Rising to the Challenge of Future Food Analytics

Robin Philp
Academia & Collaborations Manager, SEA

Global Summit on the Future of Future Food
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Bangkok, Thailand

Agilent
Trusted Answers

DE38576194

Who We Are at Agilent

A global, collaborative team, serving vital industries in 6 key markets

Pharma and Biopharma

Food and Feed

Chemicals and Advanced Materials

Environmental and Forensics

Diagnostics and Clinical

Academia and Government

Committed to

Accelerating the **advancement of science**

Providing **complete, integrated solutions**

Championing **your success**

Agilent in **Food and Feed Safety, Quality, and Authentication**

- Agilent supports the **testing and surveillance of the supply chain** to ensure the world´s food supply is safe and wholesome
- Agilent helps **labs set/ensure the highest standards** of food safety, quality, and authenticity
- Agilent works with leading researchers and labs **to develop new standards for detecting** pesticides, veterinary drug residues, and emerging contaminants

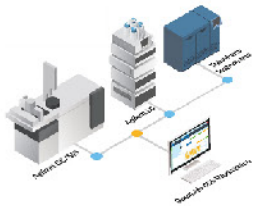
Agilent Serves the **Entire Food and Feed Analysis Value Chain**

Research → Development → Quality Assurance and Compliance

Sample preparation

Separation

Detection



Data analysis

Reporting

Agilent CrossLab
From Insight to Outcome

- Instrument service
- Training, consulting and operational expertise
- Enterprise lab management
- Columns, supplies and chemical standards

1000 Pesticide Residues Analyzed Following SANTE 12682/2019 Guidelines

Challenges in Pesticide Analysis

- Diversity of pesticides
- Complexity of food matrices
- Low limits of detection

Agilent Solution

- Wide Coverage
  - >1000 targets in dMRM
  - tailored QuEChERS kits for commodity groups
- Entire Pre-verification
  - Verified-based SANTE
  - Intra-Lab
  - Inter-Lab
- Excellent Sensitivity
  - LODs for >99% targets meet MRL
- Innovations in HW and SW

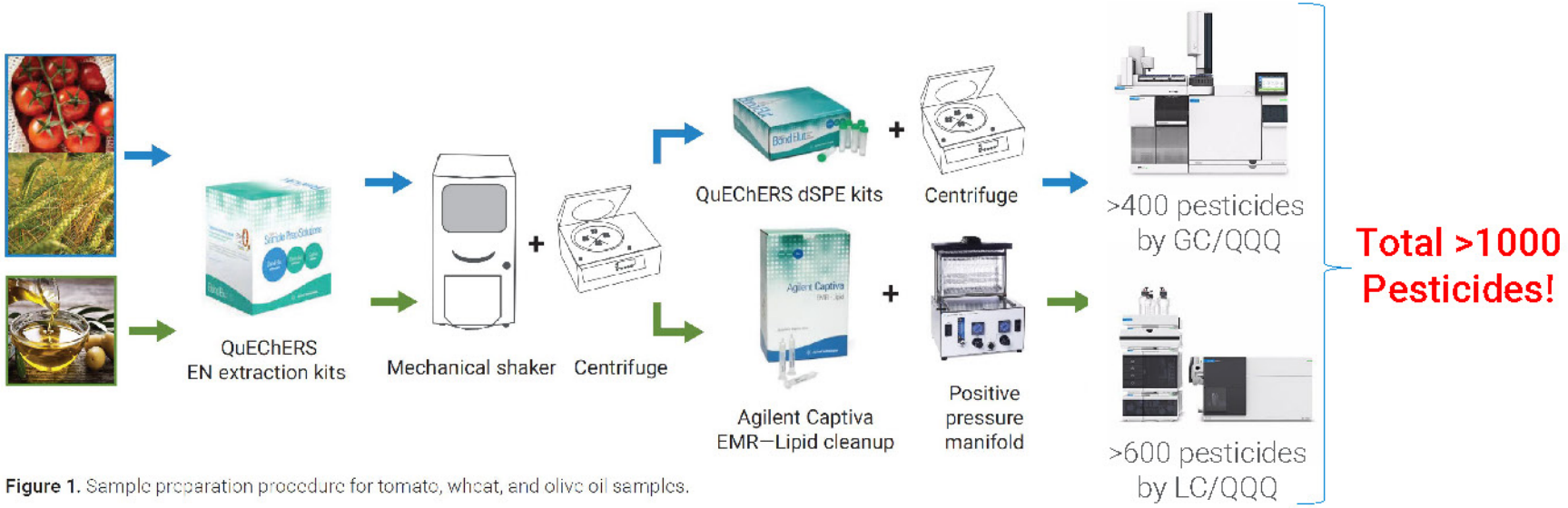
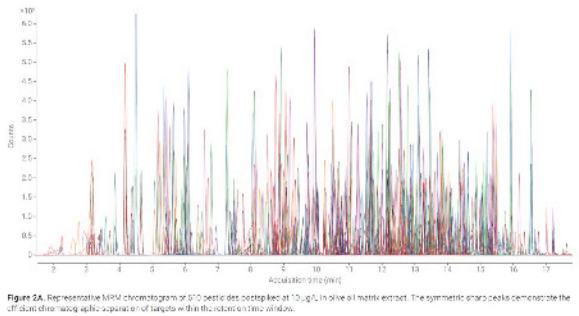
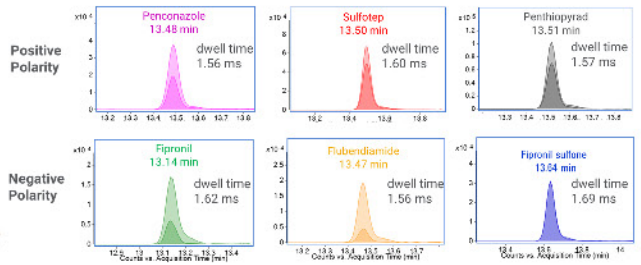


Figure 1. Sample preparation procedure for tomato, wheat, and olive oil samples.

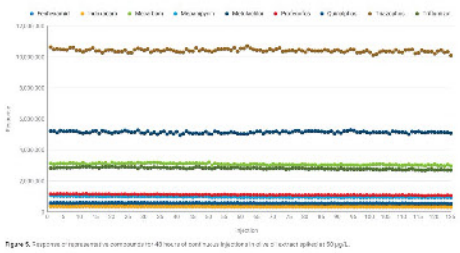
Simultaneous Analysis of Hundreds of Compounds



Excellent Chromatograms with Low Average Dwell Times



Outstanding Robustness



Webinar by Marcus Chadna, A Novel Workflow to Determine over 1000 Pesticide Residues in Compliance with SANTE 12682/2019 Guidelines in Various Food Matrices; App Notes: 5994-2370EN and 5991-7303EN; and work by Linfeng Wu

The 6475 LC/QQQ: Consistently Robust and Versatile hardware and End-to-End System Intelligence – Many new features

Maximize instrument uptime with VacShield

No venting required: perform maintenance in 30 minutes

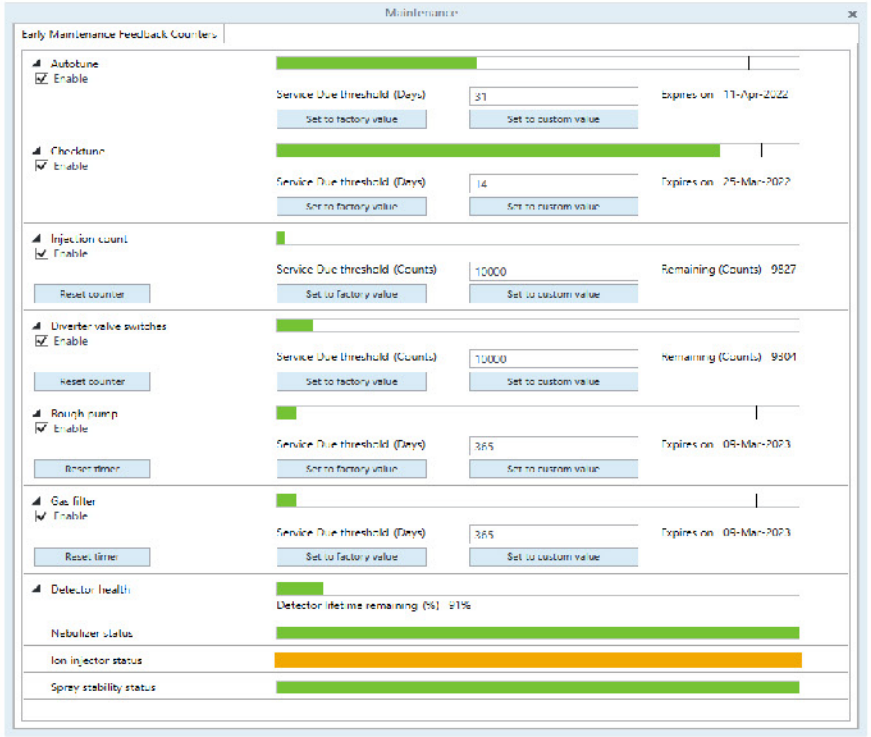
Routine Maintenance Speed

Procedure	Time Without VacShield (min.)	Time With VacShield (min.)
Cool down to acceptable temperature	15	Not needed
Break vacuum and leak air into the instrument	15	Not needed
Remove and clean ion injector capillary	20	20
Power on and pump down	300 (5 hours)	Not needed
Check tune or autotune instrument	10 (Check tune) 45 (Autotune)	10 (Check tune) 45 (Autotune)
Total	360 to 395 (6.0 - 6.6 hours)	30-65 (0.5-1.1 hours)

Active System Monitoring

Early Maintenance Feedback
helps keep an eye on system health

Event timers read like a battery bar to help anticipate maintenance events



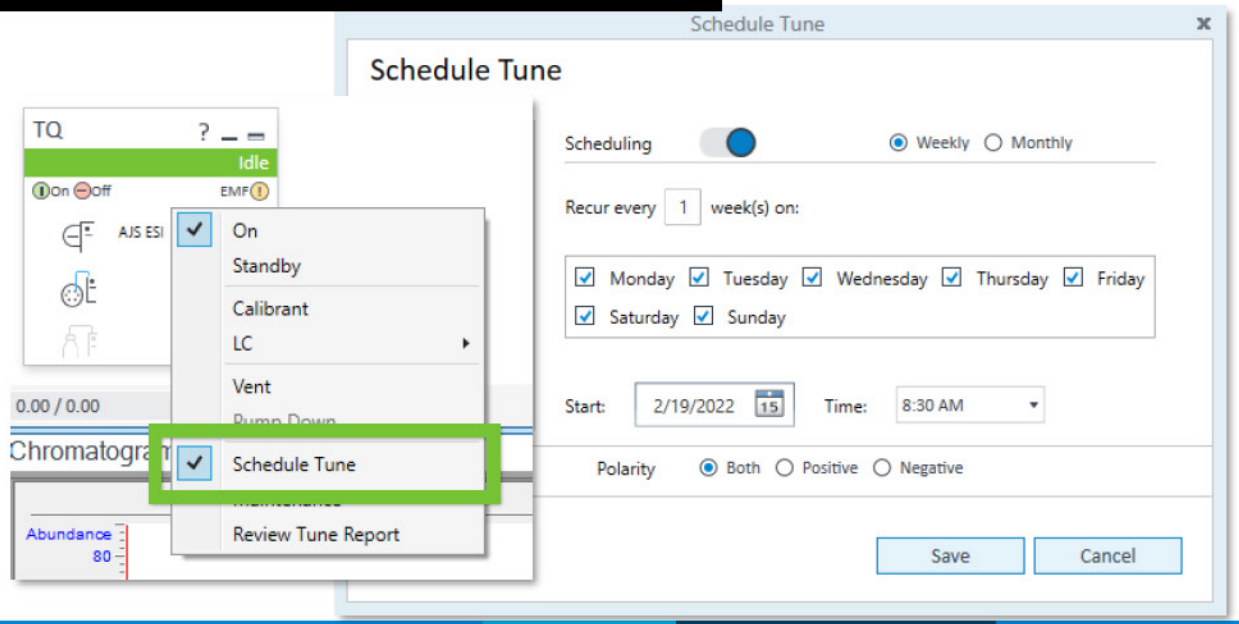
Event flags detects and pinpoints when an adverse event has occurred

Maintenance Automation

Scheduled Autotune/Checktune
automatically verifies system readiness

5AM → *Instrument tunes before anyone arrives*

Scientist arrives → *Instrument is ready to go*



Method Development Automation

Fully Automated MRM and Ion Source optimizer helps develop new methods or fine-tune existing methods quickly

Create new or load existing method

Input chemical formulas

Select optimization parameters

Select "Guided" or "Automated"

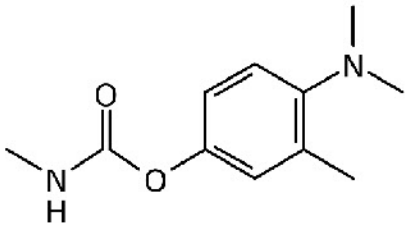
Execute workflow

Review Results

Finalize and Save to database

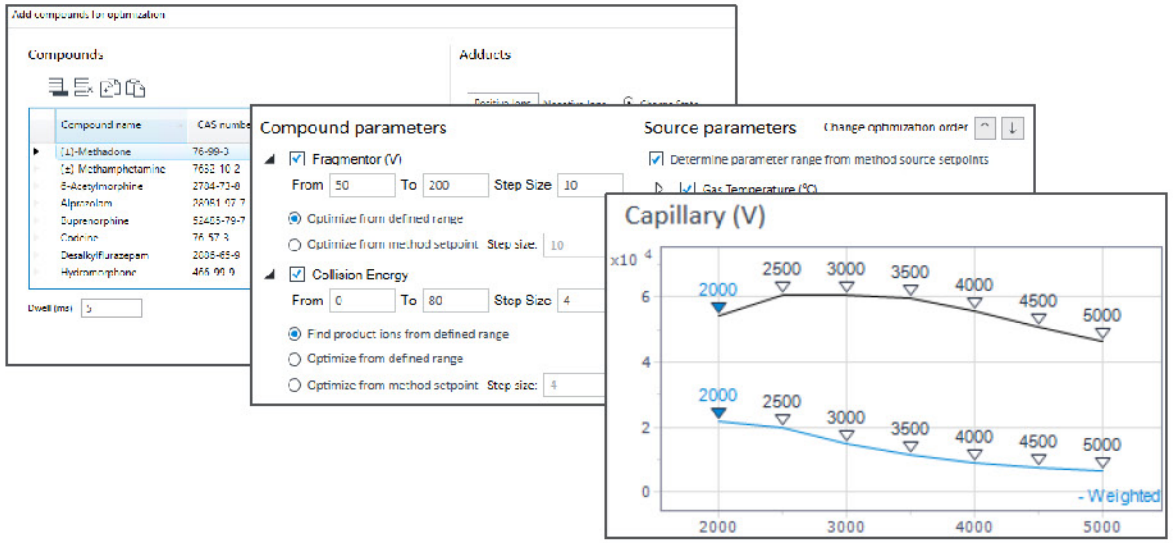
Define Target:

Aminocarb



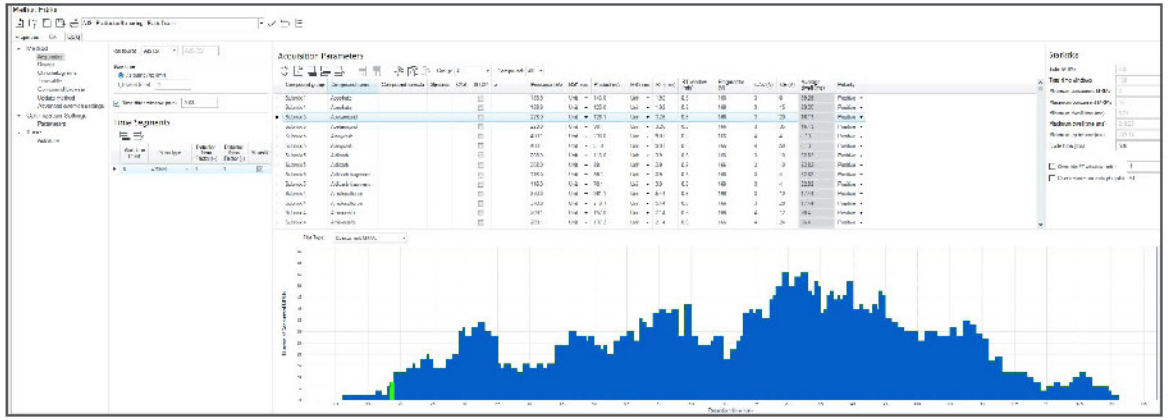
Automatically find MRMs

MRM1: 209.1 → 152.0
MRM2: 209.1 → 137.2



Automatically find Parameters

Collision Energies, Fragmentor

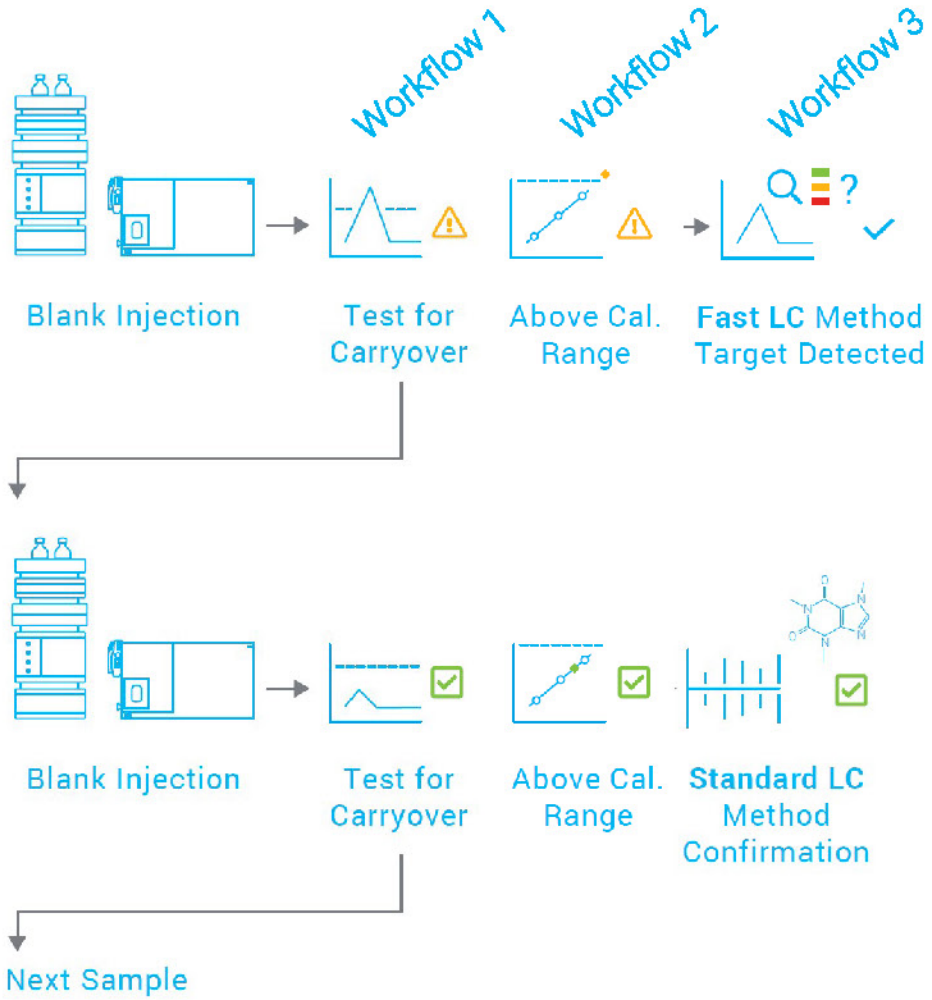


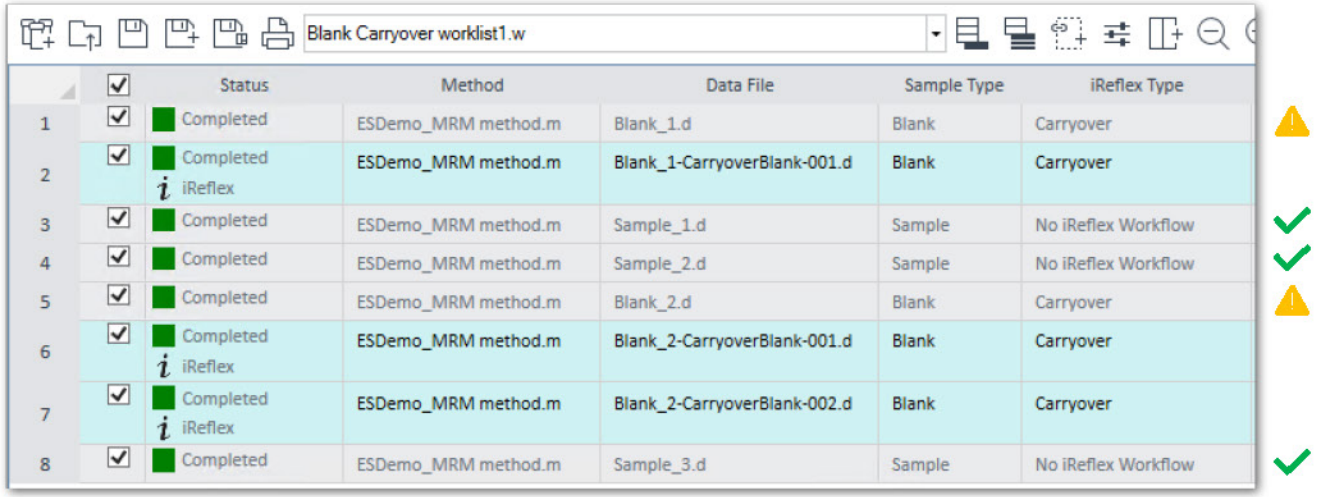
Consolidate Method

MRMs Defined
MRMs Optimized
Ion Source Optimized

Reflexive Injection Logic

Intelligent Reflex helps assure samples are in spec or to increase throughput





		Status	Method	Data File	Sample Type	iReflex Type
1	☑	Completed	ESDemo_MRM method.m	Blank_1.d	Blank	Carryover
2	☑	Completed iReflex	ESDemo_MRM method.m	Blank_1-CarryoverBlank-001.d	Blank	Carryover
3	☑	Completed	ESDemo_MRM method.m	Sample_1.d	Sample	No iReflex Workflow
4	☑	Completed	ESDemo_MRM method.m	Sample_2.d	Sample	No iReflex Workflow
5	☑	Completed	ESDemo_MRM method.m	Blank_2.d	Blank	Carryover
6	☑	Completed iReflex	ESDemo_MRM method.m	Blank_2-CarryoverBlank-001.d	Blank	Carryover
7	☑	Completed iReflex	ESDemo_MRM method.m	Blank_2-CarryoverBlank-002.d	Blank	Carryover
8	☑	Completed	ESDemo_MRM method.m	Sample_3.d	Sample	No iReflex Workflow

Additional blank injections inserted if carryover was detected

Food Authenticity/Identity

Food Fraud

The deliberate and intentional substitution, addition, tampering or misrepresentation of food, food ingredients or food packaging, labelling, or false or misleading statements made about a product for economic gain.

- Substitution
- Addition/Dilution
- False Claims

Challenges

- Meeting regulatory requirements
- Availability of authentic samples
- Speed of analysis
- Extensive method development required
- Extensive validation required



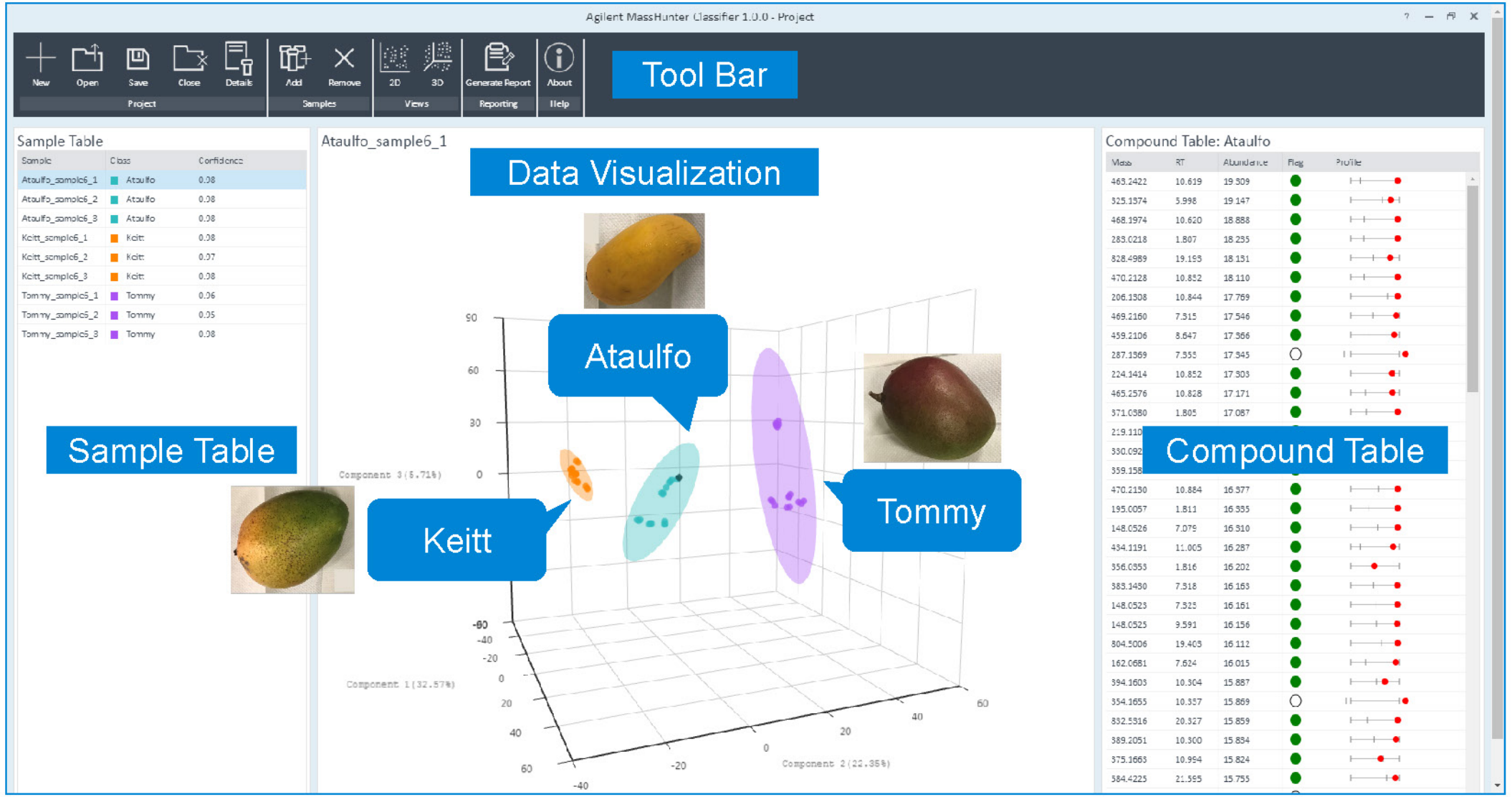






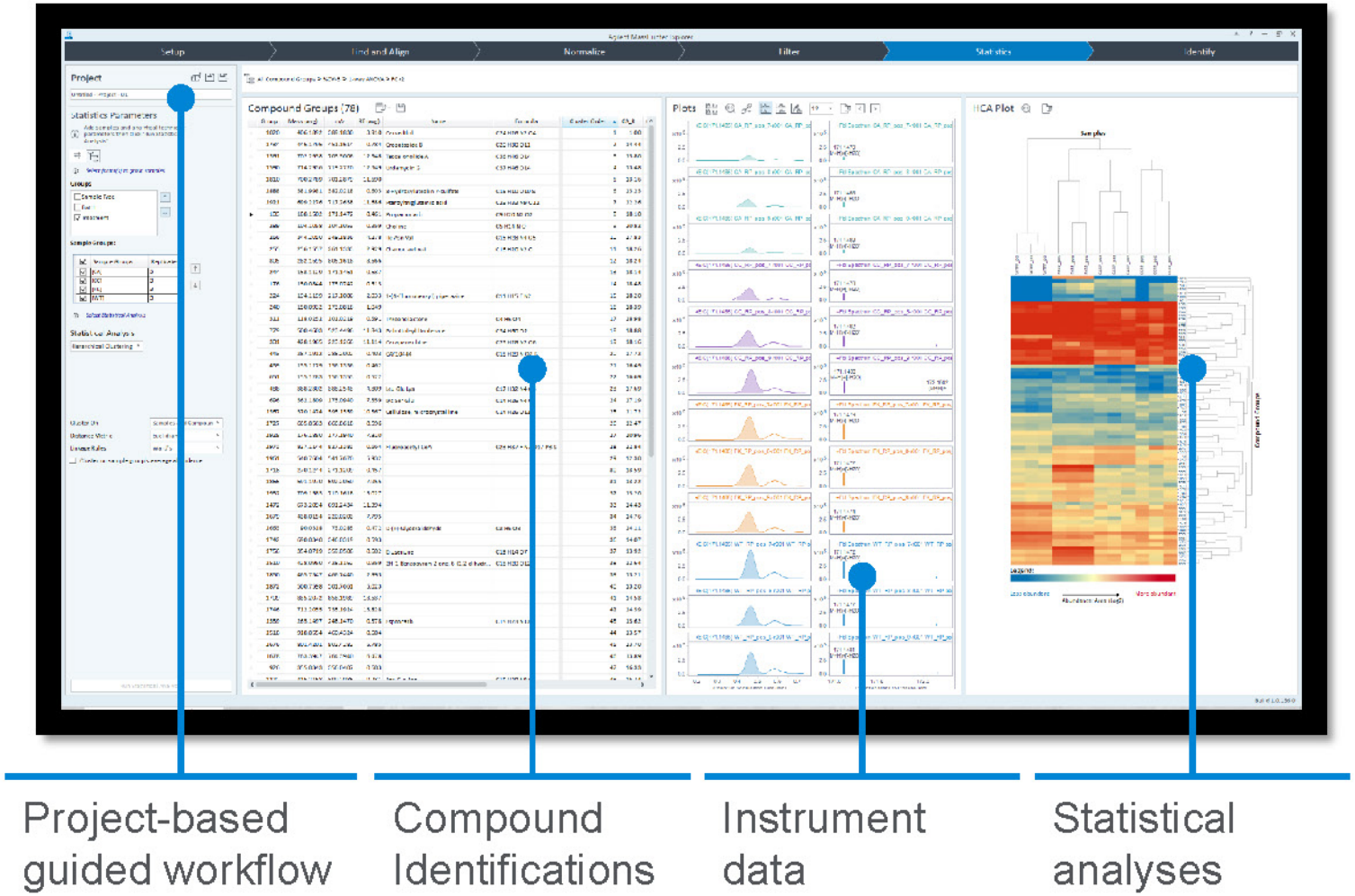
MassHunter Classifier

A simple tool for automated sample classification



MassHunter Explorer: for non-targeted LC/QTOF applications

Draw critical insights from complex data - Simple, efficient path to differential analysis



Linked interactive navigation of all results in one application

Project-based guided workflow

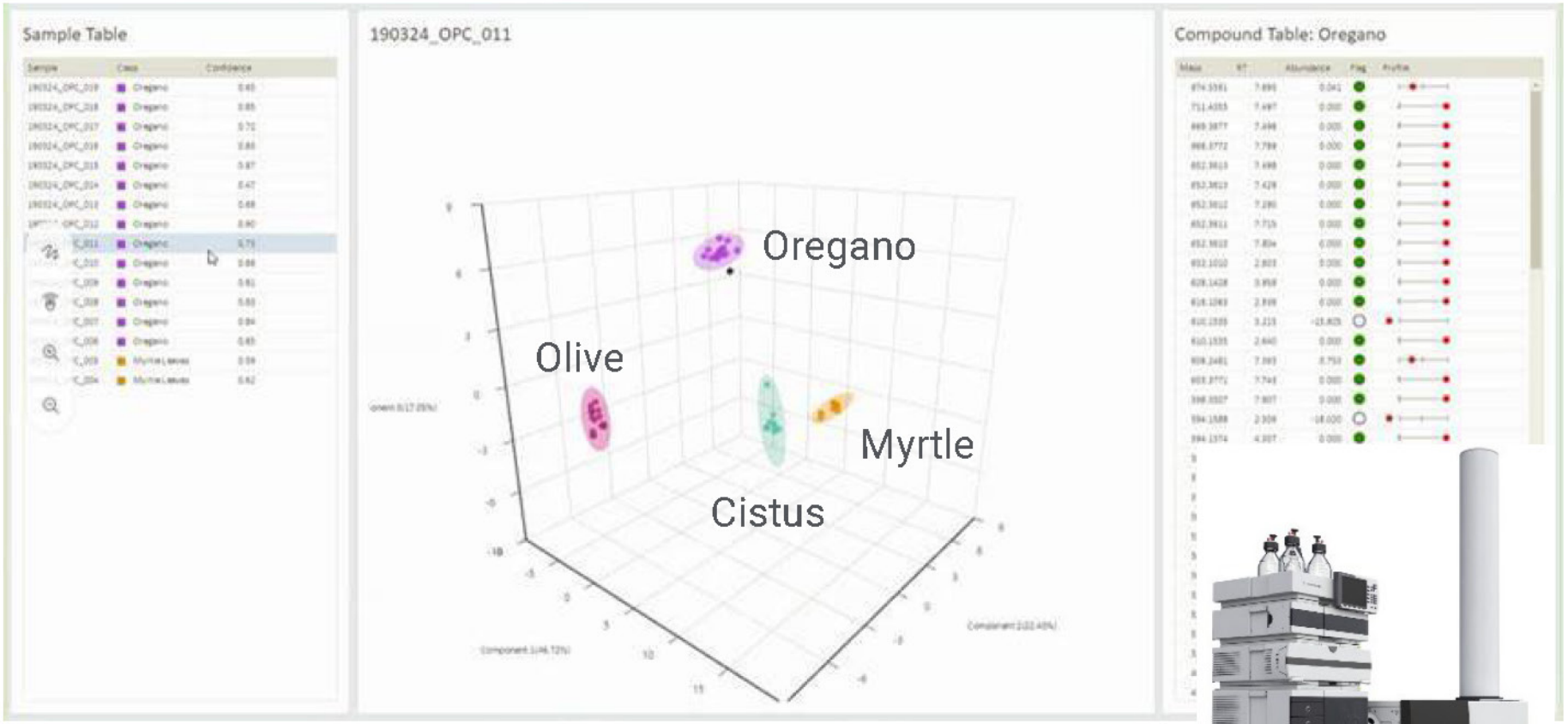
Compound Identifications

Instrument data

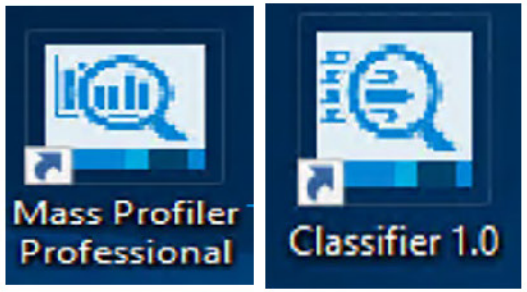
Statistical analyses

Agilent

Identity Fingerprinting of Herbs with LC QTOF



Oregano (Purple 14 samples) Myrtle (Yellow 10 samples)
Cistus (Green 10 samples) Olive leaves (red 15 samples)

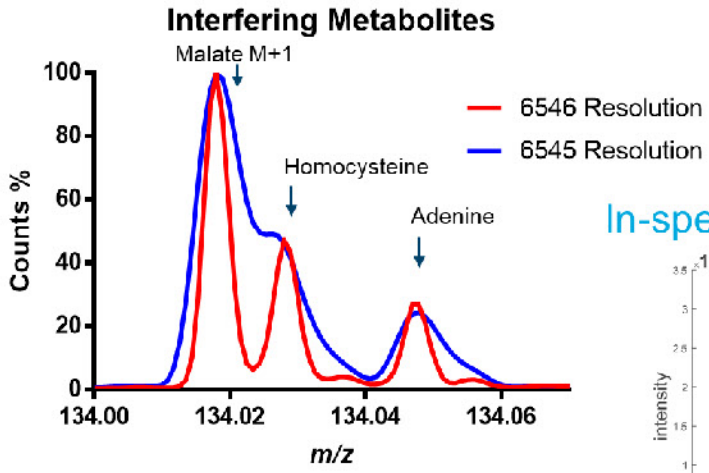


Professor Chris Elliott, OBE
Institute for Global Food Security,
Queens University, Belfast

6546 LC/Q-TOF MS for Food Analysis

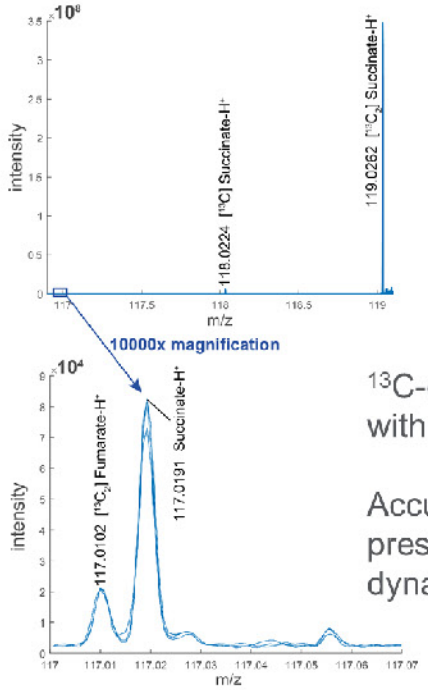
Benefiting from the design innovations

Resolving coeluting metabolites



Malate M+1 $[M-H]^-$ is 134.0176
Homocysteine $[M-H]^-$ is 134.0281
Adenine $[M-H]^-$ is 134.0472

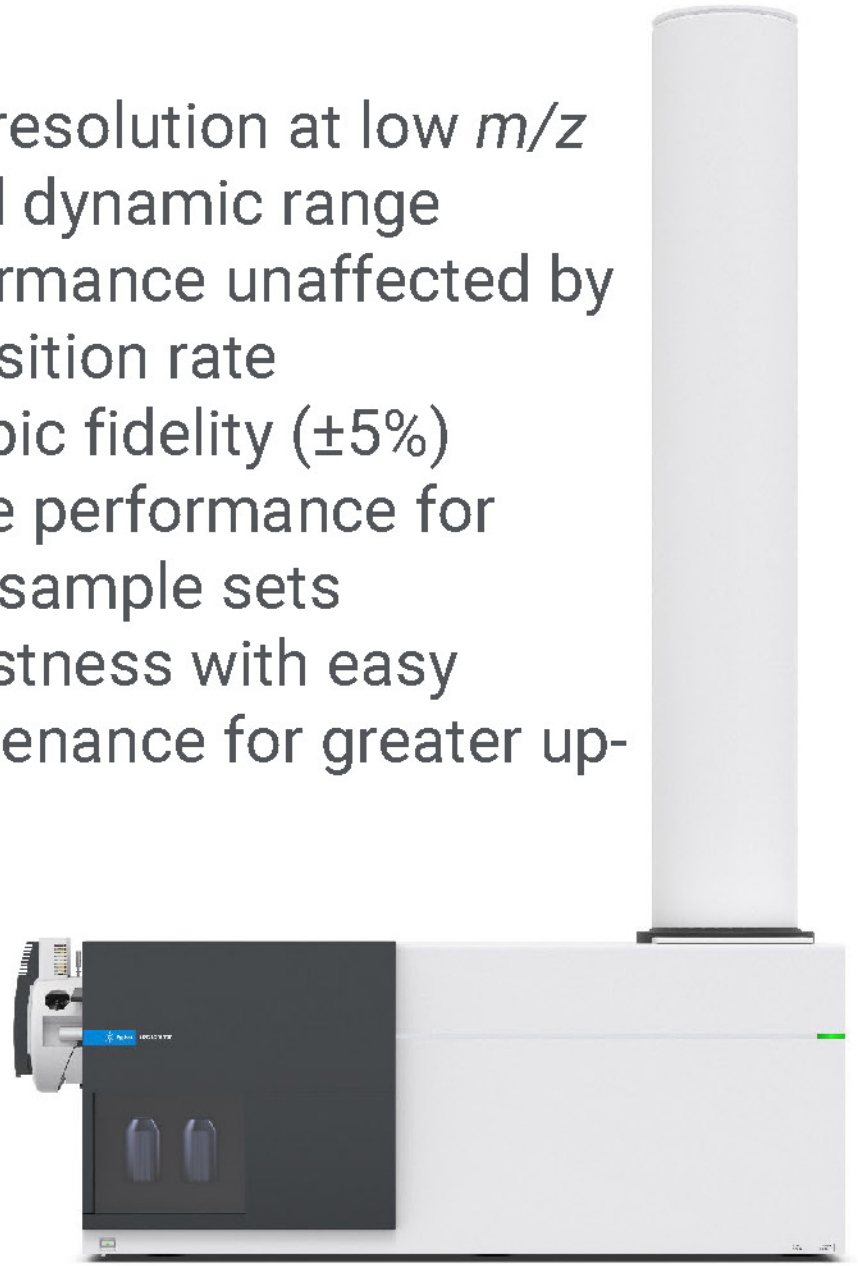
In-spectrum dynamic range: >4 orders



^{13}C-enriched *E. coli* spiked with $^{13}C_2$-succinate (n=3)

Accuracy and resolution preserved across wide dynamic range

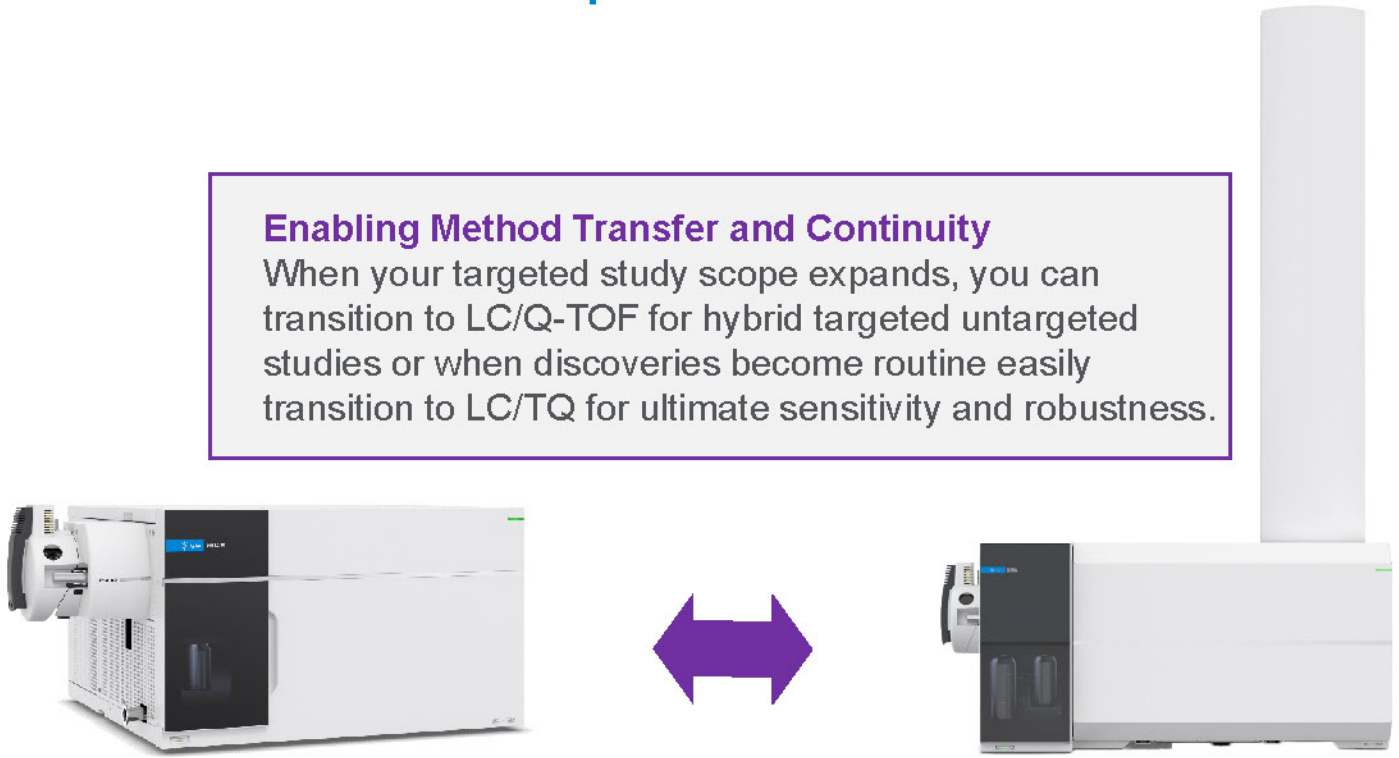
- High resolution at low *m/z*
- Broad dynamic range
- Performance unaffected by acquisition rate
- Isotopic fidelity (±5%)
- Stable performance for large sample sets
- Robustness with easy maintenance for greater up-time

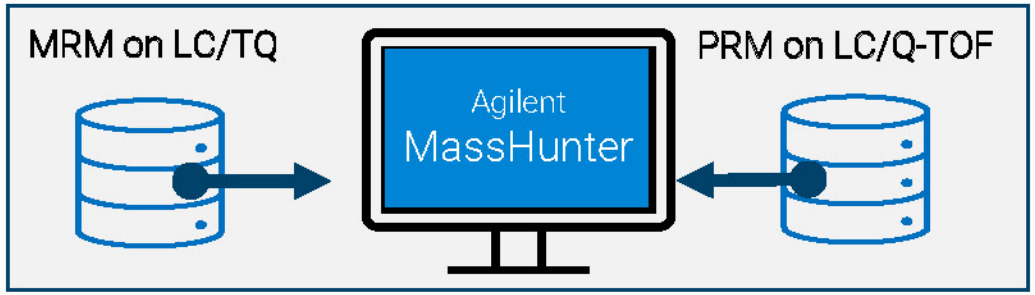


Agilent 6546 LC/Q-TOF: Gaining Higher Confidence and Throughput in Metabolite Analysis. Agilent application note 5994-0724EN

Intelligent Mass Spectrometers are Backed by Highly Curated Workflows to Decrease Method Development Time And Accelerate Research

Enabling Method Transfer and Continuity
When your targeted study scope expands, you can transition to LC/Q-TOF for hybrid targeted untargeted studies or when discoveries become routine easily transition to LC/TQ for ultimate sensitivity and robustness.

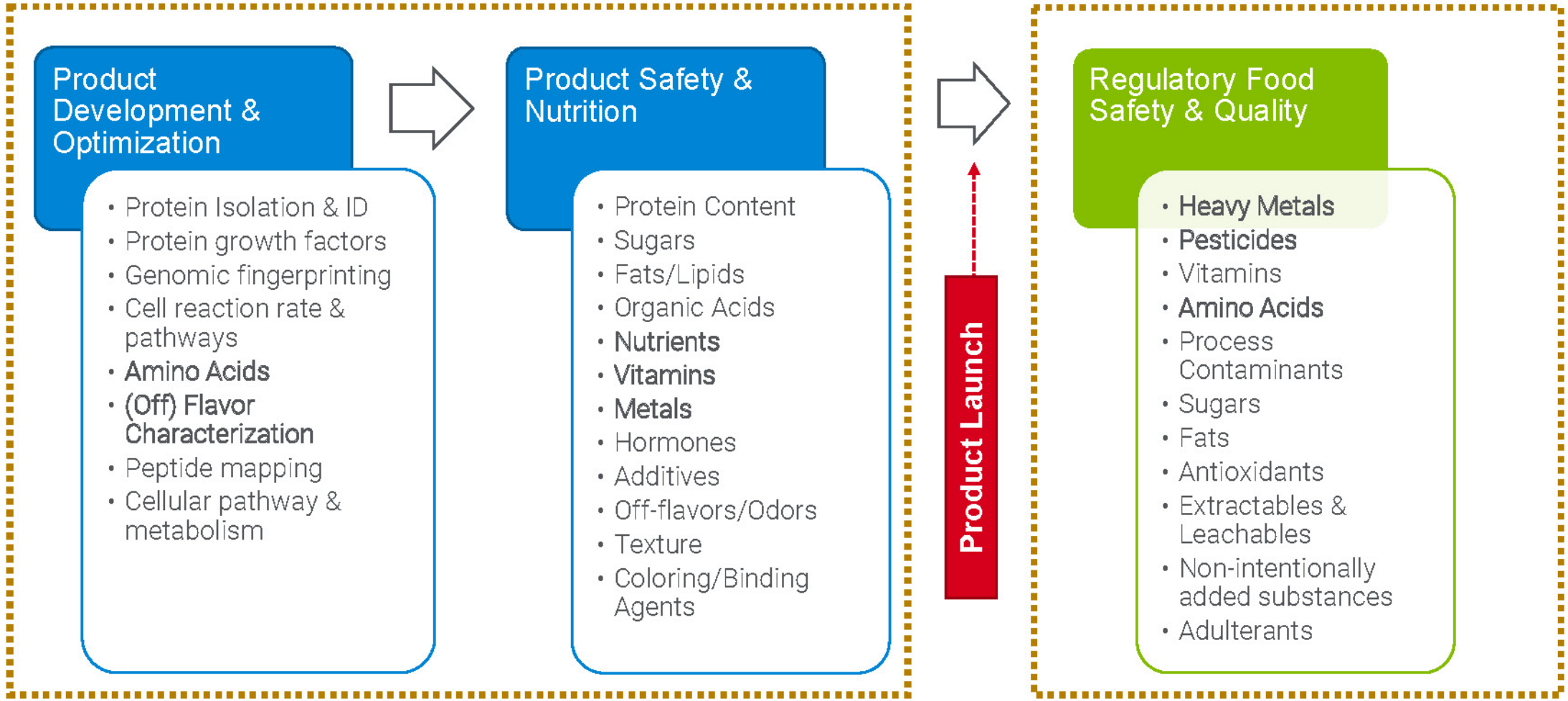




Testing Workflow for Alternative Proteins

Testing needs vary based on protein source

Testing needs vary based on regulations and final product type, with similar tests used in conventional products



Upendra Khurana, Tarun Anumol

Application Note

Food Testing

Agilent

Trusted Answers

LC/Q-TOF Analysis and Nontargeted Chemometric Profiling of Meats and Plant-Based Alternatives

Food sensory testing using the Agilent 1290 Infinity II LC and Agilent 6546 Q-TOF

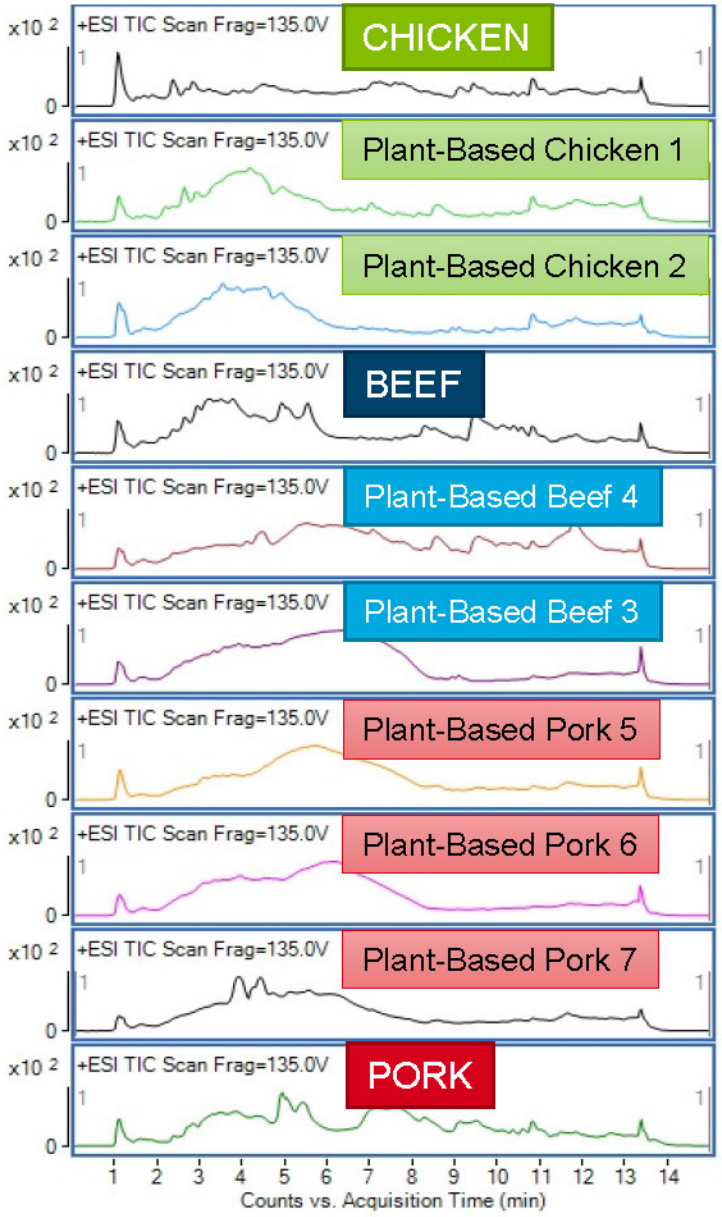
Authors

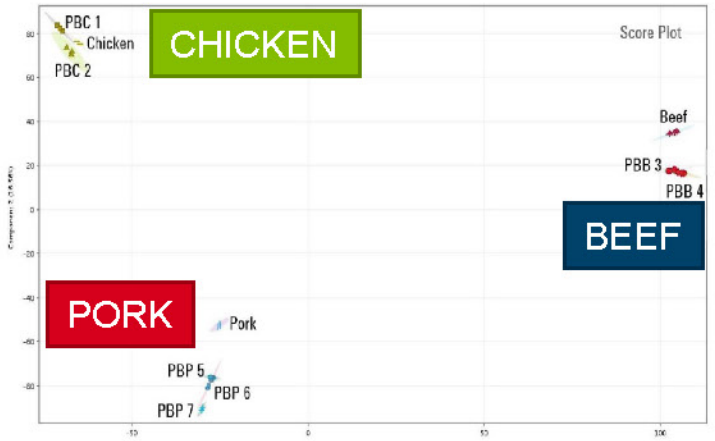
Toh Seok Hwa,
Upendra Khurana,
Tarun Anumol, and
Daniel Cuthbertson
Agilent Technologies, Inc.

Abstract

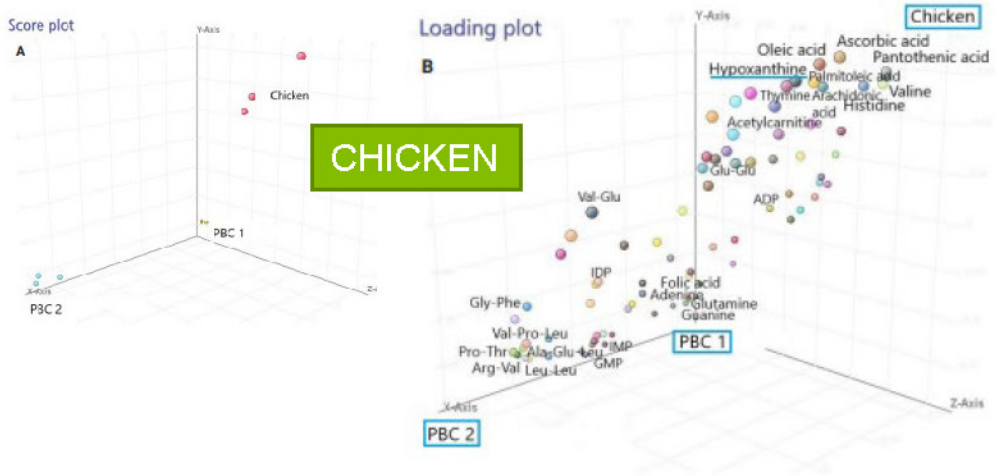
Meat-alternative sources of protein, including plant-based and cell-based foods, are gaining popularity globally due to a combination of consumer interest, regulatory changes, and global food systems. For example, as Singapore aims to achieve 30% of its food production levels through self-production by 2030, many established food companies and startups are developing meat-substitute products. The main drivers of Singapore's food production target are around health and environmental concerns. Historically, plant-based meat substitute foods have struggled to achieve the same texture and taste as animal meats. However, recent analogs of plant-based meats are significantly more similar in taste, texture, and composition as traditional meats due to technological advances in production methods. This application note describes a nontargeted profiling method to characterize chemical components of unknown foods, using a high-resolution accurate mass LC-Q/TOF. Also, various statistical tools are presented that translate accurate mass LC/Q-TOF data into more easily understandable information. Principal component analysis (PCA) of the data can be used to identify compounds, abundance distribution of the compounds in different samples, and how the compounds correspond to target taste profiles. Heat maps and hierarchical clustering of raw ingredients show similar distribution of proteins with target taste profiles.

Chemometric Profiling of Meat & Plant-Based Alternatives using LC-QTOF MS

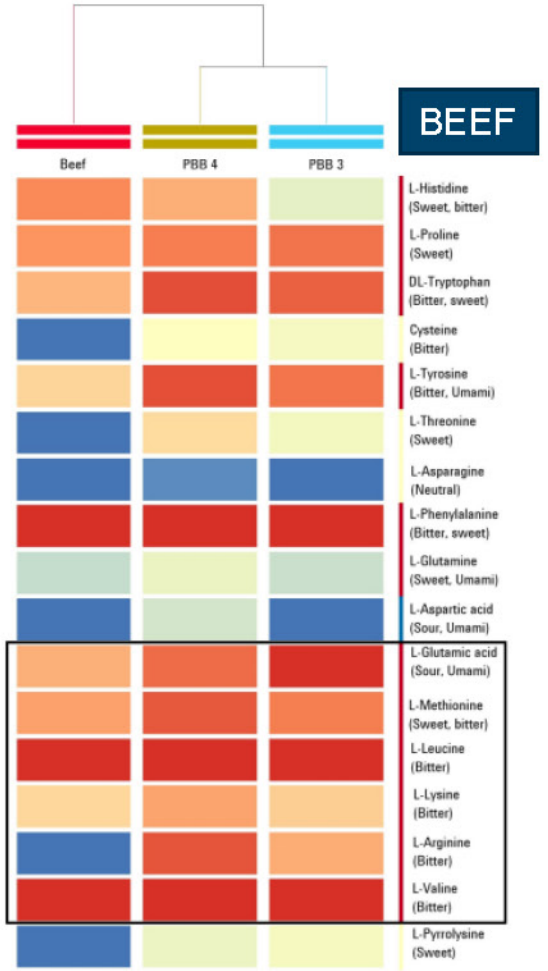




3D PCA plots of chicken and alternatives



Heat map of amino acids in beef and alternatives



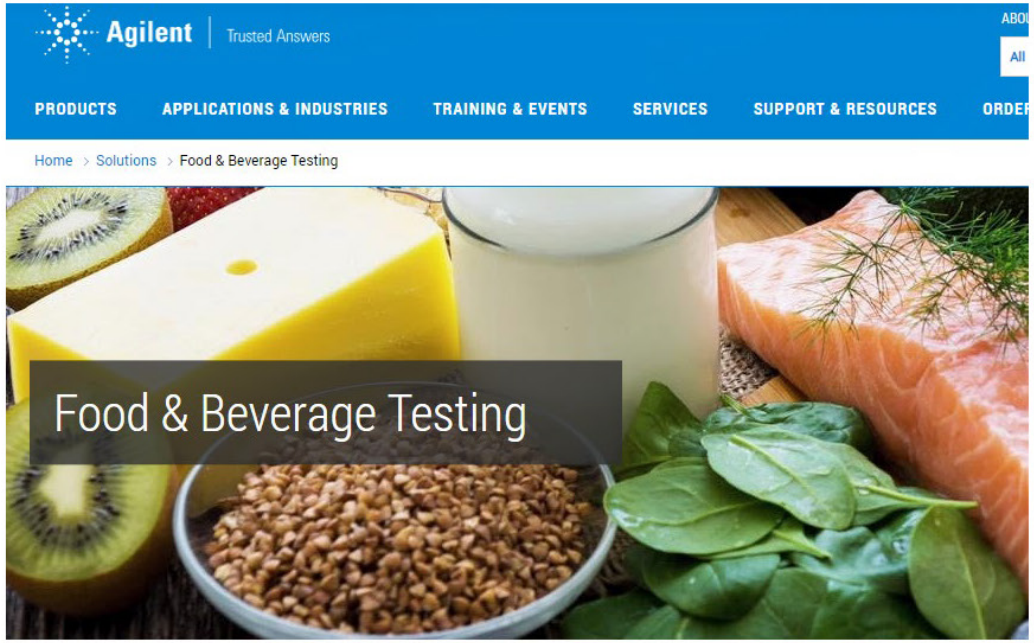
[App Note: 5994-5130EN](#)

Toh Seok Hwa et al.

For more info: lorna.deleoz@agilent.com

Agilent

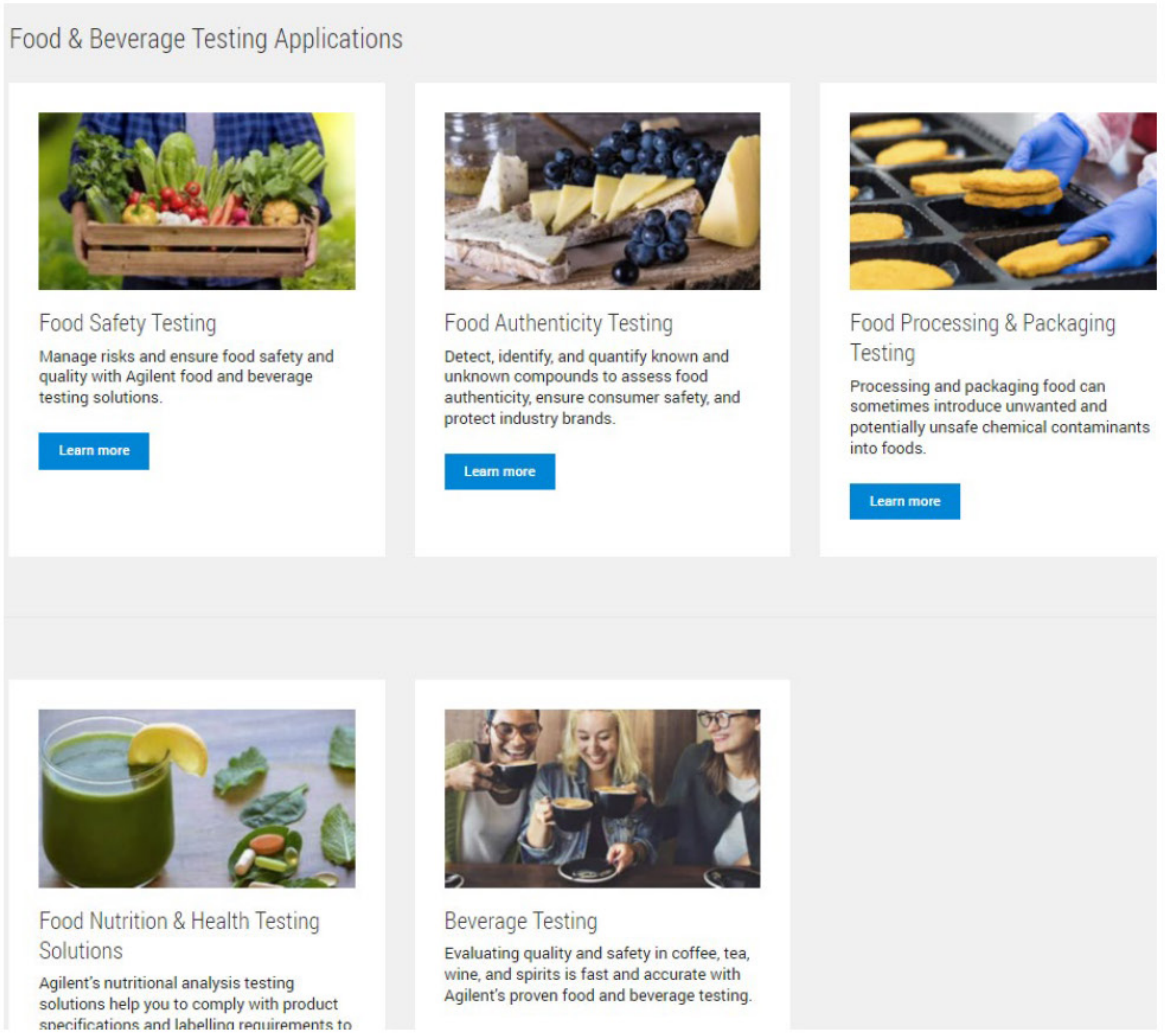
For more information, check out www.agilent.com



Agilent Food and Beverage Testing Solutions: Helping You Achieve Food Safety, Quality, and Authenticity

Ensuring food safety and quality is increasingly challenging. Whether you're analyzing for pesticide residues, ensuring that label claims are correct and accurate, or profiling for food authenticity, Agilent works with you, helping you deliver what your customers demand. Agilent Technologies food and beverage testing products and services keep you at the forefront of the latest trends, ahead of issues, and focused where you need to be – delivering highest quality and value to your customers.

Contact Us

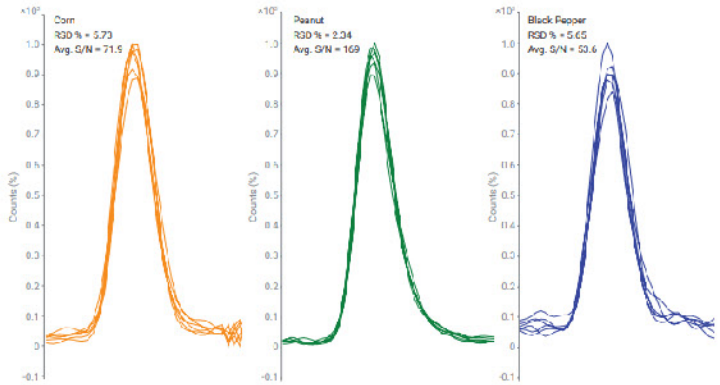


Summary: Agilent Provides Complete Solutions for Testing **Food and Feed Safety, Quality, and Authenticity**

Continuous innovation to increase productivity, lower costs, and increase compound coverage in one test. New regulations monitored to ensure Agilent solutions stay relevant.

Agilent workflows

- Enable laboratories conducting surveillance and food-safety risk assessments from imported and exported food.
- Provide industry with approaches for testing vitamins, minerals, and oils in food, helping to ensure label claims are correct.
- Support food chemists working to ensure the authenticity of food products.



Agilent strengths

- Solutions for quantification and food profiling.
- Highly skilled chemists who develop unique and differentiated workflows.
- Outstanding service and support for hardware, software, and applications.

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