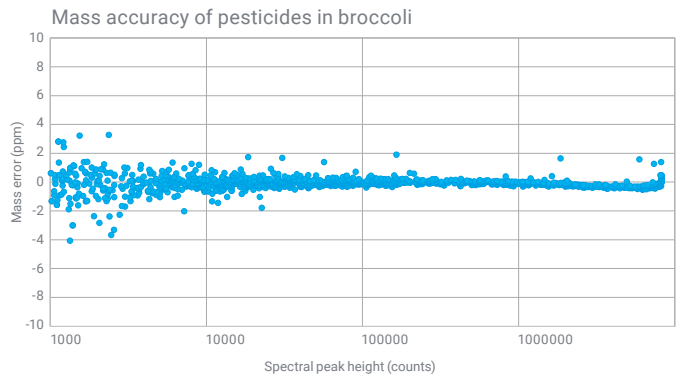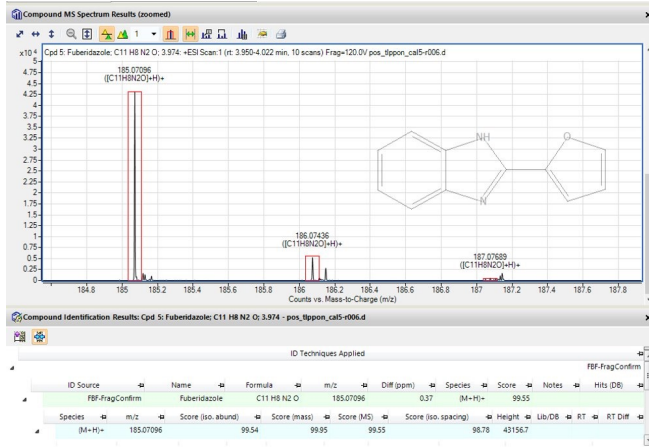


Excellent mass accuracy is obtained with the Revident LC/Q-TOF over a wide range of abundances.

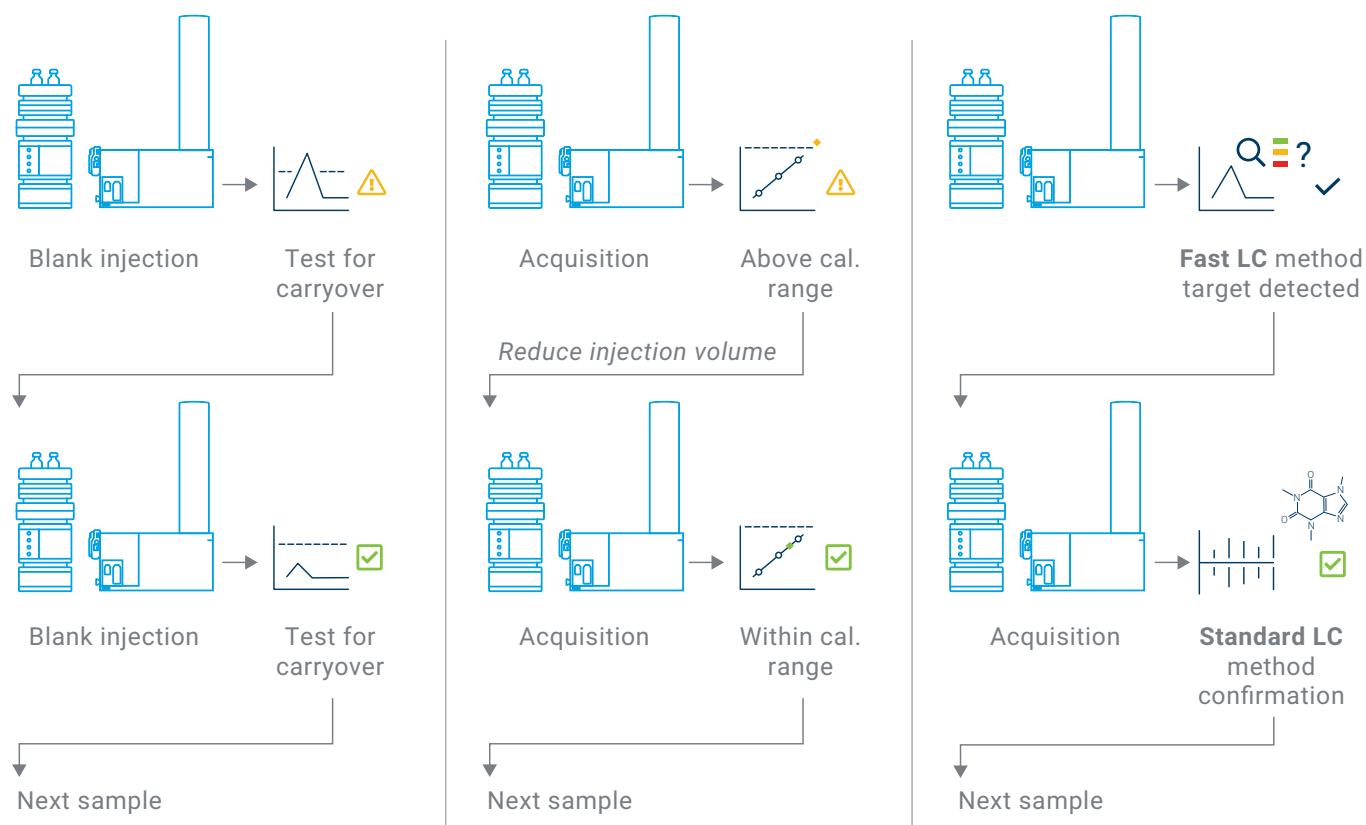| Reserpine Amount Measured | Replicates | %RSD | t(99%) | Reserpine IDL |
|---|---|---|---|---|
| 100 fg | n = 8 injections | 6.7 | 2.998 | 20.1 fg |



Extracted ion chromatograms (EIC) of eight consecutive runs close to the detection limit (DL) of the Revident LC/Q-TOF. Multiple injections of 100 fg reserpine near the lower DL on the Revident LC/Q-TOF. The table shows both EICs and RSDs.

# Increase confidence and throughput with Intelligent Reflex

Intelligent Reflex enables an automatic reflexive reinjection logic without user intervention, so you can be certain that your results are trustworthy and within operational limits.

1. Carryover detection inserts extra blanks, ensuring that the previous sample does not affect the next sample.

2. The above calibration range function detects if a sample is outside of the calibration range. If so, it automatically reinjects the sample with less volume.

3. Fast screening function samples with incredible speed. If a target analyte is detected with a fast screening method (short LC gradient), an analytical method (standard gradient) is run on that sample automatically. If the target isn't detected, the system skips to the next sample.

**Intelligent Reflex dramatically improves lab throughput for these workflows**

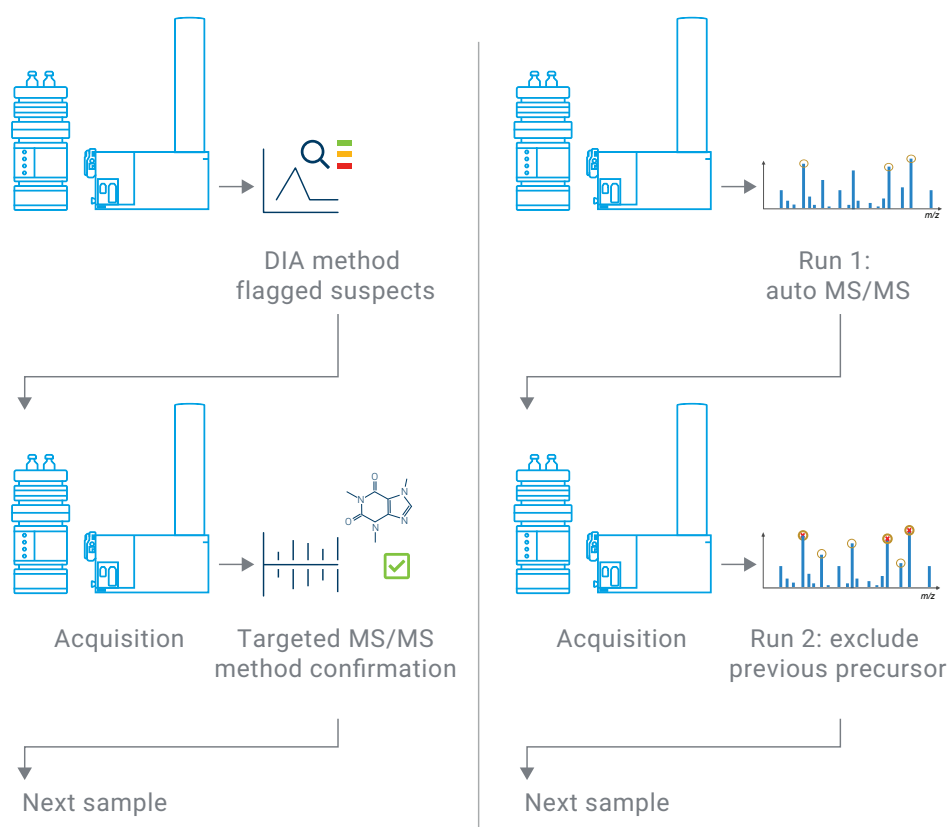| Blank injection | Test for carryover | | Acquisition | Above cal. range | | **Fast LC** method target detected |
|---|---|---|---|---|---|---|
| | | | | *Reduce injection volume* | | |
| Blank injection | Test for carryover | | Acquisition | Within cal. range | | Acquisition | **Standard LC** method confirmation |
| Next sample | | | Next sample | | | Next sample | |

# Targeted MS/MS for suspect confirmation and iterative MS/MS

1. The target/suspect screening Intelligent Reflex workflow keeps the instrument productive. After a data independent acquisition (DIA) screening, the LC/Q-TOF screener automatically evaluates the data, and follows up with a targeted MS/MS sample run at the end of the worklist to confirm suspects with highest selectivity by quadrupole isolation.

2. Iterative MS/MS allows you to dig deeper into the sample. After an auto MS/MS analysis, precursor ions in a defined retention time window will automatically be excluded in the subsequent run. This exclusion can be repeated multiple times to analyze low-abundant compounds.

## Intelligent Reflex also boosts lab throughput for these workflows

DIA method
flagged suspects

Run 1:
auto MS/MS

Acquisition

Targeted MS/MS
method confirmation

Acquisition

Run 2: exclude
previous precursor

Next sample

Next sample

# Unleash the power of every Agilent LC/MS system

Agilent MassHunter acquisition software for LC/MS systems provides powerful instrument control and data acquisition. Instrument and method setup are fast and easy, with automated tuning for straightforward, reliable operation. With its intuitive design and easy-to-access instrument-specific features, MassHunter software lets you focus on your sample analysis, not instrument setup.

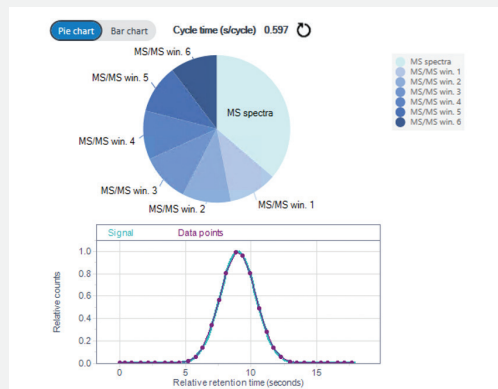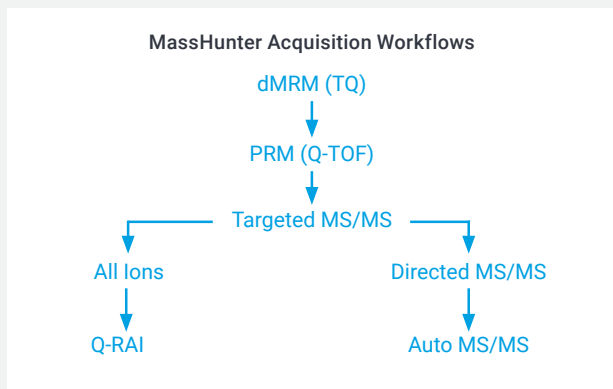## Unified control with LC/TQ systems

Now it's easier than ever to migrate an existing LC/TQ method to an LC/Q-TOF system. Simply use the same method file for LC and source conditions, and import compounds and transitions with the help of the compound browser.
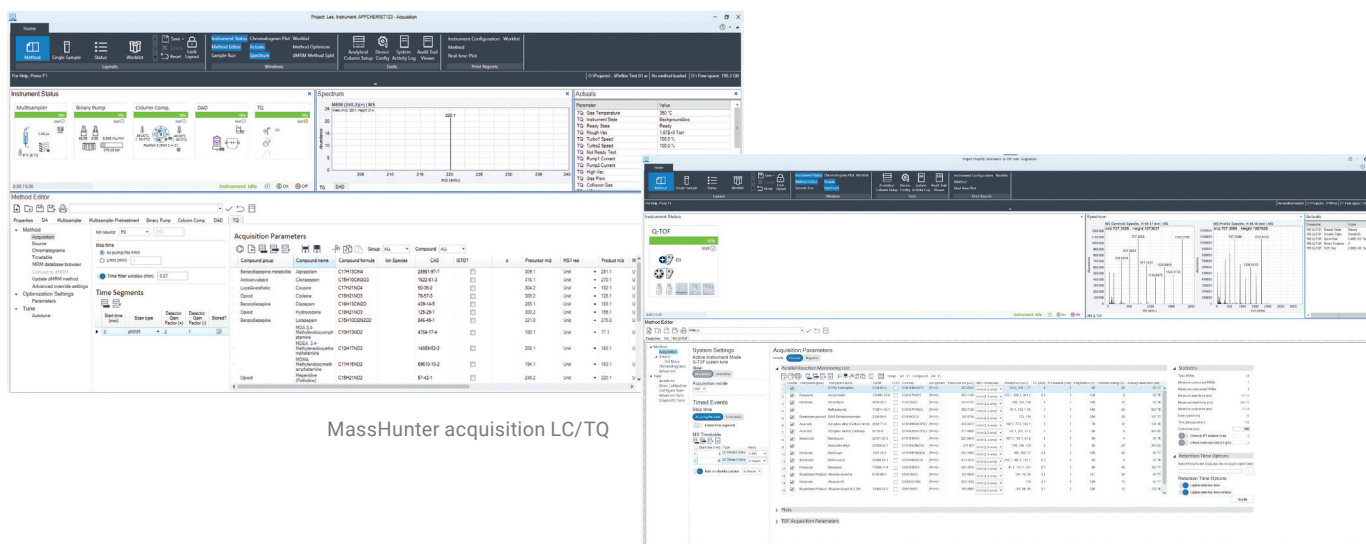


MassHunter acquisition LC/TQ



MassHunter acquisition LC/Q-TOF

You can easily develop LC/Q-TOF-specific workflows using parallel reaction monitoring (PRM) as a first step in method migration. These workflows include data independent aquisition All ions or quadrupole-resolved All Ions (Q-RAI) and data-dependent analysis (directed MS/MS or auto MS/MS). A new duty cycle chart assists with method development.



**MassHunter Acquisition Workflows**

dMRM (TQ)
↓
PRM (Q-TOF)
↓
Targeted MS/MS
↓                    ↓
All Ions          Directed MS/MS
↓                    ↓
Q-RAI             Auto MS/MS

# Perform suspect screening for food safety

European SANTE guidelines for pesticide residue analysis in food and feed require specific analytical quality control and method validation procedures for simultaneous quantitation and identification of compounds. The LC/Q-TOF screener tool simplifies the setup and provides a user-friendly overview of results.

| Status | Promoted | Compound Name | CAS# | Formula | R.T. | R.T. Diff. | Final Conc. | Mass Match Score | Target Ion | Mass Accuracy | # of Verified Ions | Area | Height |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ✕ | ☐ | Teflubenzuron | 83121-18-0 | C14H6Cl2F4N2O2 | 12.651 | 0.109 | 109.1676 | 14.6 | 380.9815 | -6.4112 | 0 | 648.0 | 141.1 |
| ✓ | ☐ | Oxadiazon | 19666-30-9 | C15H18Cl2N2O3 | 12.932 | 0.010 | 85.5098 | 91.2 | 345.0767 | -2.0051 | 7 | 8282.4 | 1815.7 |
| ✓ | ☐ | Ethion | 563-12-2 | C9H22O4P2S4 | 12.988 | 0.001 | 95.4903 | 99.3 | 384.9949 | -0.2621 | 8 | 626622.6 | 148734.2 |
| ✓ | ☐ | Pyriproxyfen (Pyriproxifen) | 95737-68-1 | C20H19NO3 | 13.044 | 0.001 | 98.3939 | 100.0 | 322.1438 | -0.2453 | 8 | 3942461.5 | 898287.3 |
| ✓ | ☐ | Quinoxyfen | 124495-18-7 | C15H8Cl2FNO | 13.157 | 0.001 | 98.1660 | 99.5 | 308.0040 | -0.7470 | 9 | 1557662.6 | 344425.2 |
| ⚠ | ☐ | Chlorpyrifos-methyl | 5598-13-0 | C7H7Cl3NO3PS | 13.269 | 0.010 | 120.2134 | 31.9 | 321.9023 | 2.5314 | 2 | 4551.7 | 1089.0 |
| ✓ | ☐ | Chlorpyrifos | 2921-88-2 | C9H11Cl3NO3PS | 13.261 | 0.001 | 97.5931 | 98.1 | 349.9336 | 0.2233 | 9 | 76177.0 | 18316.3 |
| ✓ | ☐ | Hexythiazox | 78587-05-0 | C17H21ClN2O2S | 13.374 | 0.001 | 97.5064 | 99.4 | 353.1085 | -0.4868 | 9 | 620389.6 | 141181.7 |
| ✓ | ☐ | Pendimethalin (Penoxalin) | 40487-42-1 | C13H19N3O4 | 13.398 | 0.003 | 96.2361 | 98.5 | 282.1448 | 0.1828 | 7 | 115512.7 | 26451.1 |

SANTE/12682/2019 sets identification requirements for pesticide residue analysis in food and feed for both unit mass resolution and accurate mass measurements. It also specifies a minimum number of ions required for identification. Here, two ions with a mass accuracy of less than 5 ppm and at least one fragment ion are required.

Easy setup for qualifiers/quantifiers—including a coelution score—quantitatively describe the overlap of molecular and fragment ions.
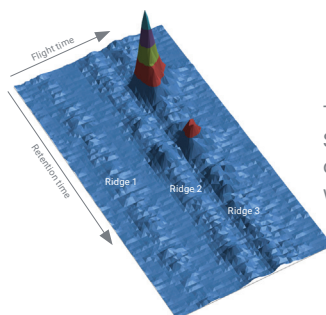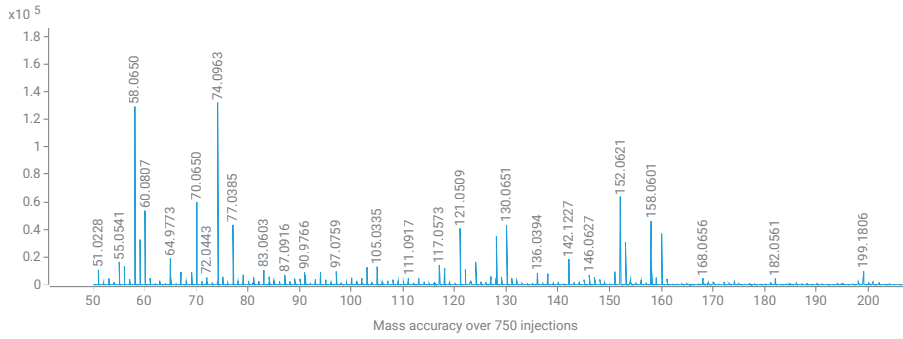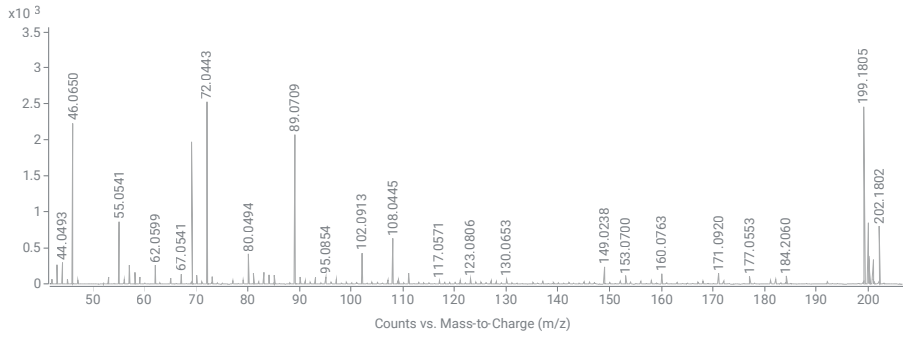
The 3D-feature detection with the Agilent SureMass detects features and ridges based on profile data, allowing sensitive detection while differentiating compounds from noise.

Another requirement for identification is that the chromatographic peaks for the precursor and/or product ion(s) must fully overlap. Therefore, screening cannot be performed in an MS-only mode. Additionally, a single-spectrum identification (typically used in auto MS/MS approaches) will not work due to the chromatographic requirement of full peak overlap. For this reason, DIA methods are the best choice.

In DIA All Ions mode, one or more collision energies are applied without isolation, and all ions present are fragmented. An MS-only spectrum with zero collision energy is acquired within this duty cycle—including molecular and fragment ions from non-zero collision energies.

This method generates fully overlapping chromatographic peaks, and will have a coelution score as a quantitative metric for the overlap displayed in the LC/Q-TOF screener.

x10$^3$

3.5
3
2.5
2
1.5
1
0.5
0

44.0493 46.0650 55.0541 62.0599 67.0541 72.0443 80.0494 89.0709 95.0854 102.0913 108.0445 117.0571 123.0806 130.0653 149.0238 153.0700 160.0763 171.0920 177.0553 184.2060 199.1805 202.1802

50  60  70  80  90  100  110  120  130  140  150  160  170  180  190  200

Counts vs. Mass-to-Charge (m/z)

x10$^5$

1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0

51.0228 55.0541 58.0650 60.0807 64.9773 70.0650 72.0443 74.0963 77.0385 83.0603 87.0916 90.9766 97.0759 105.0335 111.0917 117.0573 121.0509 130.0651 136.0394 142.1227 146.0627 152.0621 158.0601 168.0656 182.0561 199.1806

50  60  70  80  90  100  110  120  130  140  150  160  170  180  190  200

Mass accuracy over 750 injections

Intelligent Reflex enables effective screening for DIA, followed by confirmation of suspects via targeted MS/MS. Fragment spectra from DIA (top) and targeted MS/MS (bottom), confirm a previously questionable compound in DIA using targeted MS/MS.

Omethoate results, mean error = 0.1 ppm

5
4
3
2
1
0
-1
-2
-3
-4
-5

mass error (ppm)

0  100  200  300  400  500  600  700

Number of stress injections
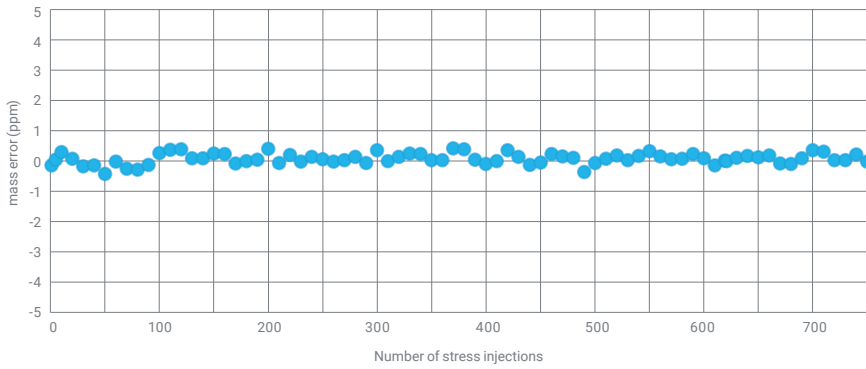
Mass accuracy of the pesticide omethoate over the course of 750 injections.
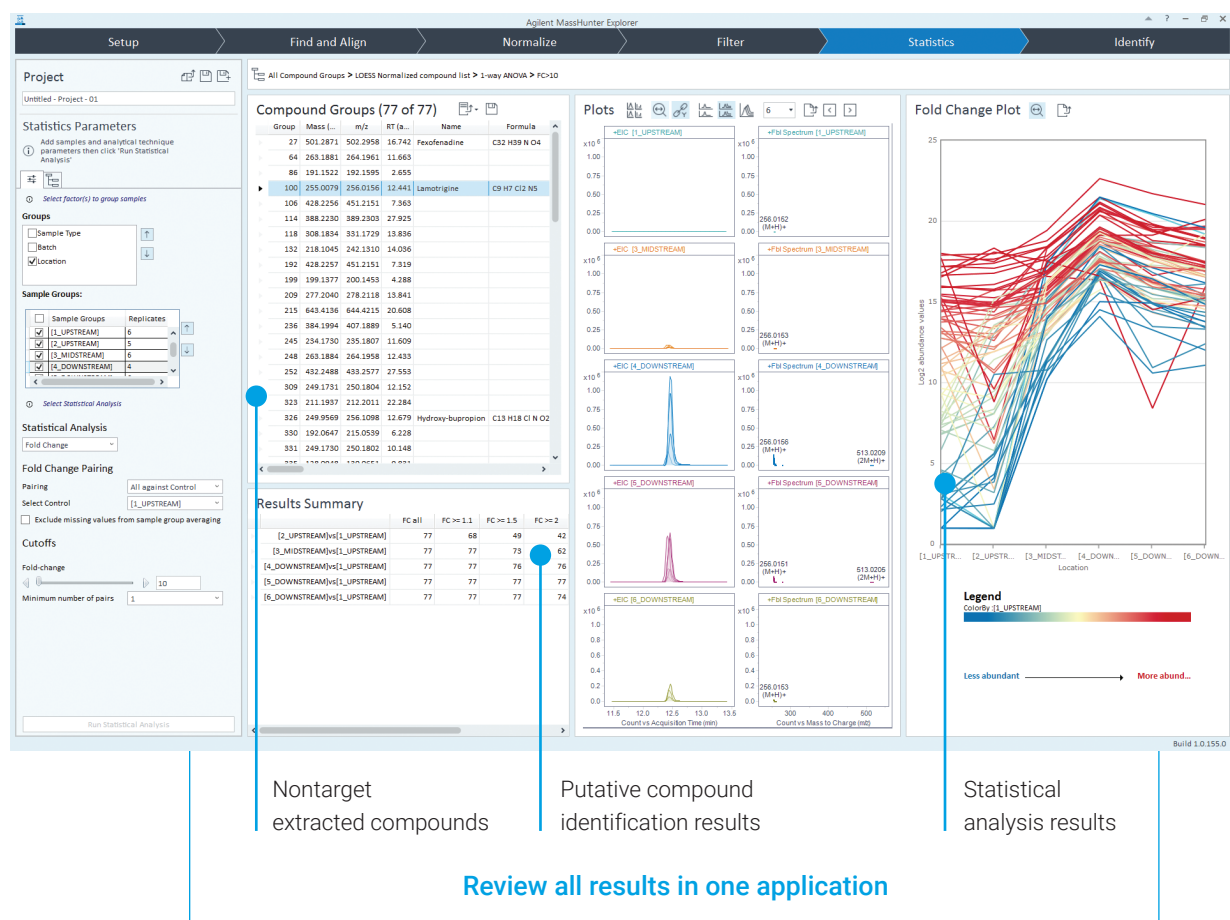
# Identify unknown emerging contaminants

Environmental contamination is an ever-increasing threat to existing ecosystems. Released chemicals of any kind can have unforeseen negative impacts, particularly if some products cannot be broken-down further. This includes the "everlasting" per- and polyfluoroalkyl substances (PFAS) such as PFOS, and thousands of similar variants.

Designed for nontargeted data extraction and differential analysis, Agilent MassHunter Explorer is a user-friendly software that combines all steps from feature finding, compound alignment, normalization, filtering, and statistical analysis to focus the analysis on the compounds of interest. Extracted compounds are putatively identified with known accurate mass, isotope patterns, and optional retention times sourced from public and private spectral libraries and databases.

## MassHunter Explorer includes integrated tools to facilitate identification



Nontarget extracted compounds

Putative compound identification results

Statistical analysis results

**Review all results in one application**

*"MassHunter Explorer software allows us to quickly move from individual samples to the big picture. It lets us see this huge amount of data in context, so we can make choices that get us to the answer as fast as possible."*

— **Imma Ferrer**
Research Scientist, University of Colorado

# Expand your identification capabilities

Agilent ChemVista software conveniently organizes, manages, and edits spectra using compound-centric architecture by facilitating identification workflows for MassHunter data analysis applications and beyond. This standalone software integrates compound, retention time, and mass spectral information from multiple sources, including MassBank or MoNA, without duplication.
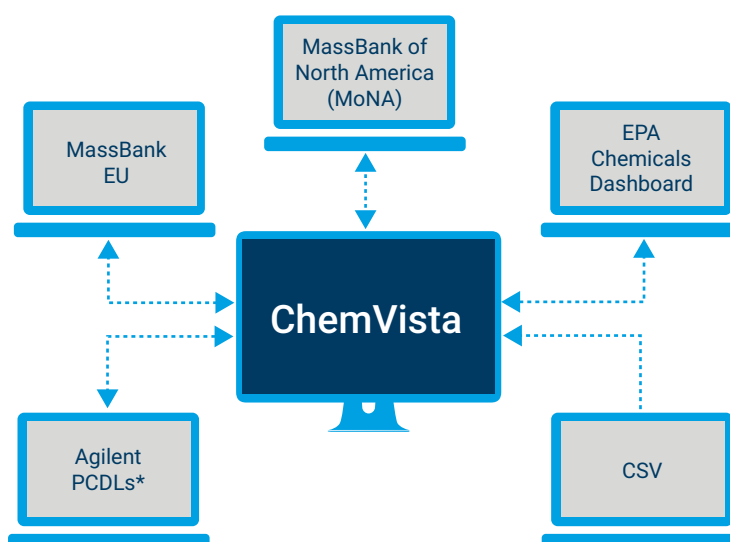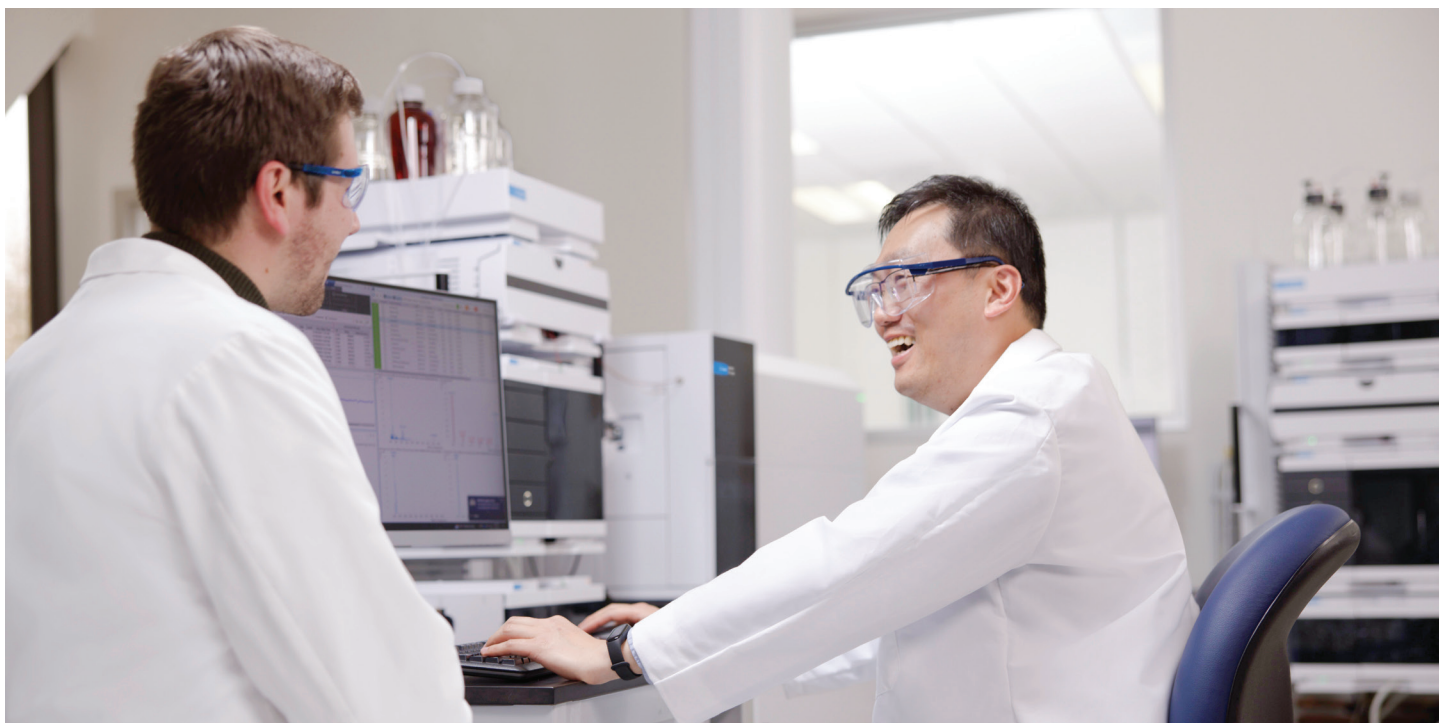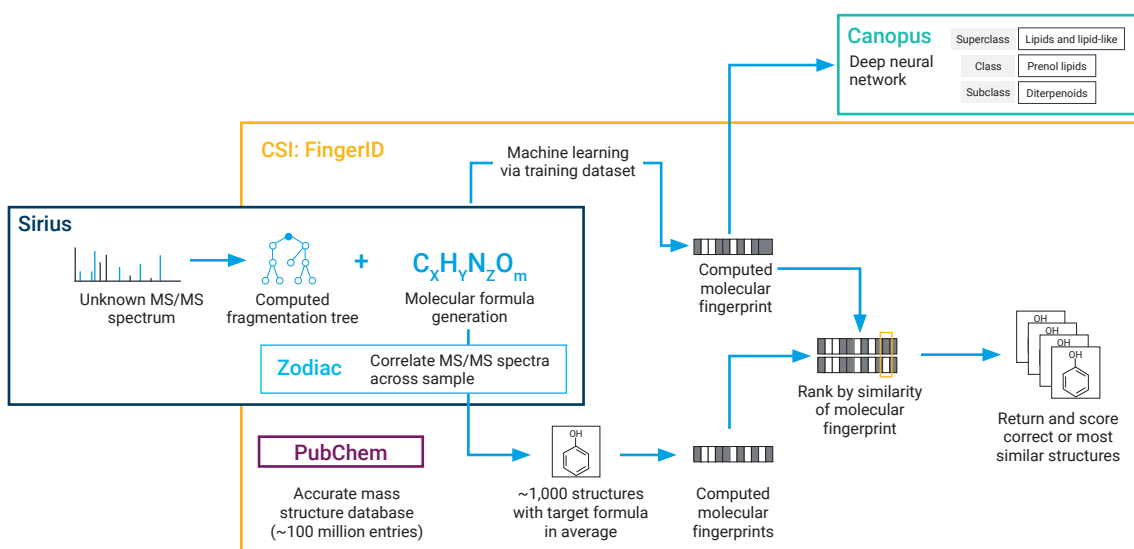




*PCDLs: curated Personal Compound Databases and Libraries

## Collaborating for rock-solid structural confirmation

With partners' software, such as Sirius and CSI:FingerID, you will receive the predicted structure of your compounds of interest.

In the first step, Sirius looks at the experimental fragment spectra and generates a fragmentation tree and a formula. Next, CSI:Finger ID enters the fragmentation tree into its machine learning data set, producing a fingerprint. The fingerprint is then compared to compounds in online databases like PubChem and HMDB. Finally, the software ranks all the options in terms of similarity and confirms a structure and ID name with certainty.



### Agilent MS data files are fully compatible with these platforms:

MD MOLECULAR DISCOVERY

Innovative Omics

Skyline

Envimass

MS-DIAL

Genedata
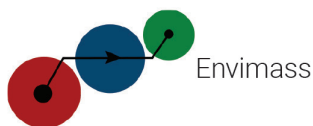
Metabolomics

# Advance your research, from sample preparation to insight

Agilent offers end-to-end solutions for lipidomics, proteomics, and genomics research. These include the Agilent Bravo metabolomics sample prep platform, Agilent 1290 Infinity II LC System, Revident LC/Q-TOF, Agilent 6495 LC/TQ system, and Agilent Seahorse XF Pro analyzer. Agilent offers omics analysis workflows that support you every step of the way.

## Quadrupole time-of-flight LC/MS:

**Agilent Revident LC/Q-TOF for untargeted analysis**
Revolutionize your identification for small-molecule analysis.

## Triple quadrupole LC/MS:

**Agilent 6495 LC/TQ system for targeted analysis**
Obtain a molecular-level view of metabolite regulation.



## Liquid chromatography:

**Agilent 1290 Infinity II LC System**
Achieve unmatched separation and detection performance.

## Sample preparation:

**Agilent Bravo Metabolomics Workbench**
Make plasma sample preparation consistent, dependable, and easy.

## Cell analysis:

**Agilent Seahorse XF Pro analyzers**
Confirm metabolic function and reveal critical drivers of cell signaling, activation, proliferation, toxicity, and biosynthesis through real-time live cell measurements.

# Illuminate cellular biology: An end-to-end workflow

Combined Seahorse XF Pro analyzer and LC/Q-TOF results let you measure metabolic pathway utilization at the cellular and molecular level.

In this workflow, the kinetic oxygen consumption rate and proton efflux rate data are converted to adenosine triphosphate production rates specific to glycolysis and mitochondrial respiration. The converted data provide a quantitative overview of drug treatment impact on cellular-level energetic phenotypes.
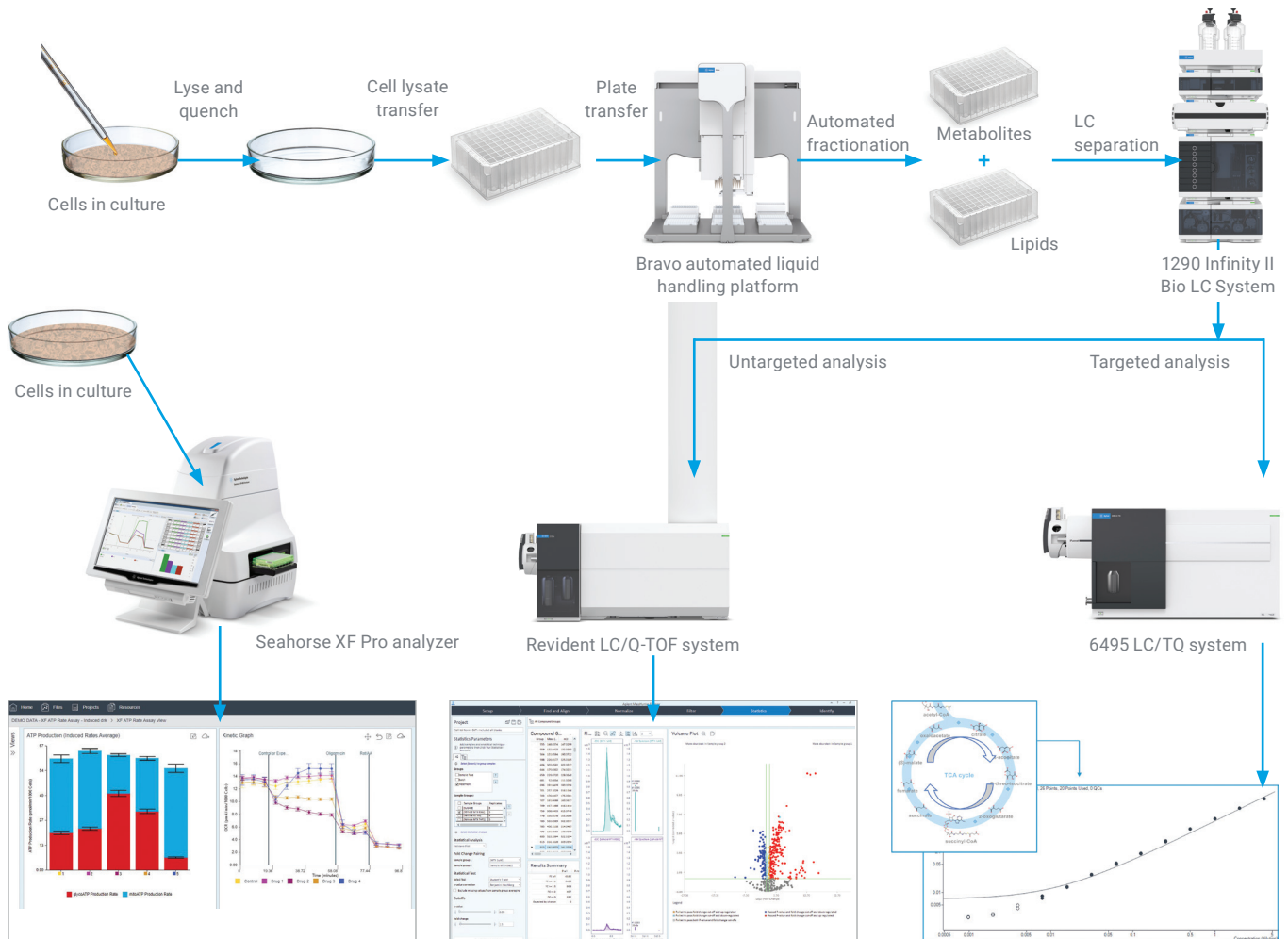
# Take control of data integrity and compliance

The complexities of safeguarding and managing lab data can be daunting, no matter which industry you're in. Partner with Agilent to implement a data system that enables you to:

- **Limit system access.** Ensure that only authorized personnel modify your LC/Q-TOF data. Assign roles to dictate unique levels of access, and use your domain to provide a unique ID and password for each user.

- **Protect records.** Be sure that all raw data, metadata, and result data are stored in a protected location. A checksum confirms whether records are valid, invalid, or altered.

- **Maintain end-to-end work attribution.** Reconstruct the who/what/where/when/why of every change that takes place by recording all user activities in secure, timestamped audit trails.

- **Document audit trail reviews.** Confirm audit trail reviews so you can review records and audit trails in parallel.

**Accommodate compliance guidelines for multiple regions:**

☑ **FDA 21 CFR Part 11**

☑ **EU Annex 11**

☑ **GAMP5**
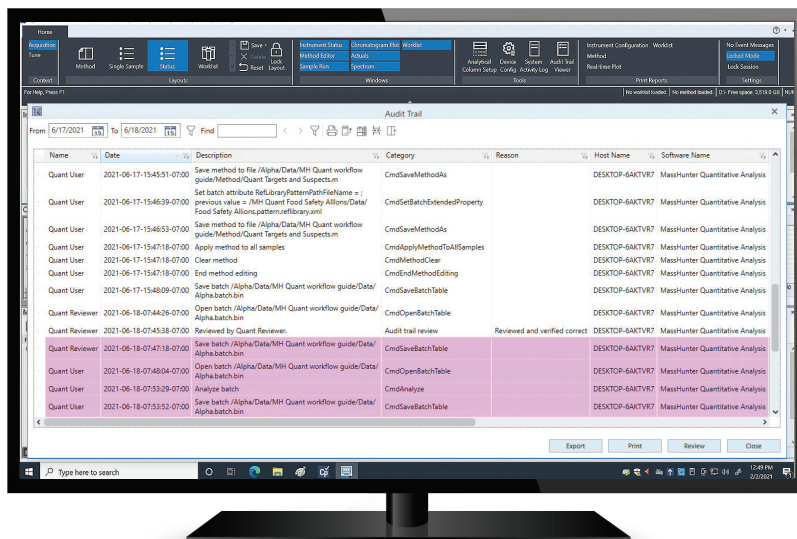
## Leverage advanced compliance expertise

CrossLab compliance services include instrument/software qualifications, consulting, and custom validations focused on data integrity so you can focus on science.

**www.agilent.com/compliance-services**

# Maximize your LC/MS efficiency with Agilent InfinityLab

Agilent InfinityLab LC instruments, columns, and supplies are designed to work together to provide efficiency gains that help you get more done and reduce operation costs.

## InfinityLab LC instruments

From routine analysis to cutting-edge research, the Agilent InfinityLab LC series offers a choice of HPLC and UHPLC systems to suit your application and budget.

## InfinityLab LC columns

With three particle sizes and 20 chemistries, Agilent InfinityLab Poroshell 120 LC columns provide a range of selectivity, making your method development fast and easy.

## InfinityLab LC supplies

The small parts of your workflow can make a big difference in the quality of your results. Agilent InfinityLab supplies are designed to improve the efficiency of daily tasks.



## Agilent CrossLab
From Insight to Outcome

### Supporting your success

CrossLab is an Agilent capability that integrates services and consumables to support workflow success, improve productivity, and enhance operational efficiency. In every interaction, we strive to provide insight that helps you achieve your goals.

Learn more about CrossLab at **www.agilent.com/crosslab**

## Want to minimize errors and improve consistency between analysts?

Agilent University offers flexible, cost-effective training options to help you plan, prioritize, and manage lab resources. Your team will also gain insights into boosting efficiency and minimizing downtime. Plus, you can choose the training format that suits you best—including in person, virtual, and online.

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