The Agilent 6545 Q-TOF LC/MS System

THE ANSWERS YOU NEED: BETTER, FASTER, EASIER

The Measure of Confidence

Agilent Technologies

FASTER ANSWERS
BETTER MEASUREMENTS
EASIER HIGH PERFORMANCE RESULTS

The new 6545 Q-TOF incorporates hardware and software innovations to enhance quality, significantly improve instrument robustness and increase overall performance.

The result: a new standard for robust, high-productivity, high-sensitivity analytical performance.

New advances in the MassHunter software suite incorporate advanced data mining and processing tools that let you rapidly and accurately extract all available information from the compounds in your samples — not just peaks and data points, but answers. The new 6545 Q-TOF is designed to make your MS analyses faster, easier, and more productive, whether you are doing pharmaceutical research, food safety analysis, forensic toxicology, environmental analysis, metabolomics, or lipidomics.

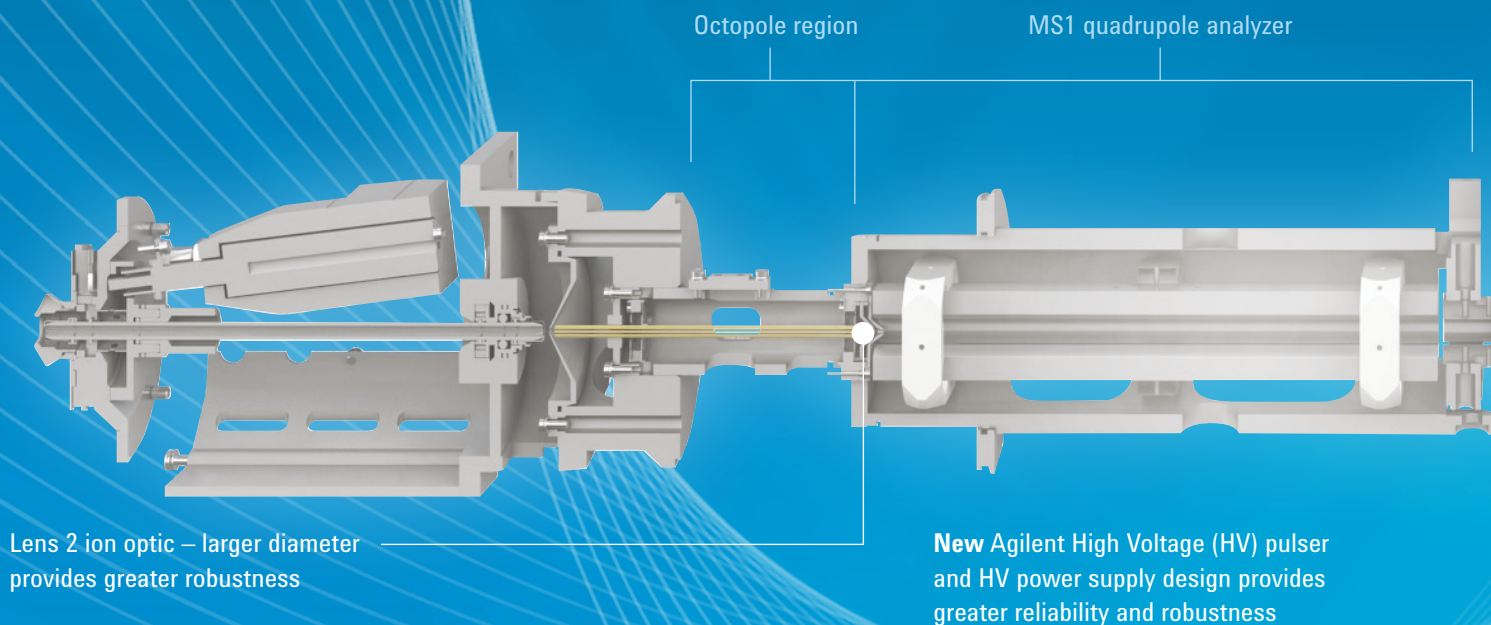| Challenge	The 6545 Q-TOF Solution
The trace level compounds you seek are inaccurately quantified or missed altogether.	The new SWARM autotune with improved optimization capabilities delivers more reliable answers, with dramatically improved analytical sensitivity for small molecule compounds. Lower ion optics voltages help to preserve fragile compounds.
Complex sample analyses require significant time and expertise.	Easy instrument optimization puts precise results within reach of the non-expert. Enhanced analytical tools promote confidence and productivity – delivering answers faster.
You need to do more with less: develop more methods, handle increased workloads.	Rugged reliability for routine screening with the analytical sensitivity needed for compound identification. Agilent databases and PCDLs reduce the time needed to get answers.
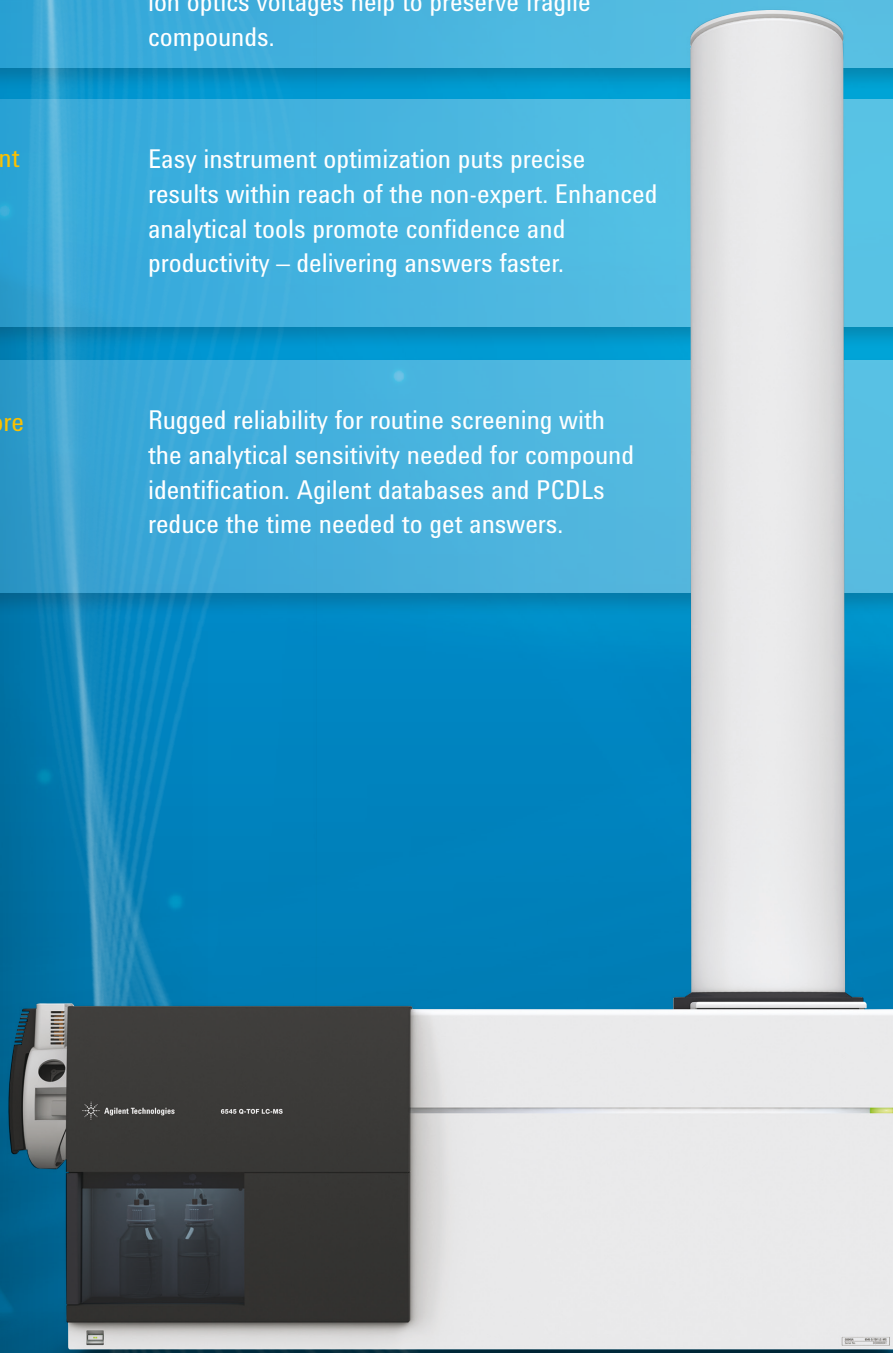
BEING THERE WHEN IT MATTERS THE MOST

Octopole region   MS1 quadrupole analyzer

Lens 2 ion optic – larger diameter
provides greater robustness

New Agilent High Voltage (HV) pulser
and HV power supply design provides
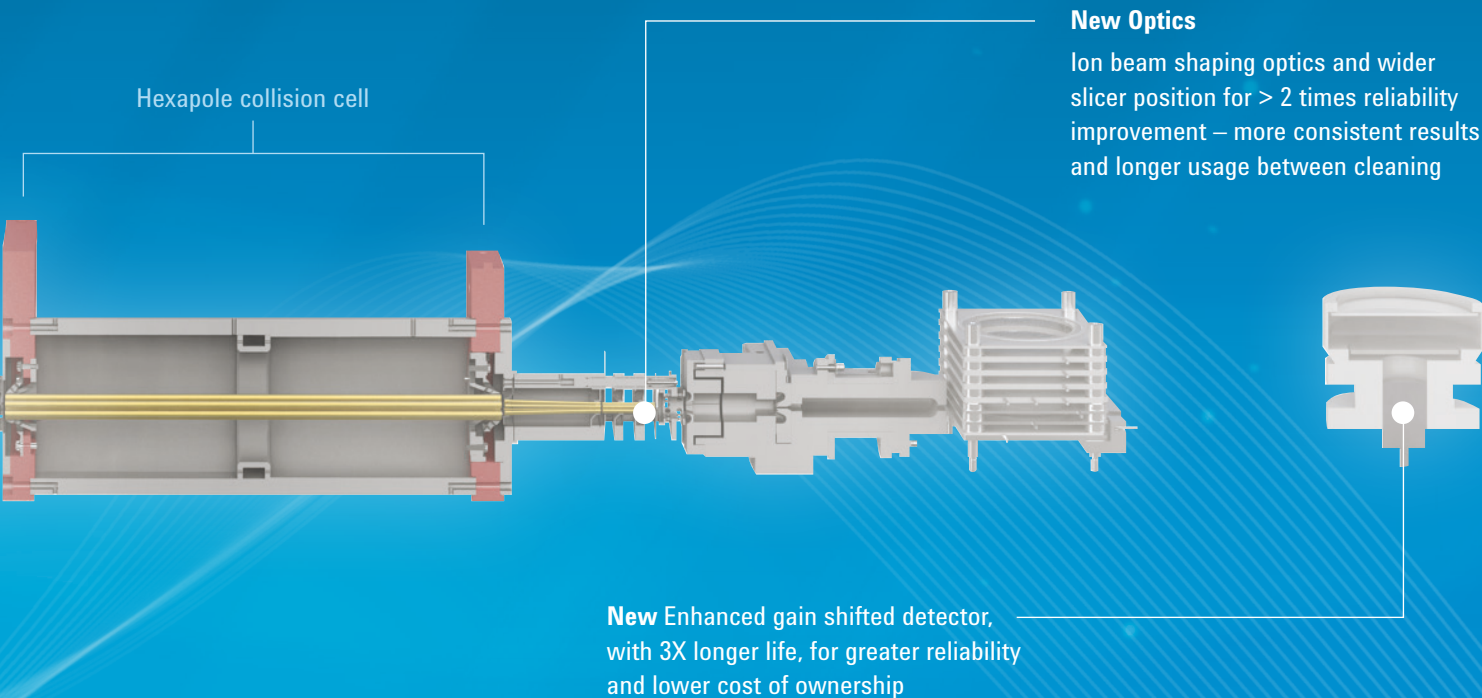greater reliability and robustness

Higher robustness than previous generation instruments

All the improvements incorporated into the Agilent 6545 Q-TOF have
produced improved resolution, enhanced analytical sensitivity and
a third important outcome: higher robustness than the previous
generation of instrument.

In addition to the high-energy optics, the 6545 features additional
improvements in two key areas that significantly enhance ruggedness
and reliability:

• A new-generation detector that offers significantly improved longevity,
  while still delivering high sensitivity and wide dynamic range.

• Next-generation electronics subsystems that substantially increase the
  robustness of our high-speed TOF electronics.

Hexapole collision cell

New Optics
Ion beam shaping optics and wider slicer position for > 2 times reliability improvement – more consistent results and longer usage between cleaning

New Enhanced gain shifted detector, with 3X longer life, for greater reliability and lower cost of ownership

Relentless attention to detail and technology development

Ion beam compression and shaping

Ion beam compression and shaping (IBCS) technology provides great analytical sensitivity while maintaining over **45K mass resolution and sub 1 ppm mass accuracy.** Enhanced electronics and software algorithms enable exceedingly high data acquisition rates–up to 50 spectra/second.

Agilent JetStream thermal gradient focusing

A precisely micro-machined sprayer surrounds ESI droplets with a sheath of superheated gas to desolvate and concentrate ions near the MS inlet for more effective sampling.

Automated slicer assembly

Continuous refinement of the ion optics design combine to deliver **robust performance for the most demanding combined qualitative and quantitative applications.**

Flight tube power supplies

Each of the three main power supplies controlling the flight tube has been redesigned to deliver substantially better **stability for mass accuracy and mass resolution.**

FASTER OPTIMIZATION: SWARM AUTOTUNE WITH PARTICLE SWARM OPTIMIZATION

Now it's easier than ever for every user to get exceptional results

What if tuning your instrument could be like autofocus on a camera? In developing the new 6545, Agilent's development team listened to customers who want ease of use together with automated optimization. The Agilent 6545 Q-TOF revolutionizes that process, with an innovative autotune that incorporates Particle Swarm Optimization (PSO).
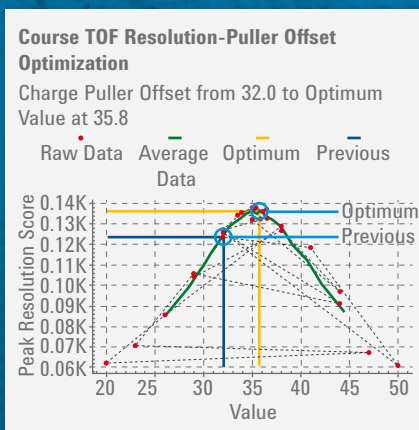
SWARM Autotune provides:

- Radically faster autotune speed – 4x faster than previous generation Q-TOFs.
- Optimization options for small molecules – automatically delivers enhanced sensitivity for the best small molecule peformance.

☒ Positive	◯ Quadrupole	◯ Mass Calibration/Check	◯ 50-1700m/z
☐ Negative	◉ TOF	◉ Standard Tune	◯ 50-750m/z
☐ Fast Polarity Switching	◯ Both	◯ Set Detector Gain	◉ 50-250m/z
		◯ Initial Tune	☒ Fragile Ions

Particle Swarm Optimization

PSO is a flexible and robust multidimensional optimization algorithm that can **optimize up to 21 parameters simultaneously** – even when no initial signal is present – and can avoid getting trapped in local optima. It can optimize elements for a target resolution, level of fragmentation, or for maximum analytical sensitivity with a simple "start tune" button. The new SWARM Autotune simplifies the optimization of multiple instrument parameters and is adjusted to allow for more ion transmission, more speed, and lower loss of fragile molecules.

Course TOF Resolution-Puller Offset Optimization

Charge Puller Offset from 32.0 to Optimum Value at 35.8

Raw Data   Average Data   Optimum   Previous

Transmission Optimization Signal Improved 7.5%

● Best Solution ▲ Particle 1 ■ Particle 2 ▼ Particle 3
✕ Particle 4 ✚ Particle 5 ● Particle 6 ■ Particle 7
▲ Particle 8 ▼ Particle 9 ✦ Particle 10

APPLICATION FOCUS: FOOD AND WATER ANALYSIS

Screen and identify pesticide residues with unsurpassed speed and analytical sensitivity

Unparalleled accuracy in mass measurements and isotope ratios make Q-TOF LC/MS systems the ideal choice for detection and identification of pesticides. Exceptional system sensitivity allows for the detection and quantitation of trace level compounds, enabling food testing labs to keep pace with evolving regulations and confidently identify new, emerging contaminants.

**Enhanced Sensitivity of 6545 Q-TOF for Pesticides in Black Tea at 2 ppb**
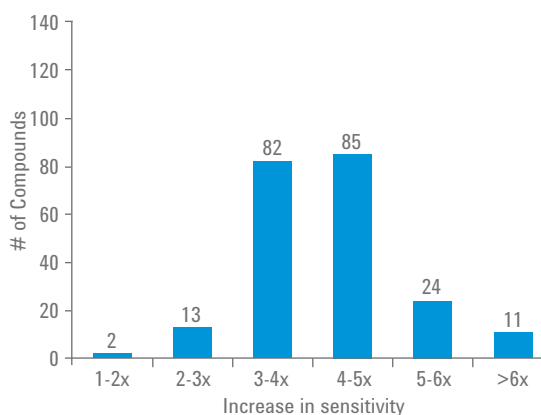
A 4-5x increase in sensitivity was observed for more than 80% of compounds detected.

Water Contaminants

The consistently superior analytical sensitivity of the 6545 Q-TOF LC/MS system makes it ideal for detection and quantitation of both targeted and non-targeted PPCP compounds.

Surface Water Analysis: 6545 vs. 6540
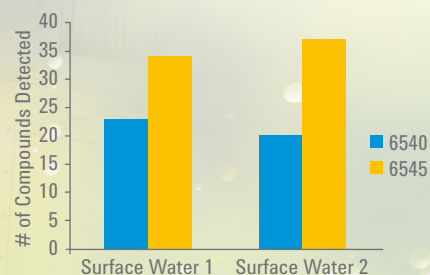
The 6545 detected a greater number of contaminants in surface water compared to the 6540 Q-TOF.

**Identification of Dextrorphan in Contaminated Surface Water**
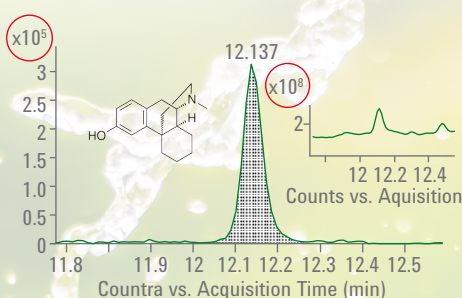
Dextrorphan can be detected in the presence of 1000x co-eluting ions by the Agilent formula-generating algorithm.

ALL IONS MS/MS

Identify and quantitate with higher confidence

All Ions MS/MS is a great solution for screening analytes in food, environmental, and forensic toxicology applications. Agilent offers a fully developed All Ions MS/MS workflow for compound confirmation and quantitation, featuring:

- Easy acquisition method setup – even for multi-compound screening.
  - Links to knowledge bank in PCDLs (extracts MS/MS fragmentation properties for all compounds in a screen).
  - Unique Co-elution score of diagnostic fragment ions used to verify hits.
  - Easily add new targets to the PCDL to continually expand the scope of screening over time.
  - A full spectrum of molecular ions plus their major fragments are always collected so data can be re-interrogated retrospectively when these new targets are added.
- Rapid quantitation method development that automatically selects two high-quality product ions for each compound.
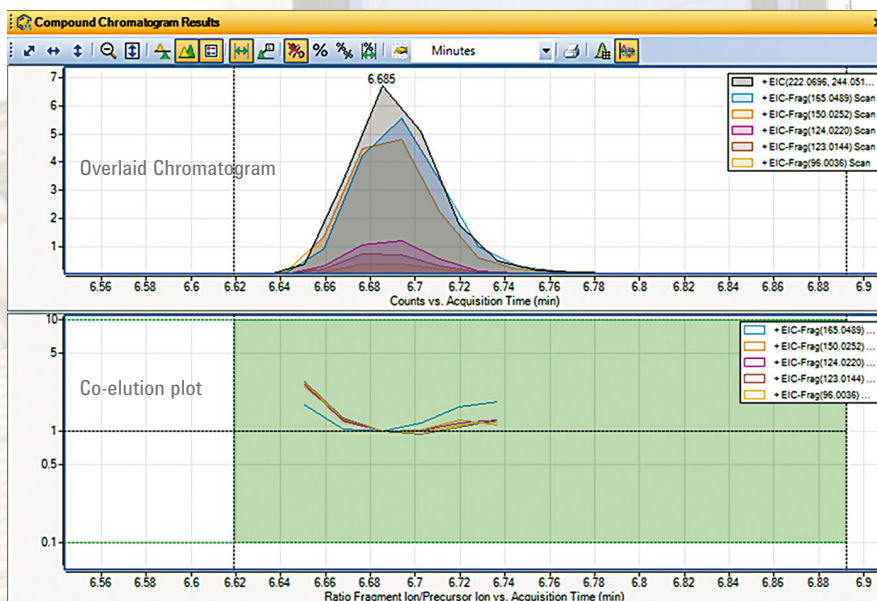
TARGETED MS/MS

Quickly quantify, find and identify compounds with targeted MS/MS, databases, and PCDLs

Targeted MS/MS and the pesticides PCDL together allow quick quantitation, identification and confirmation of unknown contaminants in a black tea sample. The 6545 Q-TOF combines quantitative requirements for screening applications with the qualitative requirements for compound identification based upon accurate mass and PCDL MS/MS library matching.

Quantitation and structure confirmation of dimethoate in avocado matrix by targeted MS/MS
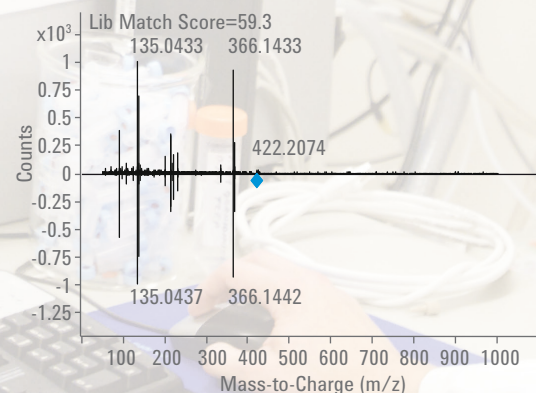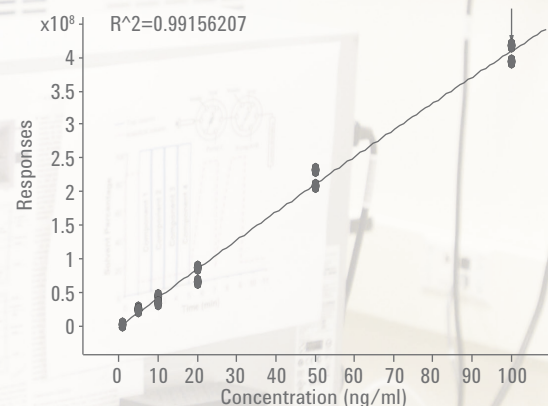
Calibration curve represents 1 ng/g to 100 ng/g at 6 levels. Most of the pesticides can be detected at or below maximum residue limit (MRL) of 10 ng/g in complex matrices, matched with the Agilent Personal Compound Database and Library (PCDL).

New PCDLs Support Easier, Accurate Results

Agilent is committed to supporting easier, more accurate results in research and regulated labs by investing in the development of personal compound databases and libraries (PCDLs). One example is the **mycotoxins PCDL**, developed in collaboration with the University of Natural Resources and Life Sciences, Vienna (BOKU), Austria. Hundreds of mycotoxins were added to the database and high resolution MS/MS spectra were obtained for those mycotoxins and related fungal metabolites. The new mycotoxins library will help food scientists to find and confirm unambiguously the presence of hundreds of contaminants without needing to actually have the standard compounds. Armed with this data, researchers and government labs can make informed decisions about which analytical standards to purchase for subsequent quantitation.
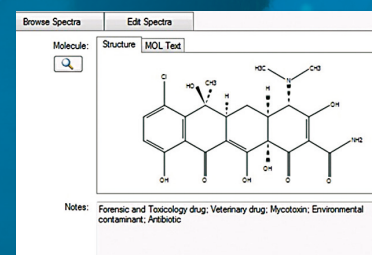
GREATER EFFICIENCY AND CONFIDENCE: A TEAM EFFORT

Agilent 1290 Infinity II LC

The Agilent 1290 Infinity II LC includes a novel multisampler, alternative pump configurations, and faster injection cycles to help you achieve unmatched separation and detection performance for data of the highest quality. Learn more at www.agilent.com/chem/1290

Agilent Poroshell 120 and ZORBAX RRHD columns

The Poroshell 120 family provides consistent, reliable performance for U/HPLC applications. Start with EC-C18 chemistry for the best all-around performance. With 13 chemistries including Poroshell HPH, designed for robust performance in high pH conditions, you can refine your methods to support the highest LC/MS sensitivity and compound identification. Learn more at www.agilent.com/chem/poroshell120.

"The Q-TOF provides data-rich files, with the accurate mass allowing very narrow extracted ion ranges to reduce noise to near-zero values, as well as the determination of chemical formulae of unknowns. I can quantitate in either MS or MS/MS mode with good linearity and dynamic range, and software tools make database and library searching very easy. I can also do retrospective searches on old data for new compounds reported in the literature or media, just by adding them to my searchable database."

RALPH HINDLE, VOGON LABORATORY SERVICES, LTD.

SOFTWARE AND SERVICES SUPPORTING YOUR WORK

Agilent MassHunter Workstation software

Agilent MassHunter Workstation software was designed to make your MS analyses faster, easier, and more productive. In addition to data acquisition, and instrument control for your Agilent LC/MS, GC/MS, and ICP-MS instruments, the software incorporates advanced data mining and processing tools.

MassHunter Workstation software data mining capabilities integrate with Agilent's Personal Compound Database & Library (PCDL), offering the ability to use accurate mass MS/MS libraries for screening and confident identification of compounds of interest, as well as the flexibility to create customized PCDLs.

- Pesticide analysis PCDL
- PCDL for mycotoxins/fungal metabolites
- PCDL for veterinary drugs
- Water Screening PCDL
- PCDL for compounds of forensic toxicology concern (Broecker, Herre & Pragst)*
- PCD/PCDL for metabolomics (METLIN)**
- Extractables & Leachables PCDL

*For Forensic Use
**For Research Use Only. Not for use in diagnostic procedures.

The Agilent Value Promise: 10 years of Guaranteed Performance

In addition to our continually evolving products, Agilent offers the industry's only 10-year value guarantee. Agilent guarantees you at least 10 years of instrument use from your date of purchase, or we will credit you with the residual value of that system toward an upgraded model.

It's our way of assuring you of a safe purchase now, and protecting your investment into the future.

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