Detecting and quantifying

new threats to the environment.

Our measure is your success.

Agilent Technologies

Emerging contaminants:
Is your lab up to the challenge?

There are growing concerns about the safety of our drinking water supplies and the purity of our natural resources. Largely driven by technology that enables detection of more substances at increasingly lower concentrations, the scientific community is turning its attention to several new classes of emerging contaminants. They include:

- Pharmaceuticals and Personal Care Products—Known collectively as PPCPs, this group of compounds includes human and veterinary drugs, as well as consumer products such as sunscreens, lotions and fragrances.

- PFOA/PFOS—Perfluorinated organics are uniquely stable molecules that are widely used in almost all industries.

- Endocrine disruptors—Endocrine disrupting compounds (EDCs) are synthetic chemicals that, even in small doses, can affect the endocrine system of living organisms. There are potentially thousands of such compounds.

Where do you start?

For more than 40 years, Agilent has been working closely with environmental testing laboratories and regulatory agencies to solve an ever-widening range of analytical challenges.

We offer today's widest range of solutions for environmental analysis, both for target and non-target compounds. Using our powerful and robust GC/MS and LC/MS methods you can:

- Achieve significantly lower LODs and LOQs for a wide range of contaminants

- Significantly shorten your analysis time

- Boost your lab's productivity

- Meet stringent regulatory and directive requirements

Agilent Solutions for Emerging Environmental Contaminants

Instrument Options	Screening	Confirmation	Quantification
LC/MS Triple Quad *Target polar or moderately polar compounds*	• Highly selective, sensitive and fast detection of hundreds of compounds in a single injection • Low detection limits in complex matrices	• MRM provides positive confirmation and low detection limits to meet all regulatory requirements • One-run screening and confirmation	• Routine high accuracy MS/MS quantification • Batch-at-a-Glance for fast review of quantification results
LC/Q-TOF or LC/TOF *Non-target polar or moderately polar compounds*	• High resolution reduces noise and matrix interference • Accurate mass provides added compound selectivity and unlimited screening using exact mass databases	• Automated accurate-mass searches against public and private databases • Molecular Formula Generator feature reduces data interpretation time	• Very narrow mass window extracted ion chromatograms provide accurate MS and MS/MS quantification • High dynamic range to quantify wide range of concentrations
GC/MS *Target and non-target, volatile and semi-volatile compounds*	• Backflushing improves retention time precision, eliminates ghost peaks and shortens cycle time • Rapid screening for 927 pesticides in a single injection without oven bakeout	• Automated Deconvolution Reporting Software (DRS) saves hours of data analysis time with fully integrated deconvolution results • Raw, deconvoluted and full spectra displayed for easy review and more confidence	• SIM/Scan capability allows spectral acquisition and high sensitivity quantification in a single injection • Trace Ion Detection (TID) lowers detection limits in complex matrices
GC/MS Triple Quad *Target volatile and semi-volatile compounds*	• Highly selective, sensitive detection of hundreds of compounds in a single injection using standard EI source • Extremely low detection limits in complex matrices	• MRM provides positive confirmation and low detection limits to meet regulatory requirements • Matrix-independent response allows one-run screening and confirmation	• Routine high accuracy MS/MS quantitation • Batch-at-a-Glance for fast review of quantification results

LC/MS: Sensitivity you can use to confirm and quantify ultra-trace polar contaminants

- PPCPs
- PFOS/PFOA

- Agilent 1200 Series Rapid Resolution LC reduces separation times to seconds.

- Agilent 6410 Triple Quadrupole LC/MS provides highly selective, sensitive detection and quantification of hundreds of targeted compounds in a single injection.

- Agilent 6460 Triple Quadrupole LC/MS, with Agilent Jet Stream thermal gradient focusing technology, delivers 6x better sensitivity than previous generation instruments—best-in-class of any available triple quad.

- Agilent 6230 Accurate Mass TOF LC/MS lets you obtain sensitive full spectra with a mass accuracy better than 2 ppm for screening and identifying non-target or target contaminants.

- Agilent 6530 Accurate Mass Q-TOF LC/MS offers unlimited target and non-target compound screening using exact mass databases as well as MS/MS confirmation/quantification in a single injection.

- Combination of TOF and Triple Quadrupole offers maximum power for unlimited target and non-target compound screening and for meeting regulatory quantification requirements; TOF provides full spectra and accurate mass for searching databases, and Triple Quadrupole provides MS/MS for confirmation and quantification.

Flexible, easy to use MassHunter MS software

From instrument tuning to final report, Agilent's MassHunter Workstation software makes all your MS analyses faster, easier and more productive, while delivering the flexibility and robustness required to meet the demands of a busy testing lab.

The software incorporates advanced feature extraction, data mining and data processing tools that let you rapidly and accurately extract the information you need from the compounds in your samples.

Reporting is fast and flexible, using preconfigured templates or customized reports in the familiar Microsoft Excel user interface.
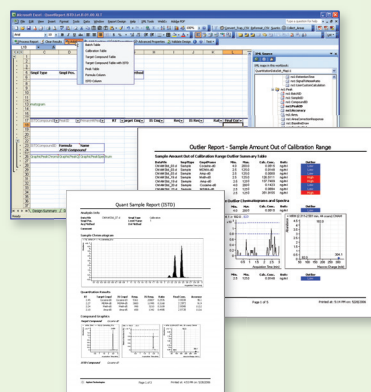
Agilent 6400 Series Triple Quadrupole LC/MS
## Lower your limits of detection and quantification
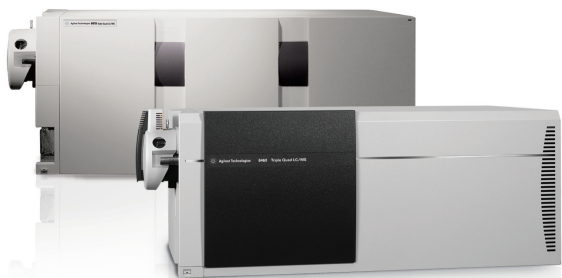
There are many ways to measure sensitivity but only one that really counts: in your lab with your samples. With Agilent Jet Stream thermal gradient focusing technology, the Agilent 6460 LC/MS delivers 6x lower LODs than previous generation instruments—to improve your results, every day.

• **Lowest limits of detection for all applications.**
  Maximized ion generation and transmission across a broad mass range ensure the lowest limits of detection and quantitation for the widest range of sample types.

• **Fast, multi-analyte quantitation.** Fast MRMs (multiple reaction monitoring) enable hundreds of compounds to be analyzed per-injection using MRM rates of 200 per second or faster.

• **Highest sensitivity in class.** With Agilent Jet Stream technology for conventional flow separations or HPLC-Chip/MS for nanoflow separations, the 6460 provides best-in-class sensitivity for a wider range of applications.
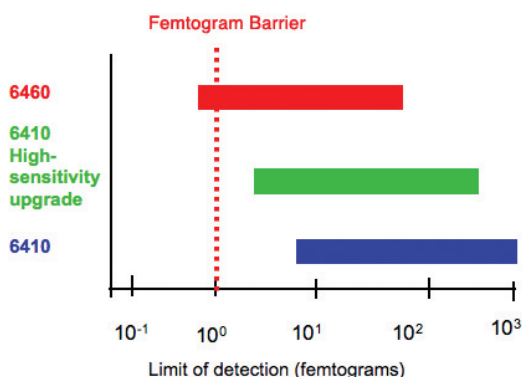

Breaking the femtogram barrier. The new 6460 system offers dramatically improved, femtogram-level sensitivity for your most demanding quantitative applications. Detection limits are shown here as a range, representing the natural spread in ionization/fragmentation efficiency for polar and non-polar compounds.

Solutions for Targeted Screening: LC/MS/MS for PPCP and PFOA/PFOS

With their unmatched sensitivity and extremely fast MRM switching speeds, Agilent 6400 series triple quads are the ideal tools for targeted screening methods such as PFOS/PFOA determination and PPCP measurement at very low levels.
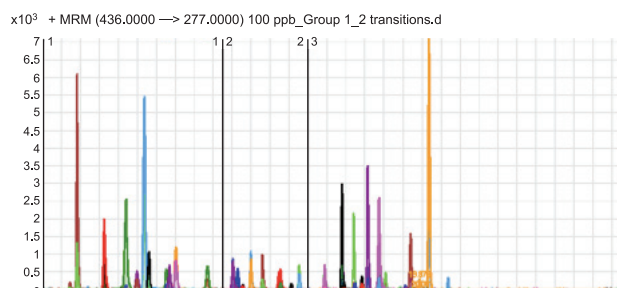
Group 1 analytes from Method 1694 for PPCPs in the environment. Note that these 48 pharmaceutical compounds are shown with two overlapping MRM transitions in three time segments. This result was obtained with a Agilent ZORBAX HPLC column, which easily meets method requirements.
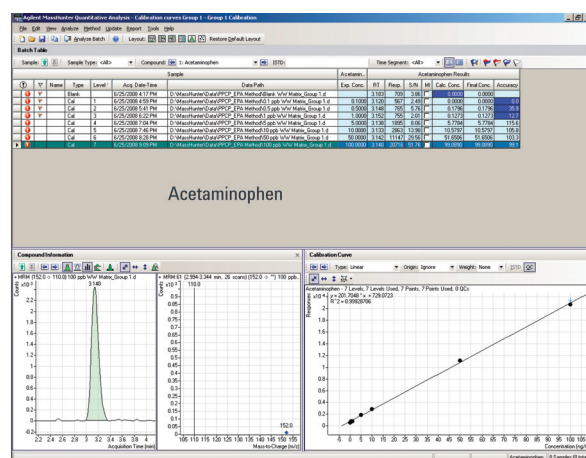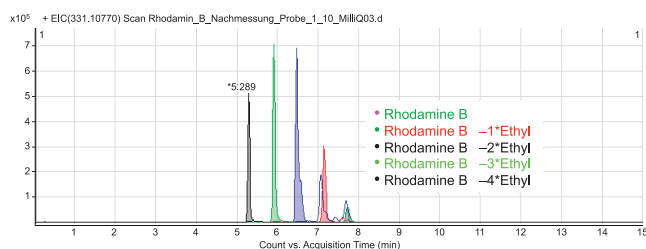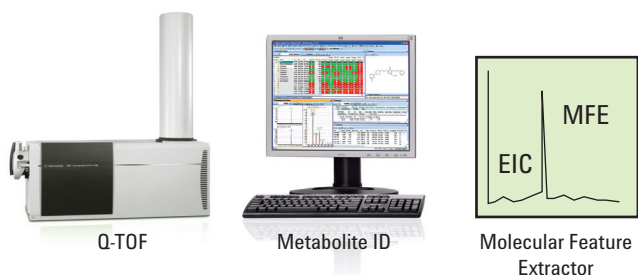

Calibration data for acetaminophen in water. With Agilent MassHunter software, all the information is on a single screen—clear and easy to understand.

Solutions for Non-Targeted Screening: LC/MS TOF and LC/MS Q-TOF

True high definition TOF technology in our TOF and Q-TOF systems coupled with powerful software tools facilitate the identification and confirmation of unknown perfluorinated organics and PPCP compounds in environmental samples. A typical workflow includes:

- Acquisition of accurate-mass full spectral data

- Data mining with Agilent Molecular Feature Extractor software

- Confirmatory tools for the discovery using MassHunter software's isotopic matching and molecular formula generator

Q-TOF   Metabolite ID   Molecular Feature
                                              Extractor

x10⁵ + EIC(331.10770) Scan Rhodamin_B_Nachmessung_Probe_1_10_MilliQ03.d

• Rhodamine B
• Rhodamine B −1*Ethyl
• Rhodamine B −2*Ethyl
• Rhodamine B −3*Ethyl
• Rhodamine B −4*Ethyl

Count vs. Acquisition Time (min)

Ground water analysis. Agilent's accurate-mass capabilities, plus powerful Metabolite ID and Molecular Feature Extractor software, identify Rhodamine B and four metabolites from a ground water sample.

Hyphenated ICP-MS: Fast, sensitive element-specific screening and quantification for emerging contaminants

Inorganic components can yield innovative solutions for emerging contaminants. Ranging from speciation of toxic elements like Cr(VI) to the herbicide example below, Agilent's ICP-MS solution gives the flexibility of analyzing a wide range of elements with superior sensitivity.

- Rapidly screen, confirm and quantify target compounds in a single injection without the need to run external standards

- Fast, accurate quantification using compound-independent calibration

- Unmatched matrix tolerance and ability to remove interferences

Glyphosate, Gluphosinate and AMPA— Rapid detection without derivatization

Glyphosate (Roundup®) and the related compound Gluphosinate are among the most widely used of non-selective herbicides.

When coupled with ion-pairing HPLC, the Agilent 7500cx ICP-MS with Octopole Reaction System (ORS) technology offers superior detection capability—without the need for derivatization—for phosphorus-containing herbicides and their metabolites.
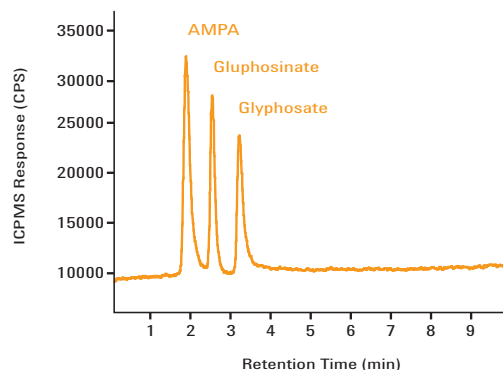
|	AMPA	Gluphosinate	Glyphosate
Regression coefficient	0.999	0.998	0.999
LOD (concentration)	25 ppt	27 ppt	32 ppt
LOD (amount)	2.5 pg	2.7 pg	3.2 pg
RSD, retention time, n=8	1.1 %	0.8 %	1.2 %

GC/MS: Sensitive confirmation, identification and quantification of non-polar contaminants

- Endocrine disruptors (EDC)

- Pesticides

- Brominated flame-retardants (PBDE, PBB)

- Polychlorinated Biphenyls (PCB)

- Polynuclear Aromatic Hyrdrocarbons (PAH)

Agilent GC-based technologies—including new Triple Quadrupole GC/MS capabilities—provide highly sensitive detection of non-polar emerging contaminants. Advanced analytical capabilities and powerful, easy-to-use software provide more information from every run. And with the industry's widest selection of inlets, detectors, columns, supplies and sample introduction choices, Agilent delivers an unbeatable combination of performance and productivity for environmental applications.

The Agilent 5975C MSD has earned its place as the industry-standard single quadrupole solution and is the best choice for screening and confirming contaminants across a range of methods, applications and matrices.

- Fast synchronous SIM/Scan mode allows collection of two data sets from one run for increased information content and more confident identity confirmation

- Trace Ion Detection technology improves signal-to-noise and lowers your detection limits in challenging matrices

- New Triple Axis Detector with off axis configuration minimizes noise and maximizes signal for the lowest detection limits

- Powerful Deconvolution Reporting Software (DRS) saves hours of analysis time, quickly finding and quantifying "hidden" compounds
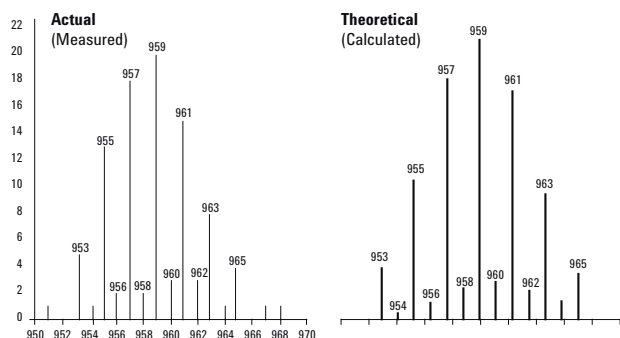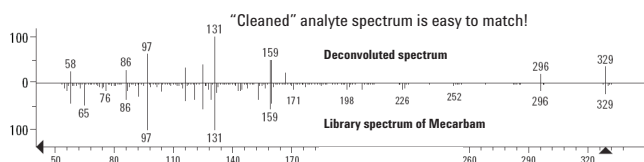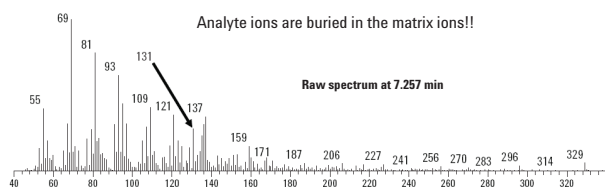

Proprietary gold quartz quadrupole ensures superior spectral reproduction across a broad mass range, as shown in this analysis of the decabromodiphenyl ether (PBDE-209) molecular ion cluster. In addition, high-temperature stability dramatically reduces maintenance, especially with complex, high boiling samples.
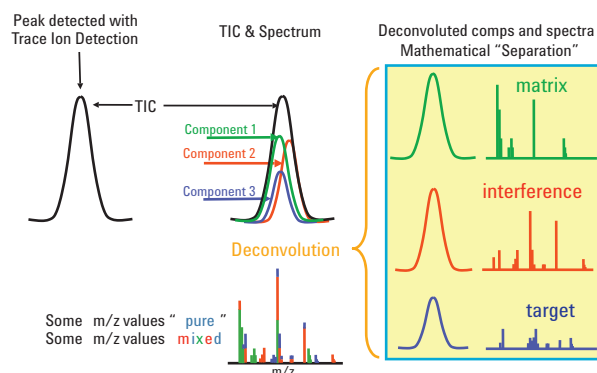
Trace Ion Detection and Deconvolution Reporting Software combine to improve the signal, reduce noise and enable faster, higher confidence spectral matching of trace level contaminants.

Analyte ions are buried in the matrix ions!!

Raw spectrum at 7.257 min

"Cleaned" analyte spectrum is easy to match!

Deconvoluted spectrum

Library spectrum of Mecarbam

Deconvolution Reporting Software (DRS) quickly finds and quantifies compounds hidden in complex matrices. *DRS fully integrates Agilent's GC/MSD ChemStation, NIST Mass Spectral Search Program with the NIST MS Library and AMDIS. The deconvoluted or "cleaned" spectra improves library search results and also ensures more accurate quantification.*

Pollutant Libraries improve identification and confirmation. *Deconvolution reporting libraries are retention time-locked and include full spectral and SIM data. A number of libraries for environmental contaminants are available, including one with 927 Pesticides and Endocrine Disruptors.*

The new Agilent 7000A Triple Quadrupole MS/MS is specifically designed for measuring the lowest levels of target compounds in difficult matrices such as sediment and wastewater. The combination of Agilent's proprietary solid inert ion source, proven quartz quadrupoles, innovative collision cell design and new triple-axis detector provides:

- Routine femtogram-level sensitivity (100 fg OFN >100:1 S/N RMS)

- Advanced, high-speed MRM data acquisition and quantification— up to 500 MRM transitions per second for reliable quantification and identity confirmation in a single run

- Superior MS resolution, ultra-low noise and exceptional spectral integrity

- Highly reliable operation under the most demanding conditions to maximize uptime and increase productivity

- Delivered with an Agilent J&W Ultra Inert GC column to help ensure the highest level of analyzer sensitivity
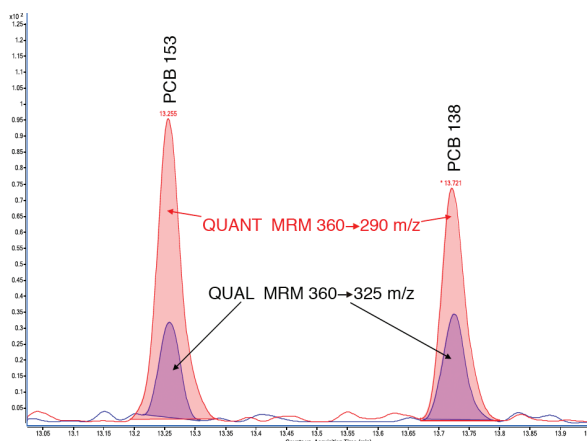
Unprecedented sensitivity for target compounds. *Chromatogram of two PCB congeners (PCB 153 and PCB 138) injected at 400 fg each on-column. Quantitation transition 360—>290 m/z, with the qualifier transition measured at 360—>325 m/z for simultaneous quantification and confirmation at the lowest detection limit.*
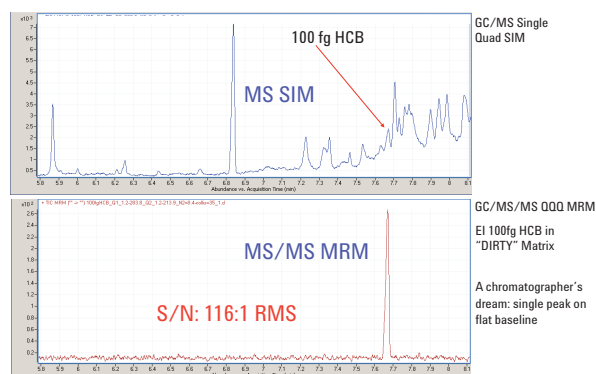
The power of Agilent Triple Quadrupole technology. *In this example, 100 fg of Lindane (BHC) is determined from a sediment matrix. No interfering peaks in MRM for reliable and faster routine analyses.*

To learn more about Agilent solutions for emerging environmental contaminants, visit www.agilent.com/chem/ppcp

High performance columns and supplies

For every environmental analysis requirement—from leading-edge methods development to routine samples—Agilent GC/MS certified supplies, Agilent J&W GC columns and ZORBAX LC columns give you the sensitivity, accuracy and reliability you need to get the job done right, the first time.

Agilent Services keep your lab running at peak productivity

With a 98% customer satisfaction rating, Agilent's service engineers are the most respected—and best-trained—in the industry. We can help you solve problems quickly, increase your uptime, and optimize your lab's resources. Through a selection of service plans tailored to your lab's needs and budget, we provide:

- On-site preventive maintenance that ensures dependable system operation and minimizes unplanned downtime

- Available remote diagnostic and monitoring capabilities that give you additional "uptime insurance"

- Expert installation, familiarization and advanced training to get you up and running as quickly as possible

Agilent: a complete range of environmental analysis solutions

In addition to our solutions for emerging contaminants, Agilent also offers complete workflow solutions for virtually all other environmental pollutants.

You can learn more about our environmental analysis solutions in our Environmental Compendium. Download a free copy at: **www.agilent.com/ppcp**

For more information

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Europe
info_agilent@agilent.com

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adinquiry_aplsca@agilent.com

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