

AGILENT FOOD SAFETY SOLUTIONS

Use the latest technologies to **protect lives** and **livelihoods**





Agilent Technologies

The pressure to meet stringent food safety standards and regulations has never been greater

Globalized food production, opportunistic pathogens, and aging populations have combined to cause *tens of millions* of food-borne illnesses each year.





In 2006, **E. coli contamination in spinach** cost California farmers more than \$70 million. *(AP)*

Melamine in milk sickened more than 13,000 Chinese children in 2008. *(CNN)*





A 2008 outbreak of **salmonella in tomatoes** resulted in more than \$100 million in losses to American farmers. *(Farm Press)*

The 2010 explosion of a drilling rig in the Gulf of Mexico – and the subsequent oil leak – threatens to **contaminate seafood supplies** for years to come. *(Time)*

Like you, Agilent is on the front line in the battle to safeguard the world's food supplies

As the food industry's premier measurement company, Agilent is uniquely positioned to help you meet *current* and *future* challenges with chemical *and* biological technologies such as:

- Powerful GC/MS and LC/MS instruments for existing and emerging applications
- LC/Q-TOF systems that support your discovery efforts by allowing you to identify, characterize, and quantify low molecular-weight compounds and biomolecules
- GC and LC systems to suit your lab's unique analytical demands and workload
- A complete line of molecular spectroscopy instruments and supplies for identification and quantification
- **Reliable bioanalysis tools**, such as PCR/RFLP species identification and MassCode PCR techniques made possible by MS detection
- High-performance autosamplers and integrated systems that process more samples, faster
- SPE products that extract and concentrate samples from complex matrices
- **High-speed, high-resolution LC/MS columns,** such as Poroshell 120 and ZORBAX Rapid Resolution High Definition, that help you meet complex analytical demands
- An ongoing application of existing technologies for the analysis of pesticides, veterinary drugs, mycotoxins, dioxins, trace metals, allergens and other categories

In addition, Agilent continually partners with global food industry leaders – including commercial laboratories, government agencies, and universities – to solve problems and bring new applications to light.

Inside: our complete food safety portfolio – with new applications

GC Applications FAMEs, plaguicides, PCBs

GC/MS Triple Quadrupole and GC/MS Applications Melamine, pesticides

LC Applications *Lipids, dyes, oils*

LC/MS and HPLC/QQQ Applications Pesticides, aflatoxins, mycotoxins, veterinary drugs

Atomic Spectroscopy (AA, ICP-OES, ICP-MS) Applications Heavy metals, trace elements, fertilizers

Molecular Spectroscopy

(NMR, Fluorescence, FTIR, UV-Vis) Applications Supplement adulteration, photosensitive samples, ethanol, enzymes

Biological Applications Speciation of fish, rice, meat, and wheat; MassCode PCR

Sample Preparation and Chromatography Columns QuEChERS, SPE, columns, and supplies

Agilent Services

Back Cover





Gas Chromatography Confidently execute your most specialized applications

For more than 40 years, Agilent GC systems have been designed with one objective – to help you achieve reliable results. We have consistently placed advanced separation capabilities, powerful productivity features, and real-time self-monitoring instrument intelligence within the reach of every lab – including:

- Industry leading GC reliability: integrated electronics and advanced mechanical design provide for superior reliability.
- Unsurpassed retention time reproducibility: full electronic pneumatics and oven temperature controls lets you quickly and easily set pressures and flows, while our 5th-generation EPC and digital electronics keep your results consistent from run to run.
- Easy method setup: powerful, user-friendly software simplifies system operation and minimizes training costs.
- Higher productivity: faster oven cool-down and faster GC oven ramps let you get more done in less time, at the lowest possible cost per sample.

· Advanced supporting techniques:

- Capillary flow and backflush technologies let you manipulate gas flows to power advanced separation techniques and reduce analytical cycle times.
- Agilent Low Thermal Mass (LTM) technology provides direct rapid heating and cooling of capillary columns to greatly boost GC productivity.
- New multimode inlet provides multiple split/splitless modes, temperature ramping and large volume injection.
- Fast, precise automated sample introduction systems also include sample preparation capabilities to help eliminate variability and rework.



The Agilent 7890A Gas Chromatograph brings important separation capabilities and productivity features to the industry-leading Agilent GC platform.







15. Endosulfan II 16. 4,4'-DDD 17. Endrin aldehyde

13. Dieldrin

14. Endrin

- 18. Endosulfan sulfate 19. 4,4'-DDT
- 20. Endrin ketone
- 21. Methoxychlor
- 22. Decachlorobiphenyl (SS)
 - SS Surrogate Standard

Plaquicides are a broad class of agrochemicals used to control and prevent harmful agricultural pests and diseases. Here, trace-level chlorinated plaguicides were analyzed using an Agilent J&W HP-1ms Ultra Inert Capillary GC column. The symmetrical peak shapes and excellent signal-to-noise ratios at trace levels emphasize the value of column inertness. Note the excellent linearity: R² values were 0.998 and higher on both primary and confirmatory columns.



GC/MS/MS and GC/MS High sensitivity and selectivity for dirty samples and demanding environments

Whether your gas phase applications goal is target compound quantitation or the discovery of unknowns, the best way to achieve the critical combination of low detection limits and high-speed measurement is with a system designed *specifically* for GC/MS/MS applications.

Agilent Triple Quadrupole GC/MS systems are designed from the ground up – not adapted from an LC/MS system – and include a proprietary solid inert ion source, proven quartz quadrupoles, innovative collision cell design, and triple-axis detector. Together, these features deliver:

- **Excellent reliability:** a high-temperature, gold-plated quartz quadrupole allows high-boiling components to be boiled away and not deposited on the quadrupoles.
- **High spectral fidelity** without the "cold spots" that can lead to condensation and signal loss.
- Flawless GC/MS integration preserves sample integrity during transit.
- **Complete confidence in your results** with data analysis, review, and reporting tools designed specifically for triple quadrupole GC/MS.
- Faster analysis: acquisition speeds of up to 500 MRM transitions per second match the front-end performance of the fastest chromatography without compromising data quality.





Triple quadrupole mass spectrometry drastically reduces or eliminates matrix interferences that impede the accuracy and detection limits of SIM methods.

In this example, a TIC chromatogram (top) was acquired in Multiple Reaction Monitoring (MRM) mode for 360 pesticides in a vegetable extract. (Each MRM segment is indicated by a grey marker line.) An enhanced overlay (bottom) shows all the MRM segments for compounds in a selected part of the analysis. As you can see, MRM mode allows for quantification of many coeluting analytes between 11.5 to 14.3 minutes.





Comparison of detection of 0.25 ppm melamine in soy meal using the Triple Quadrupole GC/MS method (a), versus the GC/MS SIM method at 2.5 ppm (b). The quantifying transition used with the Triple Quadrupole GC/MS method was m/z 327.1 \rightarrow 171.1, and the qualifying transitions were m/z 342.1 \rightarrow 295.1 (2.5% of the peak area of the quantifying transition) and m/z 342.1 \rightarrow 217.1 (4.8% peak area). The uncertainty bands are shown in (a) as well. The SIM ions used in the GC/MS method were m/z 342.2, 327.2, and 171.1 (b).

In response to the threat of food adulteration with melamine, many countries have established strict allowable limits for this adulterant. For example, the U.S. FDA maximum residue limit (MRL) is 1 part per million (ppm) for infant baby formula and 2.5 ppm for other products.

Here, the Agilent Triple Quadrupole GC/MS system screened, quantified, and confirmed the presence of melamine and its analogs in approximately 15 minutes – while demonstrating a sensitivity of 0.25 ppm, and a linearity of quantification up to 2.5 ppm. The accuracy of quantification was greater than 97%.

Count on the best GC/MSD systems in the business for dependable, consistent, and affordable routine analysis

Agilent's 5975 Series GC/MSD lets you spend *more time* running your analyses and *less time* maintaining your system. It brings together these essential elements for trace-level analysis:

- Advanced capabilities: a solid inert ion source, quartz quadrupole analyzer, and high signal-to-noise Triple-Axis Detector dramatically improve MS resolution, spectral integrity, and detection limits.
- **Higher throughput:** comprehensive automation, faster separations, and shorter detection cycles enable you to process more samples in less time.
- **Maximum uptime:** real-world engineering and system intelligence features ensure easier upkeep, predictive support, enhanced self-maintenance and powerful remote diagnostics.



Deconvolution Reporting Software (DRS) lets you quickly identify and quantify compounds in high-matrix samples

Data review and processing are the greatest bottlenecks in today's high-volume laboratories. In fact, even an experienced analyst can take more than *one hour* to review and confirm one data file and identify target compounds from a high-matrix background.

DRS gives you the tools to discover more compounds and contaminants faster – and with greater precision

Together with Retention Time Locking, this automated reporting package *quantitates* and *screens* for compounds more quickly than you ever thought possible. It combines the power of three distinct compound identification programs:

- 1. **MSD ChemStation** Identifies and quantifies targets based on locked retention time and four qualifier ions.
- AMDIS 32 Identifies targets based on deconvoluted full spectra, and qualifies targets using Retention Time Locking.
- 3. **NIST 05** Confirms targets using deconvoluted full spectra from AMDIS, along with a 163,000-spectra library.

Additionally, DRS condenses the results generated by these software packages into one easy-to-read report. The process takes only 2 to 3 minutes per sample and is more reliable than conventional GC/MS methods.



The Agilent 5975C Series GC/MSD combines innovative hardware and software features to optimize performance from injection to final report – and to take your LODs and LOQs to an all-time low.





Here, a green pepper extract was spiked with 229 pesticides, of which approximately 148 could be analyzed by GC/MS. The total ion chromatogram for this extract is shown in the first box.

The second box shows the undeconvoluted spectrum at 17.840 minutes (top) and the deconvoluted spectrum (middle). The deconvoluted spectrum is an excellent match to the fenhexamid library spectrum (bottom).





Raw (dirty) spectrum, deconvoluted (clean) spectrum, and library spectrum of cabaryl found in peach, from AMDIS.



An analysis of cabaryl in peach using AMDIS. The top spectrum (scan) from the TIC is the only spectrum that would be available for library searching without deconvolution – obviously quite useless. Compare that with the middle box, which shows the deconvoluted spectrum, and the bottom box, which shows the target compound's library spectrum.

Keep in mind that deconvolution lowers the demand for chromatographic resolution. Therefore, the Agilent system with Deconvolution Reporting Software allows you to shorten your chromatographic run times – increasing your productivity.



Liquid Chromatography Flawlessly execute chemical and biological applications

When you apply LC technologies to the analysis of substances such as mycotoxins, marine toxins, and allergens, precise retention times and accurate quantitation are critical. Agilent LC systems are designed to generate reliable data in real food samples – regardless of variables such as pressure, flow, column dimension, and particle size.

Whether you need a "workhorse" LC system for routine analysis or a sophisticated, high-resolution LC/MS instrument, Agilent LC systems deliver ultimate resolution and sensitivity, while helping you boost your separation power per time. They also ensure easy method transferability between systems, without redevelopment or revalidation.

Agilent 1290 Infinity LC: *Infinitely more powerful* Now you are no longer limited in your choice of column dimension, particle type, mobile and stationary phase, flow rate, or pressure. Agilent's 1290 Infinity LC gives you the foundation for method transfer to or from any Agilent or non-Agilent UHPLC or HPLC system. You also get the confidence that comes with high-performance features like binary pump, active damping, and Infinity Diode Array Detector.

Agilent 1260 Infinity LC: *Infinitely more confident* Finally – an LC system that meets your demands for chromatographic performance while matching the constraints of your budget. The Agilent 1260 Infinity LC sets a new standard for analytical HPLC with a 600 bar, high-speed 80Hz detector, and up to 10x greater sensitivity. It is also 100% compatible with HPLC and RRLC.

Agilent 1220 Infinity LC: *Infinitely more affordable* With its 600 bar pressure capabilities and 80 Hz detector speed, the Agilent 1220 Infinity LC gives you RRLC capabilities at an HPLC price. Its integrated design is both robust and easy to use, and the system is fully compatible with HPLC and RRLC.



Agilent 1220 Infinity LC



Agilent 1260 Infinity LC



Agilent 1290 Infinity LC

A high-resolution separation of complex lipids (triglycerides) using the Agilent 1290 Infinity LC with ZORBAX RRHT and RRHD 1.8 µm columns.

The low flow rate and high resolution also make it easier to interface this separation with high-resolution TOF and QTOF mass spectrometers for reliable peak identification and compositional data.

Sudan dyes are Azo-dyes and classified as Group 3 of the potential carcinogenic compounds based on findings of the IARC (International Agency for Research on Cancer).

Here we see how the Agilent 6140 Single Quadrupole LC/MS was used in SIM mode to analyze the Sudan red compounds with highest sensitivity. The target masses were 215, 249 and 277, and the detection conditions were evaluated by injecting 5 μ L of the standard sample. The resulting chromatograms show that the max pressure achieved was approximately 825 bar.



Analysis of soybean triglycerides on the 1290 Infinity LC. Sample: soybean oil, 10 mg/mL, 30 μg on-column. Conditions: 0.29 mL/min, 10% to 40% MTBE vs. ACN at 42 minutes, hold to 55 minutes, run 60 minutes, 210 nm UV. ZORBAX RRHD StableBond C18, 2.1 x 400 mm (2-150 and 1-100 mm length in series), 1.8 μm, 20 °C. Operating pressure 730 bar.



Overlay of standard and sample extract chromatograms using Agilent 6140 single quadrupole MS in SIM mode.



LC/MS Confidently perform discovery, quantitation, and target compound analysis

From best-in-class LC technologies, to MS spectral accuracy and precision, to TOF-MS systems that let you identify empirical formulas *without a spectral library*, Agilent LC/MS instruments are specifically designed to help you meet tough qualitative and quantitative challenges. Our powerful data analysis tools and workflow productivity enhancements include:

- Jet Stream technology increases LC/MS and LC/MS/MS sensitivity five-fold by improving the spatial focusing of electrospray droplets.
- Maximum ion generation and transmission across a broad mass range ensure low detection limits and quantitation for the widest range of sample types.
- Automated method development and optimization: MassHunter Optimizer software automatically finds the best transitions for each compound and determines the optimal fragmentor voltage and collision energies.

Agilent 6100 Series Single Quadrupole LC/MS:

Proven day-to-day performance and reliability

Whether you're performing routine QC or research-level applications, Agilent 6100 Series Single Quadrupole LC/MS systems put the speed sensitivity, selectivity, and information content of mass spectrometry into a compact package that integrates seamlessly with Agilent's ChemStation LC control.

Agilent 6400 Series HPLC/000:

Clearly better sensitivity for better results

The 6400 Series HPLC/QQQ delivers sub-Femtogram sensitivity for trace analysis, and features an innovative dynamic MRM acquisition mode that lets you quantify up to 4,000 compounds without manually setting up time segments.

Agilent 6200 Series Accurate-Mass TOF:

Putting the power of ultra-high definition behind your discovery

Our 6200 Series Accurate-Mass Time-of-Flight (TOF) LC/MS systems combine the speed you need for ultra-fast UHPLC separations with the MS and MS/MS performance you need to glean critical data from challenging samples. Features like **sub-ppm mass accuracy** reduce the likelihood of false positives, while resolving powers of up to **20,000** distinguish desired compounds from interferences.

Agilent 6500 Series Accurate-Mass Q-TOF:

Unambiguous structural clarification and target identification

With their sub-ppm mass accuracy and ultra high definition, Agilent's 6500 Series Accurate-Mass Q-TOF systems can help you reduce uncertainty, minimize false positives, improve database search scores, and generate molecular formulas for unknowns. Their enhanced resolving power of up to **40,000** reliably detects mass peaks of interest, while a dynamic range of up to five orders in-spectrum uncovers low-abundance compounds in the presence of higher-abundance components.





The following chromatograms demonstrate how the application of high-end HPLC systems – combined with next-generation triple quadrupole mass spectrometers – facilitate the analysis of contaminants in challenging matrices.

This example shows the quantifier and qualifier transition signal for fluazifop and propoxur in a spiked baby food sample. From these traces, it is clear that excellent selectivity and sensitivity were obtained, while the relative response of the quantification and qualifier transitions are within the limits for positive identification.



Meet the quantitation and confirmation demands of today's emerging applications



Aflatoxins are carcinogenic mycotoxins produced as metabolites by the fungi Aspergillus flavus and Aspergillus parasiticus. They can be found in foods such as grains, nuts, and spices.

Traditional aflatoxin analysis techniques lack confirmation power; conversely, Agilent HPLC/QQQ systems can achieve *simultaneous quantitation and confirmation* using multiple ions.

In this method, the top overlay represents an extract with Aflatoxins B_1 , B_2 , G_1 , and G_2 at concentrations of 1 ppb with isotopically labeled internal standard concentrations of 2.5 ppb shown in the bottom overlay. Confirmatory ions are shown for all compounds. Note that all LODs were less than 140 ng/g – less than 530 fg on-column.

The power of Q-TOF for screening and confirming compounds you didn't know were there. Here, a strawberry extract was spiked with a pesticide mix, and analyzed using an Agilent 1200 Series SL LC with an Agilent 6520 Q-TOF.

Top: EIC generated from a standard of over 200 pesticides detected in a "find compounds by molecular feature" extractor with database search. This sensitive configuration meets the stringent demands of multiresidue analysis.

Bottom: High-quality mass spectral data collected at a rate of 10 spectra per second.



Extracted compound chromatogram (from compounds found by MFE) of 200 pesticides using the Agilent 1200 Series SL LC with the Agilent 6230 TOF.



Example mass spectrum from data on 3 min run with Agilent 1290 Infinity LC an Agilent 6540 Q-TOF. Note the mass resolution at 10 spectra per second.





Atomic Spectroscopy (AA, ICP-OES, ICP-MS) Industry-leading technologies that fit your workflow and analytic needs

Some metals are essential to human nutrition; others are highly toxic. For this reason – and to confirm a food's origin and authenticity – trace metals are monitored at nearly every stage of food production.

Traditionally, the analysis of metals in foods requires multiple techniques to cover the range of elements, concentrations, and food types. This approach is both slow and expensive.

In contrast, atomic spectroscopy permits large numbers of samples to be quickly screened for total toxic metals. Samples that are found to contain trigger levels of metals with important chemical forms (or species) can be analyzed further using Agilent-supported speciation techniques, such as LC-ICP-MS or GC-ICP-MS.

Clearly better... together.

The acquisition of Varian – a company with more than 60 years of atomic spectroscopy innovation – has added AA and ICP-OES instruments to Agilent's existing ICP-MS products. The range now includes:

- Atomic Absorption Spectroscopy (AA) with superior flame, graphite furnace, and vapor generation precisely matched to your lab's analytical needs.
- Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES) with radial or axial plasma viewing, and simultaneous wavelength measurement using a single view for extended dynamic range and reduced interference.
- Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) with high-matrix tolerance, 9 orders dynamic range, and He mode collision/reaction cell for reliable interference removal in any sample.

Now you can find the most accurate, robust, and reliable Atomic Spectrometry instruments *all in one place*.



Agilent's 7700 Series ICP-MS provides unparalleled accuracy in high-matrix samples, redefining He mode cell performance with a revolutionary 3rd generation cell design – the ORS³.

With near-universal elemental coverage, and wide dynamic range, the 7700 operating in He mode delivers the highest accuracy and productivity in the analysis of trace elements in foods and related sample types.



Agilent's 700 Series ICP-OES offers the finest performance, speed and flexibility.

The axially-viewed 720/730 provides maximum sensitivity for trace-level applications. Using MultiCal, major elements can be simultaneously quantitated accurately, providing the dynamic range needed for determination of major, trace and toxic elements in food and agricultural samples.



The Agilent 240FS/280FS AA with GTA 120 Graphite Furnace is built for determining very low detection limits (low ppb or ppt). The system is particularly useful when only a small number of analytes are required, or when sample amounts are extremely small.

Results for NIST 8435 Milk Powder using Fast Sequential AA

049 0.914	0.8	0.916
6 820	0.7	812
047 1.364	1.0	1.351
040 0.366	0.8	0.372
oles		
	047 1.364 040 0.366 vles	047 1.364 1.0 040 0.366 0.8 oles

Accurately determining major and toxic elements in milk samples is a public health necessity. Here, a NIST 8435 whole milk powder sample was measured using Fast Sequential AA after preparation in a trichloroacetic acid solution. Results show good agreement with the certified values, and were achieved with a *30% time savings* compared to conventional AA.

Results for fertilizer samples using ICP-OES

Sample labels Units	As 188.980 mg/kg	Expected mg/kg	Ca 370.602 %	Expected %	Cd 214.439 mg/kg	Expected mg/kg	Cr 267.716 mg/kg	Expected mg/kg
Sludge B Magruder 4B Magruder 6B	141 2.05 5.75	141 1.75 5.66	0.0233 2.71 4.93	0.0242 2.48 5.94	0.64 12.31 1.51	NA NA NA	110 125.2 50.88	111 132.6 51.08
Sample labels Units	Cu 327.395 %	Expected %	Fe 261.382 %	Expected %	K ₂ 0 404.721 %	Expected % K ₂ O	Mg 279.078 %	Expected %
Sludge B Magruder 4B Magruder 6B	0.0407 0.0461 1.010	0.0398 0.0307 0.976	0.012 0.350 0.500	0.014 0.400 0.500	NA 11.02 21.37	NA 10.54 20.54	12.6 1.62 0.53	12.2 1.64 0.62
Sample labels Units	Mn 294.921 %	Expected %	Na 589.592 %	Expected %	P 214.914 % P ₂ 0 ₅	Expected % P ₂ O ₅		
Sludge B Magruder 4B Magruder 6B	0.51 0.036 0.014	0.48 0.039 0.015	0.94 0.31 0.57	0.94 0.29 0.58	0.51 8.1 9.1	0.50 9.1 9.9		
Sample labels Units	Pb 220.353 mg/kg	Expected mg/kg	Se 196.026 mg/kg	Expected mg/kg	Zn 213.857 %	Expected %		
Sludge B Magruder 4B Magruder 6B	6.8 1.16 1.88	5.7 2.18 2.15	NA 0.43 0.13	NA 0.44 0.12	0.0244 0.043 0.003	0.0249 0.048 0.003		

Fertilizers play a vital role in sustaining crop yields by supplying essential nutrients such as nitrogen (N), phosphorus (P_2O_5), and potassium (K_2O).

This table summarizes the results obtained when fertilizer samples were prepared by microwave digestion/extraction and evaluated for macro, secondary and micro nutrients by simultaneous ICP-OES. The combination of microwave and ICP-OES techniques resulted in fast, simple sample preparation and analysis, and required *only one* analytical system to measure all elements of interest.



	Determi	nation of tox	ic elements	in Iraditional	Chinese Medici	ne(ICIVI) usi	ng ICP-IVIS	
Name of	f sample	Gegen	Zhike	Guifudihuang	Huanglianshangqing	Jinsangsanjie	Naodesheng	Shugan
Element		Soup	San	Pill	Pill	Pill	Pill	Pill
Be	Found value	0.020	0.009	0.032	0.034	0.060	0.037	0.013
	RSD%	5.2	2.6	1.0	5.1	2.0	1.4	5.2
Cr	Found value	0.34	0.46	1.40	1.58	4.89	1.74	4.76
	RSD%	2.0	2.0	1.9	2.6	2.3	2.5	0.8
Mn	Found value	34.77	17.80	54.78 3	0.37	87.23	23.96	124.4
	RSD%	0.7	2.4	1.1	2.20	1.21	2.62	3.10
Ni	Found value	1.09	1.17	1.24	1.64	3.09	1.50	3.15
	RSD%	0.6	0.9	1.4	0.8	2.2	1.8	1.8
Cu	Found value	1.49	1.68	4.08	8.85	15.23	3.56	5.38
	RSD%	0.6	0.6	0.6	2.5	2.3	2.38	0.46
Zn	Found value	5.66	4.82	21.27	18.57	37.07	15.33	22.59
	RSD%	0.6	1.1	2.4	1.3	1.5	1.7	1.7
As	Found value	N.D.	0.26	0.46	0.79	0.89	0.56	29.14
	RSD%	1.6	1.4	3.9	3.5	5.7	3.3	1.5
Ag	Found value	0.0009	0.0008	0.005	0.007	0.079	0.006	0.007
	RSD%	5.3	6.3	2.1	5.8	3.5	5.6	4.3
Cd	Found value	0.022	0.042	0.10	0.11	0.15	0.077	0.082
	RSD%	5.5	1.5	1.2	2.7	1.9	3.6	2.0
Ва	Found value	5.86	8.94	15.32	44.76	167.8	136.7	12.98
	RSD%	1.1	1.7	1.4	2.1	2.8	0.3	0.9
Hg	Found value	0.003	0.002	0.85	0.088	0.027	0.076	5.05
	RSD%	6.8	5.8	3.3	5.5	5.0	3.5	0.6
TI	Found value	0.008	0.027	0.025	0.020	0.033	0.036	0.014
	RSD%	1.3	2.4	2.7	3.6	3.2	1.1	4.1
Pb	Found value	0.15	0.16	0.93	1.54	2.14	0.68	1.69
	RSD%	0.7	1.1	2.6	2.1	1.7	1.5	1.3

Analytical results of TCMs (n = 8). Unit: $\mu g g^{-1}$.

In the past, herbal remedies have been analyzed by a combination of time-consuming, costly spectroscopic methods, including atomic fluorescence spectroscopy (AFS) and atomic emission spectroscopy (AES).

Today, however, ICP-MS is fast becoming the technique of choice for element determination, because it delivers nearuniversal elemental coverage, low detection limits, and the widest dynamic range (nine orders of magnitude, from 1 pg/mL to 1000 μ g/mL).

Here, thirteen toxic elements were determined in seven Traditional Chinese Medicine (TCM) mixtures, using an Agilent ICP-MS, following sample preparation by microwave digestion. The study showed that some TCM preparations contained toxic elements that are well above legal limits. For example, the Shugan Pill exceeded both the limit for Hg (0.2 ppm) and As (2.0 ppm), as defined in the 2010 Pharmacopoeia of the People's Republic of China. Although it should be noted that total digestion of the sample does not give an accurate indication of patient exposure.

Satisfy your growing demands for analyzing large numbers of food samples, faster

Measuring the elemental content of foods took a giant leap forward with the introduction of Inductively Coupled Plasma Mass Spectrometry (ICP-MS). ICP-MS provides rapid multielement analysis at trace levels, breaking the bottleneck created by slower, single-element techniques such as graphite furnace atomic absorption spectroscopy (GFAAS). With unmatched matrix tolerance, 9 orders dynamic range, and reliable interference removal in He cell mode, the Agilent 7700 Series ICP-MS provides accurate measurement of all regulated elements in foods, regardless of the sample matrix.

The 7700 also offers simple coupling to Agilent LC and GC systems for high performance speciation applications, including monitoring toxic forms of elements such as As, Sn and Hg in foods.

As Speciation using LC-ICP-MS

In this separation, HPLC-ICP-MS was used to separate toxic inorganic forms of As (As(III) and As(V)) from the less harmful organic species. Separation of all 5 species in human urine was completed within 12 minutes. The method is robust enough for the analysis of undiluted urine with limits of detection of 0.1 μ g/L or less for the individual As species.



Sn Speciation using GC-ICP-MS

This chromatogram illustrates a mixed organo-tin standard containing 20 ng/mL (ppb) of each compound. The elution order is Sn, MBT, TPrT, DBT, MPhT, TBT, TeBT, TPeT, DPhT, TPhT.

GC-ICP-MS determination of Sn and Hg compounds can benefit from species-specific isotope dilution (SS-IDMS), which has the advantage of lower uncertainty than external calibration, and is independent of compound loss during extraction or derivatization.





Molecular Spectroscopy Identify. Confirm. Solve. Explore!

With the acquisition of Varian, Agilent has added depth, breadth, and expertise to our capabilities – including these fresh ideas for identifying and confirming target and unknown molecules in difficult matrices:

- Nuclear magnetic resonance spectroscopy (NMR): takes screening and characterization to a new level by revealing how atoms are *organized in space*.
- **UV fluorescence:** analyzes molecular fluorescence using a beam of ultraviolet light that excites specific electrons, causing them to emit lower-energy light.
- Fourier transform infrared spectroscopy: identifies functional groups based on their IR radiation absorption frequencies – a must for structural elucidation and compound identification.
- UV-VIS spectroscopy: provides direct, non-destructive measurements that enable both quantitative analysis and spectral data gathering.

NMR: Complete spectral analysis and interpretation

The Agilent 400-MR DD2 is your instrument of choice for fast, reliable NMR analyses in a compact footprint. It features:

- **DirectDrive electronic architecture** precisely captures RF and gradient events, and provides total pulse programming control. Demanding data acquisition sequences with numerous selective excitation events (such as Hadamard NMR) can be achieved with push-button ease, allowing you to spend less time on method optimization and more time analyzing your experimental output.
- **DirectDigital receiver system** makes quadrature detection obsolete by reproducibly delivering flat baselines and fewer artifacts *without extensive post-acquisition algorithms*. This unique receiver system also ensures reliable detection and quantitation of minor components in complex matrices with minimal sample preparation.
- Easy-to-use software simplifies your compound detection, confirmation, and quantitation including mixture analysis.

In addition, the Agilent 400-MR DD2 delivers outstanding cryogenic performance for longer stretches of uninterrupted uptime.



The Agilent 400-MR DD2 is your instrument of choice for fast, reliable NMR analyses in a compact footprint.

Fourier transform infrared spectroscopy: superior analytical performance under real-world conditions

Thanks to the addition of Varian, you can now find the fastest, highest performance Infrared (IR) systems under one name: Agilent. You can also find powerful, flexible software that allows you to transform your IR instrument into a dedicated analyzer that automates data collection and analysis. So you can identify more compounds, faster, and with greater clarity than ever before.

IR spectroscopy is an important identification and quantification method for the world's food, animal feed, pet food, and nutrition industries. The Agilent Cary 600 series of versatile, high-performance spectrometers and microscopes are designed for applications involving foods/beverages, flavors, food packaging, foodborne pathogens, edible oil testing, food contaminants/adulterants, fermentation control, vitamins, food additives, and nutritional supplements.





Vibrational spectrum of edible oil. FTIR is an ideal tool for QC/QA applications, such as measuring trans fat content using the AOAC method for classifying and discriminating food adulterants. It is also useful for Halal applications, as well as the analysis of emulsions in food and beverage processing.



 β -Lactoglobulin (β -lg) is the most abundant globular protein in milk, and the major component in the whey fraction of milk. In this example, the thermal properties of β -lg A (5% w/v) in deuterated phosphate buffer at pH 8.6 were investigated in real time by monitoring changes in the secondary structure using intuitive kinetics software. Shown is the stacked plot of deconvolved infrared spectra during heating from 40° C to 92° C. This information provides a useful model for studying the relationship between protein structure and function.





Fluorescence spectroscopy: pushing the limits of measurement

The Cary Eclipse Fluorescence Spectrophotometer leverages the world-class technology of Cary UV-Vis spectrometers. With its unique Xenon flash lamp, the Cary Eclipse is the *only* fluorescence spectrophotometer with room light immunity. Sample size need no longer be a restriction – just leave the sample compartment open while you are collecting data.

Specialized accessories for food-based applications are available, including peltier thermostat multicell holders, polarizers, fiber optic liquid, solid sampling probes, and a microplate reader capable of reading 96 and 384 well plates.



UV-Vis spectroscopy: the gold standard for research and reference

The Agilent family of Cary UV-Vis and UV-Vis-NIR spectrophotometers deliver unsurpassed photometric accuracy and linearity, superior optical stability, and the highest spectral resolution.

From QA/QC and remote fiber optic measurements, to method development, to fundamental and applied research, Agilent has the right UV-Vis system for your food chemistry needs. You can also choose from a wide range of accessories, such as peltier thermostat cell holders, autosamplers, fiber optic probes, and integrating spheres.

Measuring tannins in wine is critical to proper fermentation. The Cary 60 UV-Vis spectrophotometer, with its unique fiber optics and Xenon flash lamp, lets you bring the instrument to the sample - minimizing sample preparation without compromising data quality.

In addition, Cary Wine Analyzer software allows even nontechnical users to analyze wine samples in seconds – and perform sixteen internationally recognized tests for color density and hue, sulfur dioxide, citric acid, and glucose/fructose.





Surface reflectance estimates derived from hyperspectral data can be used to assess spatial variance in crop condition and biomass over large agricultural fields.

This comparison between healthy and etiolated wheat leaf spectra shows the distinct impact of pigment content on reflectance and transmittance. As you can see, visible red reflectance is reduced considerably in the etiolated leaves due to the inhibition of chlorophyll synthesis. The etiolated leaf spectra still exhibit a significant response drop in the visible blue region due to carotenoid leaf pigments, which develop even in the absence of light.



Biological Food Testing Harness the very latest methods to identify species, confirm pathogens, and detect allergens

Electrophoresis and PCR are two of the most common biological food testing techniques. Typically, the acid-PAGE (polyacrylamide gel electrophoresis) method is used in electrophoresis; however, highly skilled operators are needed to prepare, run, and scan the gels – and interpret band patterns. In addition, this routine method can take up to two days, which is too slow for many food applications in which decisions must be made within hours or minutes. Nucleic acid-based assays (including PCR) are increasingly being applied as rapid alternatives to conventional bacteriological culture techniques when testing for microbial pathogens.

Real-time quantitative PCR (qPCR) takes measurements *kinetically in real time*, conferring significant advantages over conventional PCR – including reaction speed, sensitivity and specificity. It also prevents cross-contamination by eliminating the need to open the reaction tubes for post-PCR analysis.



Multiplex pathogen detection

New developments in Mass Codes/qPCR enable you to open individual genes and react them with appropriate tags (primers). This allows you to access and manipulate DNA on a *chemical* level and identify unknown pathogens based on precise mass measurements.

Species identification

Heating and cooling proteins can cause them to fold and unfold, allowing you to force specific reactions or search for individual DNA sequences. For example, you can combine genetic data (from qPCR) with the 2100 Bioanalyzer's separation capability to accurately identify fish species.

Agilent's 2100 Bioanalyzer and qPCR products allow you to take advantage of quick, cost-effective nucleic acid-based methods for establishing food authenticity. You can also use the 2100 Bioanalyzer to generate follow-up quantitation estimates.

Common protein-based seafood speciation methods (such as isoelectric focusing) require a skilled analyst, cannot readily distinguish closely related species, and are unsuitable for processed foods. In contrast, DNA methods such as PCR-RFLP provide more objective, specific, and robust results, for highly processed or mixed samples.

Here, cod DNA extract was blended with tuna DNA in a 1:20 ratio; the mixture was then PCR amplified, and digested with Ddel. Cod peaks are circled in green, and can be identified by RFLP Matcher using a mixture algorithm.

The correct labeling of rice is critical to ensuring quality and regulatory compliance. In 2003, the UK Food Standards Agency carried out a surveillance exercise on basmati rice products using a DNA variety testing method with PCR amplification of eight rice microsatellite sequences. The survey found that 74% of the sampled products contained > 7% non-basmati varieties of rice.

Given the clear need for varietal verification, a bioanalyzer assay was developed to differentiate approved and non-approved rice varieties using three primer sets. As shown below, the assay can also use reference admixtures to estimate the level of non-basmati rice.

The combination of Agilent's 2100 Bioanalyzer and RFLP Decoder software generates highly reproducible data. This figure demonstrates the intralab method reproducibility for Alaskan pollock (A) and coley (B).









Sample Preparation Reliably extract and concentrate samples from complex matrices

Agilent Bond Elut QuEChERS Kits make sample preparation easier and more reliable

Pre-packaged Agilent QuEChERS Kits are an easy way to capture the time-saving benefits of QuEChERS sample preparation.

- **Extraction kits** with pre-weighed salts in anhydrous packets allow you to add salts *after* you add organic solvent to your sample avoiding an exothermic reaction that can compromise analyte recovery.
- **Dispersive kits** with sorbents and salts supplied in 2 mL or 15 mL centrifuge tubes accommodate the aliquot volumes specified by current AOAC and EN methodologies.
- **Ceramic homogenizers** break up salt agglomerates, promoting consistent sample extraction and increasing product recovery during extraction and dispersion.

Agilent SPE products help ensure accurate, reproducible measurements right from the start

By harnessing the principles of LC, Agilent SPE products selectively remove interferences and/or analytes from complex matrices such as foods and biological specimens. They feature:

- A unique, proprietary three-tier QC process that confirms the correct particle size while delivering superior flowthrough and performance.
- **Trifunctional bonding chemistry** that provides greater stability than monomeric bonding approaches.
- A wide selection of silica, non-silica, and polymer phases in formats ranging from cartridges to 96-well plates.
- · A complete range of manifolds and accessories.



Agilent's QuEChERS procedure for determining 11 Quinolone

antibiotics in bovine liver. Extraction was performed using Agilent EN extraction kits and 5% FA in Acetonitrile. Clean-up was accomplished using Agilent dispersive SPE kits (25 mg C18 and 150 mg MgSO₄). The extracted samples were then analyzed by LC/MS/MS.

The limits of quantitation (LOQ) were 5.0 ng/g, and the calibration curves were linear over the range of 5.0 to 400 ng/g. Pre-fortified recoveries were between 90% and 110% for 10 of 11 compounds (pipemidic acid was 65%), and RSDs were between 2% and 13.4%.



QuEChERS extraction procedure



Agilent's QuEChERS flow chart procedure for antibiotics

To learn more about Agilent food safety technologies and

applications, visit www.agilent.com/chem/food



Recovery of aflatoxin B_1 , B_2 , G_1 and G_2 from food matrices using a) C_{18} or b) MycoSep clean-up.

Here, we extend the QuEChERS approach beyond produce to grains and nuts for the analysis and confirmation of aflatoxins B_1 , B_2 , G_1 and G_2 . The detection limit was <0.15 μ g/kg – and the quantitation limit was <0.5 μ g/kg – for all four sample matrices.

Toxin	Recovery [%] ± RSD [%], 3 levels, n = 3								
	Wheat	Corn	Durum	Oats	Bread	Muesli	Infant Food		
DON	90 ± 5.2	93 ± 2.8	98 ± 3.8	96 ± 5.1	87 ± 1.7	87 ± 3.7	88 ± 12		
NIV	67 ± 5.9	74 ± 2.5	67 ± 6.3	73 ± 10	65 ± 5.7	71 ± 13	66 ± 10		
3ADON	89 ± 9.3	88 ± 7.6	97 ± 6.6	93 ± 11	100 ± 5.5	101 ± 7.1	91 ± 9.4		
15ADON	92 ± 13	87 ± 15	89 ± 11	89 ± 11	96 ± 9.5	98 ± 8.3	96 ± 6.6		
FUS	91 ± 10	94 ± 4.2	91 ± 7.8	91 ± 7.8	98 ± 8.5	97 ± 6.4	6 ± 4.3		
T-2	87 ± 7.6	88 ± 8.8	84 ± 2.2	84 ± 2.2	83 ± 8.2	75 ± 11	70 ± 7.3		
HT-2	82 ± 7.3	91 ± 3.3	85 ± 5.0	85 ± 5.0	79 ± 3.3	70 ± 7.7	74 ± 0		
NEO	91 ± 2.6	78 ± 11	68 ± 18	68 ± 18	80 ± 2.0	104 ± 10	71 ± 6.3		
DAS	82 ± 8.3	89 ± 3.6	85 ± 5.2	85 ± 5.2	75 ± 3.7	82 ± 6.8	68 ± 4.6		
MAS	86 ± 13	85 ± 12	93 ± 4.2	93 ± 4.2	86 ± 11	88 ± 16	91 ± 14		
T-2 triol	69 ± 9.1	66 ± 1.2	83 ± 2.8	83 ± 2.8	76 ± 9.3	82 ± 3.3	71 ± 7.9		
T-2 tetraol	69 ± 12	75 ± 6.8	73 ± 10	73 ± 10	65 ± 11	67 ± 17	70 ± 16		
ZEA	110 ± 5.9	113 ± 5.0	108 ± 4.8	108 ± 4.8	111 ± 6.0	102 ± 2.7	116 ± 6.7		

Trichothecene contents of six naturally contaminated samples analyzed with DONPrep[®] IAC, MycoSep[®] 227 and Bond Elut Mycotoxin cartridges, (n=3). Data reported by Klötzel et al.

Fusarium are toxin-producing fungi commonly found on cereals grown in the temperate regions of America, Europe, and Asia. This table shows the average recoveries and RSDs obtained for 12 trichothecenes and ZEAs from spiked wheat, corn, durum, oats, bread, muesli and infant cereal samples after clean-up with Bond Elut Mycotoxin columns.

As you can see, recoveries – especially for the polar toxins DON, NIV, 3ADON and T-2 tetraol – were increased up to 31%, compared to the extraction method on charcoal-alumnia cartridges.



Chromatogram of 10 ng/g fortified apple extract.

Here, the Agilent AOAC Buffered Extraction kit and Agilent AOAC dispersive SPE kit for General Fruits and Vegetables provided a simple, fast, and effective method for purifying representative pesticides in apple.

Based on matrix spiked standards, both recovery and reproducibility were acceptable for multiclass, multi-residue pesticide determination. The apple's impurities and matrix effects were minimal, and did not interfere with the quantitation of target compounds. Additionally, the pesticide LOQs were significantly lower than required by European and North American regulated MRLs.



The oil crisis in the Gulf of Mexico has underscored the need for fast, dependable analysis of environmental matrices contaminated with petroleum hydrocarbons. QuEChERS with GC/MS or GC/MS/MS with backflush can simplify sample preparation and reduce cycle time.

Here, 50 ppb EPA PAHs were extracted from Swai fish using QuEChERS DB-5ms 20 m x 0.18 mm, 0.18 μ m GC/MS in the SIM mode.





Determination of Sulfonamide Antibiotics in Bovine Liver Using Agilent Bond Elut QuEChERS EN Kits by LC/MS/MS.

Recovery and reproducibility, based on matrix-spiked standards, were acceptable for multiresidue sulfonamide determination. In addition, the impurities and matrix effects from liver were minimal and did not interfere with the quantification of target compounds. Note that the LOQs of the quinolones were much lower than their regulated MRLs in animal food products (20-100 ng/g).





Overlay HPLC – FLD chromatograms of the spiked fish sample containing: 1. Nap 2. Acy 3. Ace 4. Flu 5. Phe 6. Ant 7. Fln 8. Pyr 9. BaA 10. Chr 11. BeP 12. BeA 13. BkF 14. DahA 15. BghiP 16. InP. The spiking level for this sample was level 1. The blue portion of the chromatogram used the following excitation/emission wavelengths: 260-nm/352-nm; the red portion 260-nm/420-nm; the light blue portion: 260-nm/440-nm. For acenaphthylene, UV detection at 230-nm was used.

PAH			Level of spiking (ng/g) (n = 6)					
	1	1			3	3		
	%Recovery	%RSD	%Recovery	%RSD	%Recovery	%RSD		
Naphthalene	94.7	1.4	97.9	1.1	93.8	1.4		
*Acenaphthylene	87.8	1.7	96.3	1.2	85.6	0.8		
Acenaphthene	92.1	1.5	93.0	1.8	96.7	0.8		
Fluorene	98.1	1.5	89.9	1.0	97.2	0.9		
Phenanthrene	90.6	0.9	93.8	0.8	83.1	1.7		
Anthracene	96.7	1.0	87.6	0.8	92.1	0.6		
Fluoranthene	83.4	1.3	93.9	1.5	95.9	1.2		
Pyrene	93.5	1.8	86.1	1.3	95.0	1.4		
1,2-Benzanthracene	94.5	1.3	89.6	1.6	94.9	1.0		
Chrysene	101.0	1.4	97.8	1.7	87.2	1.6		
Benzo[e]pyrene	88.8	1.5	85.2	1.9	95.0	1.4		
Benz[e]acenaphthylene	95.5	0.7	92.7	0.7	89.2	0.9		
Benzo[k]fluoranthene	93.5	0.8	94.6	0.9	98.9	0.8		
Dibenzo[a,h]anthracene	88.2	0.9	97.3	1.1	97.1	0.6		
Benzo[g,h,i]perylene	98.4	0.8	95.5	1.6	98.2	0.7		
Indeno[1,2,3-cd]pyrene	91.5	1.5	97.9	0.9	94.3	0.7		

* UV detection at 230 nm

Recoveries and RSDs for the Sixteen Polycyclic Aromatic Hydrocarbons in Fish Sample (n = 6)

This example shows an analysis of polycyclic aromatic hydrocarbons in fish using Agilent QuEChERS AOAC Kit and HPLC-FLD. Recovery and reproducibility (RSD) were evaluated on spiked samples at three different levels, and the analysis was performed in replicates of six (n = 6) at each level.

As you can see from the table above, very good recoveries – and excellent RSD values – were achieved for the sixteen polycyclic aromatic hydrocarbons.



Columns and supplies

Keep your methods safe, keep your workflow running smoothly, and keep contamination to a minimum

The stakes have never been higher in food safety testing, and you cannot afford to let "little things" like columns and supplies jeopardize your productivity and results. That is why Agilent-engineered columns and supplies are designed to outlast the competition, while ensuring a lifetime of peak instrument performance essential for complex food applications.

LC Columns

From research... to leading-edge method development... to routine quality assurance... **Agilent ZORBAX HPLC columns** are optimized for high throughput analysis, and feature the sensitivity, accuracy, and reliability that demanding food applications require.

For example, our new **Poroshell 120 columns** give you speed and resolution that are comparable to sub-2 micron columns. Because they use a standard 2 μ m frit, however, they resist plugging with complex food samples.

GC Columns

Agilent J&W GC columns are designed and manufactured to give you excellent, reproducible performance for benign and difficult sample types. With the lowest bleed levels, the best inertness, and the tightest column-to-column reproducibility, Agilent J&W GC columns perform better than any other columns on the market.

Poroshell 120 columns give you speed and resolution similar to sub-2 micron columns, but they use more forgiving 2 micron frits, so they are more forgiving for food safety samples.



Backflush techniques can reduce the time it takes to remove unwanted matrix from the GC. This increases column life by eliminating cycle time between runs.



Parts and supplies

As the world's premier measurement company, Agilent is uniquely positioned to offer you the widest selection of parts and supplies. All are engineered or selected by our experienced instrument design teams, manufactured to our demanding specifications, and tested under the strictest conditions.

And remember, all Agilent columns and supplies are backed by unmatched technical support – on the Web, by phone or in person – plus a 90-day warranty from the date of shipment.











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Agilent is uniquely equipped to support your food testing efforts with unmatched expertise, training, and services

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Whether you need support for a single instrument or a multi-lab, multi-vendor operation, Agilent helps you solve problems quickly, increase your uptime, and optimize your resources – from installation and upgrade to operation and repair.

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We *guarantee* you at least 10 years of instrument use from your date of purchase, or we will credit you with the residual value of the system toward an upgraded model.

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