Pesticide Analysis in Food

Faster, more confident

screening, confirmation and quantification

Our measure is your success.

products | **applications** | software | services

Agilent Technologies

There are more than 900 pesticides in use around the world. Agilent can help you screen, confirm and quantify all of them.

Most of the fruit and vegetables we eat are produced with the help of chemicals that protect against insects and weeds. All of these compounds are potentially harmful to humans—and every month the list keeps growing.

Agilent GC/MS and LC/MS solutions enable you to confidently monitor ultra-trace levels of pesticides—target and non-target—faster and easier than ever. Using powerful, multi-residue MS-based methods, you can achieve significantly lower LODs and LOQs for a wide range of food matrices. You can routinely screen for hundreds of compounds in a single analysis. And by taking advantage of productivity enhancements such as Agilent's GC Capillary Flow Technology, easy-to-use software tools and ultra-fast Rapid Resolution LC, you can significantly shorten your analysis time.

Result? You'll not only boost your lab's productivity; you'll reduce your cost per sample.

Pesticides Workflow

Sample Prep	Instrument Options	Screening	Confirmation	Quantification
QuEChERS Extraction Clean-up	**GC/MS** ***Target and non-target, volatile and semi-volatile compounds*** 	• Backflushing improves retention time precision, eliminates ghost peaks, 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
	LC/QQQ ***Target polar or moderately polar compounds*** 	• Highly selective, sensitive 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 chromato-grams provide accurate MS and MS/MS quantification • High dynamic range to quantify wide range of concentrations

Applications support and deep regulatory knowledge

Agilent scientists work closely with major testing laboratories and regulatory agencies. This in-depth experience can be a valuable resource for your lab, helping you address your most demanding analytical and productivity challenges.

GC and GC / MS — Speed up and simplify pesticide analysis in complex matrices

Agilent GC-based technologies provide accurate, sensitive detection—even in complex food matrices. Advanced analytical capabilities help you get more information from every run, and with the widest selection of inlets, detectors, columns, supplies and sample introduction choices, Agilent delivers an unbeatable combination of performance and productivity.

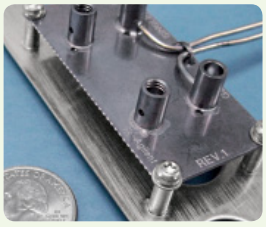
- Get more done in less time, at the lowest possible cost per sample, through faster oven cycle times and advanced automation and maintenance features
- Lower detection limits in complex matrices using Trace Ion Detection technology
- Simplify in-oven connections and improve analytical results with Agilent's exclusive Capillary Flow Technology
- Save hours of analysis and simplify the data review process with powerful Deconvolution Reporting Software option and Pesticide Library

A complete technology portfolio

Agilent offers today's widest range of solutions for pesticide residue analysis, both for target and non-target compounds. We can help you select the Agilent-reliable platform and the method that best meets your needs and your budget, while also giving you the lab management benefits of a single trusted source of supply.

Agilent Capillary Flow Technology. Something new in GC!

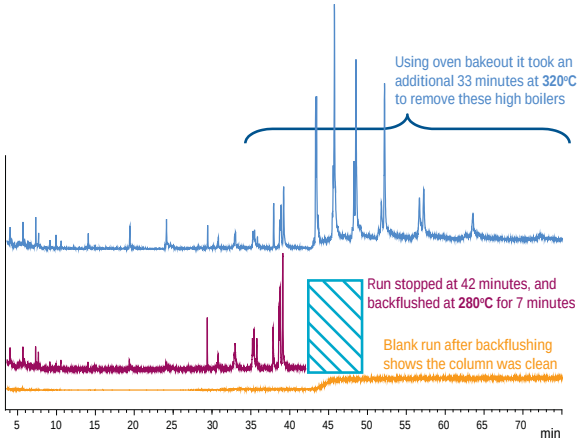
Agilent's proprietary Capillary Flow modules enable reliable, leak-free, in-oven connections. Available in a number of useful configurations, these inert, low-mass, low-dead volume devices not only make it easy to make secure connections; they give you the ability to precisely divert your gas flow, where and when you want. This opens the door to valuable techniques such as flow splitting, backflushing and Deans switching that can improve your analytical results, as well as save time and resources.



Backflushing shortens analysis time by 33 minutes

In this analysis of pesticides in milk extract, *the top trace employing oven bakeout takes an additional 33 minutes at 320°C to remove the high boilers that elute after the analytes of interest. Backflushing (middle trace) removes all the high boiling components in seven minutes, at only 280°C.*

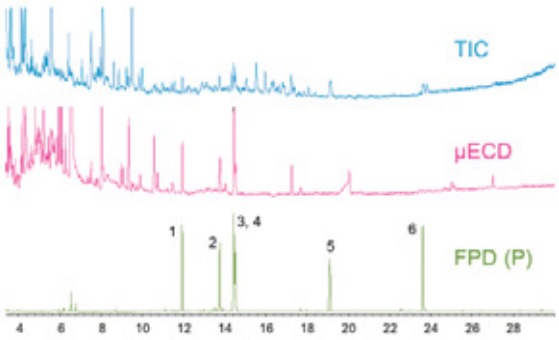
Backflush capability improves data quality, while shortening cycle time and increasing column life. It reduces ion source contamination by keeping excess column bleed and heavy residues from being introduced into the MSD. It also eliminates ghost peaks, providing a significant improvement in data integrity. (Agilent 7890A GC with Agilent 5975C MSD and Agilent J&W HP-5ms GC column)



Three total ion chromatograms comparing the results with and without backflush.

Screening and quantification in the same run

Agilent's Capillary Flow 3-Way Splitter consolidates a multi-instrument, multi-injection analysis into a single injection. *In addition to offering significant timesaving, the dual-detector (µECD and FPD) method provides excellent sensitivity and selectivity that allow for both screening and quantitation of trace level pesticide residues. (Agilent 7890A GC with Agilent 5975C MSD and Agilent J&W HP-5ms GC column) (1)*

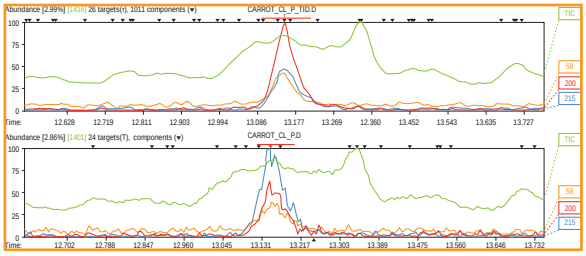


1. *Phorate*
2. *Terbufos*
3. *Diazinon*
4. *Disulfoton*
5. *Fenthion*
6. *Phenamiphos*

Trace Ion Detection lowers MDL in complex matrices

Agilent Trace Ion Detection (TID) technology provides enhanced spectral fidelity and higher library match quality *in this analysis of carrot. With TID enabled (top), a clear AMDIS hit was achieved for atrazine; without TID (bottom), atrazine was missed as a poorly defined component under a larger peak.*

Trace Ion Detection reduces false negatives and enables higher confidence in detecting trace level residues in complex matrices by reducing noise and improving signal-to-noise ratio. In addition, the technology dramatically reduces the number of manual interventions during peak integration. (Agilent 7890A and 5975C GC/MSD) (2)

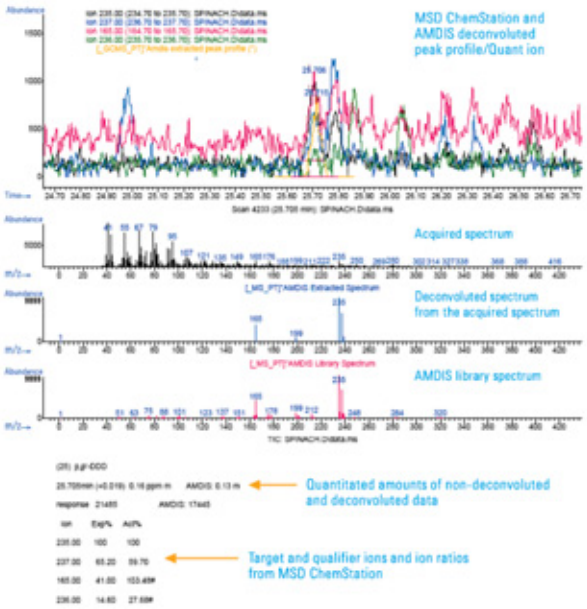


(1) 5989-6007EN: Using RTL and 3-Way Splitter to Identify Unknowns in Strawberry Extract

(2) 5989-7670EN: Replacing Multiple 50-Minute GC and GC-MS/SIM Analyses with One 15-Minute Full-Scan GC-MS Analysis for Non-targeted Pesticides Screening and >10x Productivity Gain

Deconvolution Reporting Software (DRS) saves hours of data review

DRS fully integrates Agilent's GC/MSD ChemStation and the NIST Mass Spectral Search Program with the NIST MS Library and AMDIS. *The deconvoluted, or "cleaned," spectra improve library search results against AMDIS or other databases, and also ensure higher quality quantification. Using DRS, this example of incurred trace level pesticides in spinach screened 927 compounds—and found 10 hits—in just 2 minutes. (Agilent 7890A GC with Agilent 5975C MSD)*



DRS software quickly finds and quantifies compounds hidden in complex matrices, as shown in this analysis of spinach.

DRS Pesticide Libraries (full spectral and SIM libraries in both Agilent and AMDIS format) have been expanded to include:

- *Japanese Positive List Pesticides (430 compounds)*
- *Pesticide and Endocrine Disruptors (927 compounds)*

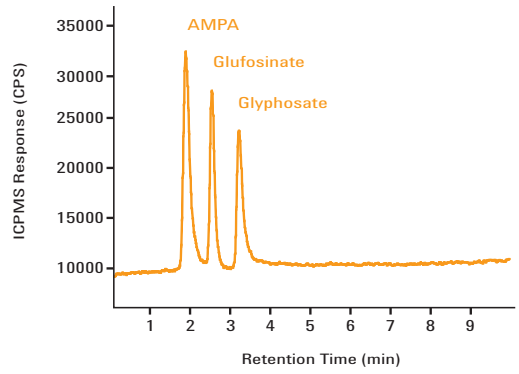
Hyphenated ICP-MS—Fast, confident, element-specific screening and quantification

- 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	Glufosinate	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 %

LC and LC / MS—Fast, sensitive analysis plus accurate ID and quantification

Agilent LC/MS gives you sensitivity you can use to confirm and quantify a large number of pesticides in food matrices. The combination of accurate-mass TOF or Q-TOF and Triple Quadrupole technologies lets you optimize screening, confirmation and quantification of target and non-target pesticides.

Agilent Series 1200 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. MRM of two transitions per compound provides confirmation and low detection limits to meet all regulatory requirements.

Agilent 6220 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 pesticides.

Agilent 6520 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.

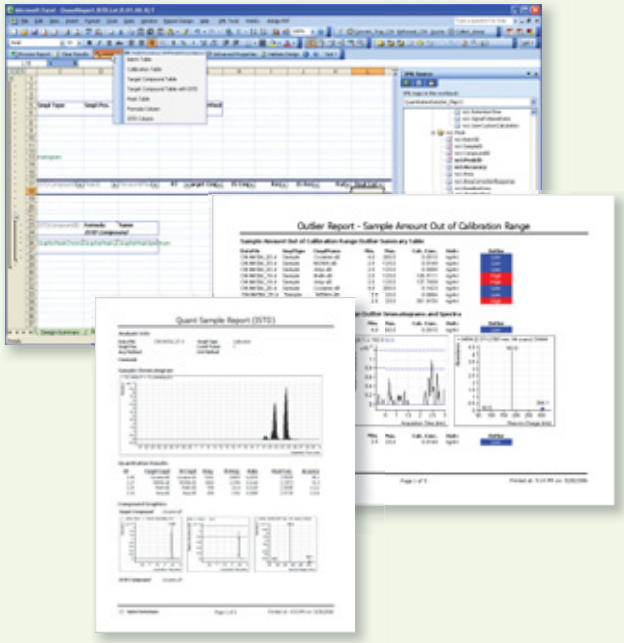
Combination of TOF and Triple Quadrupole offers maximum power for unlimited target and non-target compound screening and for meeting regulatory quantification requirements; TOF provides full spectra and accurate mass for searching databases, and QQQ provides MS/MS for confirmation and quantification.

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.

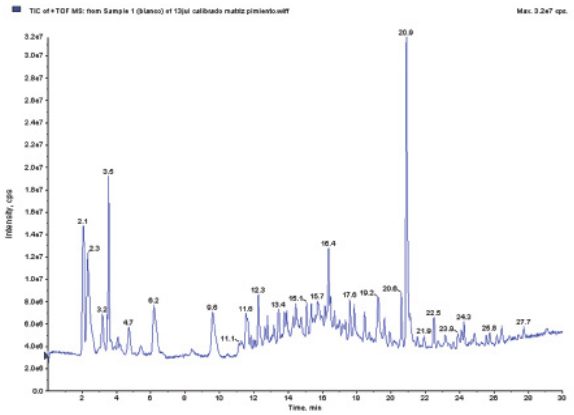
The software incorporates advanced feature extraction, data mining and data processing tools that let you rapidly and accurately extract the information you need from the compounds in your samples.

Reporting is fast and flexible, using preconfigured templates or customized reports in the familiar Microsoft® Excel user interface.

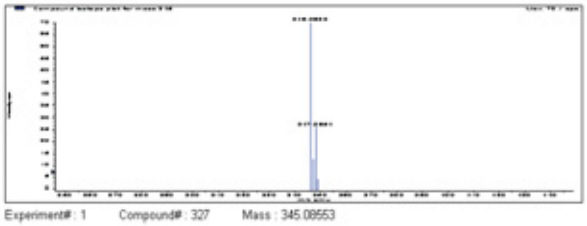


Accurate-mass LC-TOF screening of an unlimited number of pesticides

In this analysis of pepper, Agilent's Accurate Mass capability provides added compound selectivity; the system's higher resolution provides added interference selectivity. Sensitivity is the same regardless of number of compounds screened. ***Non-targeted compounds can be automatically flagged for subsequent database search and identification*** *using Agilent's Molecular Feature Extractor (MFE) and exact mass databases. (Agilent 1200 HPLC with Agilent 6220 TOF and ZORBAX Eclipse XDB-C8 4.6x 150mm, 5µm) (3)*



Blank pepper sample showing complexity of the sample; approximately 3,000 accurate mass peaks were detected in this sample at S/N of 10:1 or greater.



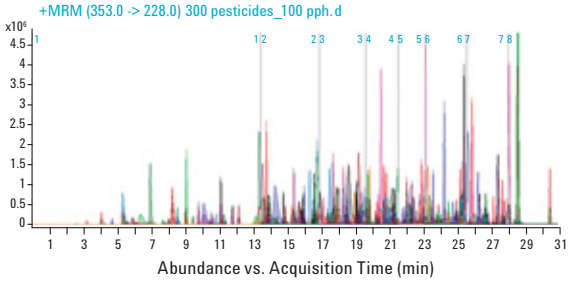
Mass Value = 345.08553

#	Formula	Compound	Mass	Error (mDa)	* Error (ppm)	Ret. Time Error	Description
1	C15H15N3OClF3	Triflumizol	345.08557	-0.04	-0.1	-0.02	

Example of a report from the exact mass database search.

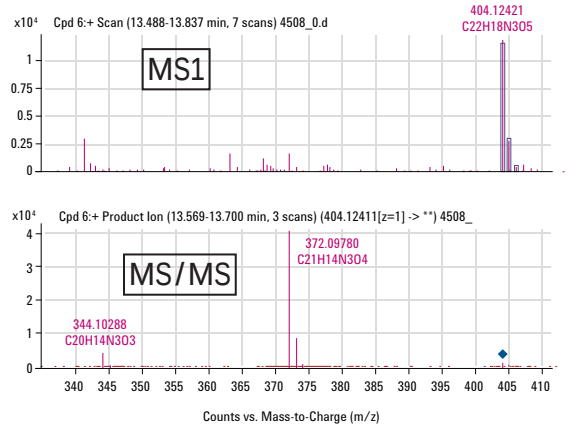
Screen and confirm 300 pesticides in a single run

LC/MS/MS MRM method detects 300 pesticides *spiked in a food extract at LOD of 10 ppb, the EU standard for baby food. The analysis demonstrates the capability of the Agilent LC/QQQ MS for rapid, reliable screening and confirmation at trace levels. (Agilent 1200 RRLC with 1.8 micron Agilent ZORBAX SB C-18 Column, Agilent 6410 QQQ) (4)*



High-confidence confirmation using both MS and MS/MS spectra

For confident confirmation of non-targets, the 6520 Q-TOF system can generate formulas for ions in both MS1 and MS/MS spectra. The system achieves low ppm (0.25 ppm in this example) mass accuracy, even in MS/MS mode.



MS/MS Formula Details: Compound 6 C22H17N3O5

m/z	Formula	Abund%	Difference (ppm)	Loss Mass	Loss Formula
344.10288	C20H14N3O3	8.08	0.25	60.02113	C2H4O2
372.09781	C21H14N3O4	91.92	0.22	32.02621	CH4O

(3) 5989-5496EN: Automated Screening of 600 Pesticides in Food by LC/TOF MS Using a Molecular-Feature Database Search

(4) 5989-5469EN: Multiresidue Analysis of 100 Pesticides in Food Samples by LC/Triple Quadrupole Mass Spectrometry

High performance columns and supplies for every pesticide analysis need

For every analytical requirement—from leading-edge methods development to routine QA/QC—our full portfolio of GC and LC columns gives you the sensitivity, accuracy and reliability required for successful pesticides analysis. We can help you increase your productivity in sample preparation, too, with industry-leading solid phase extraction (SPE) products including the most popular Florisil and C-18 cartridges that can streamline and simplify your lab's food analysis workflows.

The Agilent Value Promise—10 years of guaranteed value

In addition to continually evolving products, we offer something else unique to the industry—our 10-year value guarantee. The Agilent Value Promise 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. Not only does Agilent ensure a safe purchase now, we help ensure your investment is as valuable to you in the long run.

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Additional Application Notes and Technical Overviews on Pesticide Analysis

The following is a partial library of Agilent application notes related to pesticide analysis. For a complete listing, please visit: **www.agilent.com/chem**

GC and GC/MS

5989-1335 Analysis of Organophosphorus Pesticides with Agilent 6820 Gas Chromatograph/Nitrogen Phosphorus Detector

5989-1334 Analysis of Carbamate Pesticides Using Agilent 6820 Gas Chromatograph/Nitrogen Phosphorus Detector

5989-7436 Screening for Pesticides in Food Using the Japanese Positive List Pesticide Method: Benefits of Using GC/MS with Deconvolution Reporting Software and a Retention Time Locked Mass Spectral Database

5989-1716 New Tools for Rapid Pesticide Analysis in High Matrix Samples

5989-1100 Validated Multi-Residue Method for Extraction and Analysis of Trace-Level Pesticides in Surface Water

LC and LC/MS

5988-5445 Creating and Using a Performance-Based LC/MSD Mass Spectral Library with NIST MS Search Software

5988-8595 Validated Method for the Determination of Phenyl Urea and Triazine Herbicides in Portable and Groundwater by LC/MS Using Selective Ion Monitoring

5988-6085 Analysis of Components, Contaminants, and Impurities in Fungicide Formulations by GC/MS and LC/MS

5989-5320 Determination of Pesticides in Water by SPE and LC/MS/MS in Both Positive and Negative Ion Modes

5989-5459 Determination of 44 Pesticides in Foodstuffs by LC/MS/MS

5989-7409 Superior Molecular Formula Generation from Accurate-Mass Data

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