

FOOD TESTING APPLICATIONS

eBook

> LECO Corporation –
company facts



> GC- and GCxGC-TOFMS
instrumentation

> Specific LECO GC-TOFMS
instrument features

> Separation Science
product portfolio

> Selection of LECO SepSci
App Notes

> LECO Food Testing
Bibliography

> Next Page



LECO CORPORATION

SOME COMPANY FACTS



SOME COMPANY FACTS

LECO CORPORATION



Established in 1936 by Carl Schultz, the Laboratory Equipment Company introduced what would be the first rapid carbon determinator to the American iron and steel industry.

Today, over 80 years later, LECO continues to be a family-owned company in its third generation of leadership and is recognised globally as a leader in the development of high-quality elemental and thermal analysis equipment, mass spectrometers and chromatographs, metallography and optical equipment, and consumables.

Our headquarters in St. Joseph, Michigan, USA, is comprised of several facilities each dedicated to improving customer success, including state-of-the-art research and development centers and rugged manufacturing facilities. Through this vertical integration system, we are able to maintain strict control over the manufacturing and assembly process in accordance with our quality standards.

LECO established its first international office in Germany in 1967, and since that time has grown to include over 25 worldwide subsidiaries and distributors who are authorised to sell our equipment to over 75 countries around the Globe.



LECO'S KEY MARKETS



Energy & Fuels

While LECO has continued to be a leader in carbon/sulfur testing of coal and coke, it has since expanded into biofuels, biomass, oil additives, petroleum products. Ensuring existing sources, and analysing fuels of the future – LECO technology is here to validate their potential and quality.



Environment & Agriculture

LECO instruments help to monitor environmental impact, manage agricultural resources more efficiently by monitoring composition of arable soils, crop and fertilisers; determining optimum nutrition values for animal feed.



Food Safety

Multi residue methods and screening all at once; food contamination; authenticity or traceability: LECO provides solutions with unrivalled performance, sensitivity, speed and robustness.



Life Science & Pharmaceutical

Academic research and drug discovery requires the instrumentation that goes beyond normal expectations. Empowered by advanced LECO mass spectrometry be more confident in your assignments.



Metabolomics

As the established leader in GCMS metabolomics, LECO products deliver the accuracy, resolving power, deconvolution, and speed to characterise the most complex biological systems. Our instrumentation has been validated by the industry's most demanding researchers.



Metallurgy & Metals

With a global reputation for rapid, accurate analysis in iron, steel, alloys, refractory metals, and ores, LECO instruments have become the brand leader for these markets.



GC- AND GCxGC-TOFMS INSTRUMENTATION



BENEFITS OF GCxGC

Comprehensive two-dimensional gas chromatography (GCxGC) is an analytical technique that has been around for over 25 years.

GCxGC increases separation capacity by using two separate columns with orthogonal selectivity connected in series through a modulator (**Figure 1**). The modulator rapidly traps and "injects" the effluent from the first dimension column onto the second dimension.

The result of a GCxGC analysis is a chromatographic plane (contour plot) (**Figure 2**), that depicts the separation over the nonpolar and polar columns. The chromatographic separation space is dramatically increased compared to a conventional 1D-GC.

Other benefits of GCxGC are structured two-dimensional chromatograms (i.e. contour plots), and sensitivity enhancement. Research has shown the advantages of GCxGC in a wide variety of applications (e.g. environmental, metabolomics, petroleum, food safety, fragrance).

The merits of GCxGC as a separation science are clear, but how will it benefit a routine laboratory?



[View the full article "Benefits of Comprehensive Gas Chromatography \(GCxGC\) for Routine Laboratory"](#)

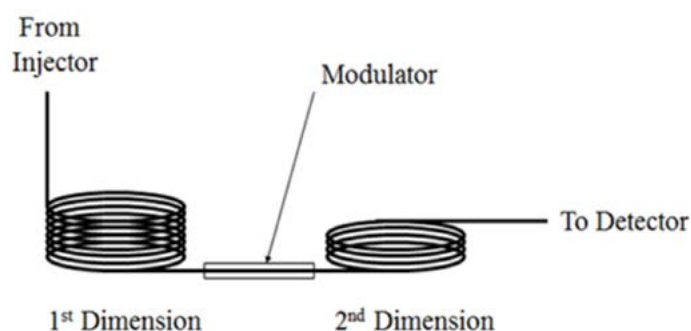


Figure 1: Principle of GCxGC

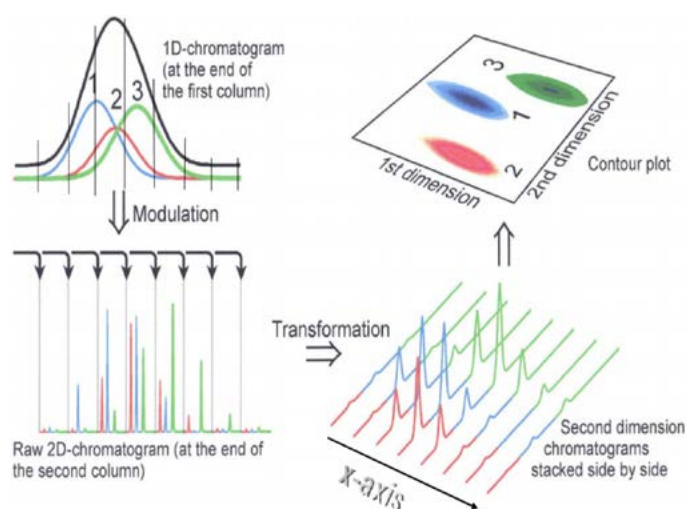


Figure 2: Data Conversion for Visualisation



BENEFITS OF TIME-OF-FLIGHT MASS SPECTROMETRY

A time-of-flight mass spectrometer (TOFMS) for gas chromatography (GC) (**Figure 3**) is the right choice for complex samples, targeted and non-targeted analysis and fast GC or GCxGC.

Time-of-flight mass spectrometry (TOF-MS) is probably the simplest method of mass measurement to conceptualise. The ion's mass-to-charge ratio is determined via a time measurement (Figure).

The ability to collect a full mass range without sacrificing data acquisition speed or sensitivity is perfectly suited for non-targeted analyses. Using a non-targeted approach is beneficial for discovery-type work. A TOFMS spectrum has better spectral continuity across a peak than with a scanning mass analyser (**Figure 4**). Spectral continuity is important for maximising the performance of mass spectral deconvolution algorithms, which results also in higher library matches.

A targeted analytical method also benefits from acquiring a full mass range. Data processing methods including the Target Analyte Finding feature can be used for both qualitative analysis of sample data and quantitation.

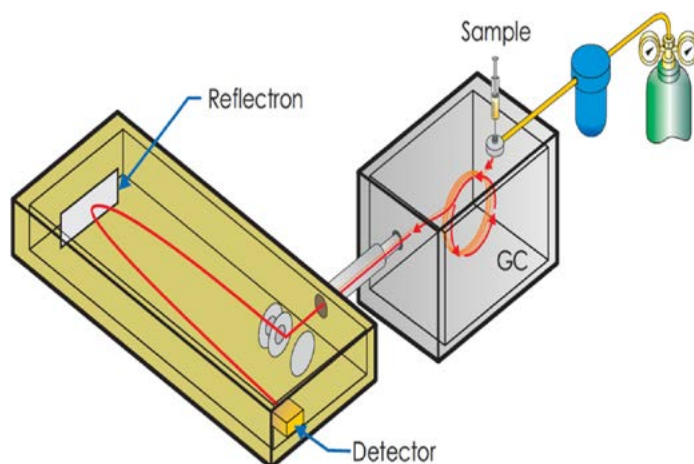


Figure 3: GC-TOFMS Setup

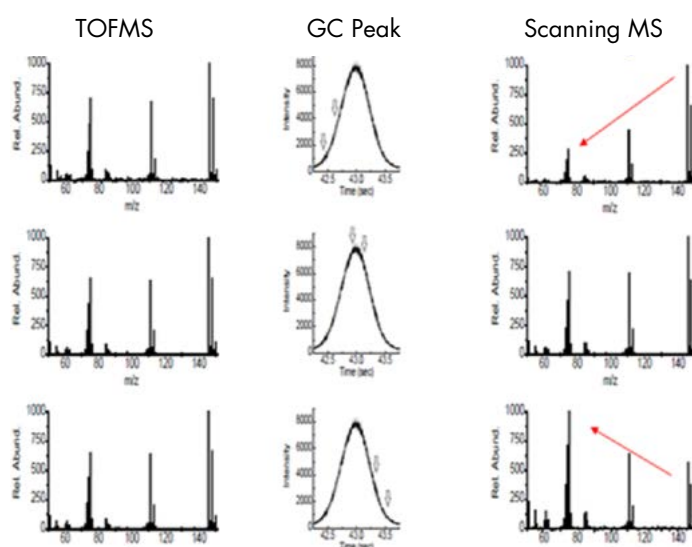


Figure 4: Spectral Continuity



View the full article "Benefits of Equipping your Lab with a Time-of-Flight Mass Spectrometer"



SPECIFIC LECO GC-TOFMS INSTRUMENT FEATURES



STAY CLEAN®

ION SOURCE STABILITY

Fouled ion sources and related issues are often time consuming to diagnosis and resolve. A definitive diagnosis can only be achieved after other preventative maintenance steps (inlet maintenance, column trimming, etc.) have been tried and tested. Once the source has been pinpointed as the issue, users have to clean the source before proceeding.

Even routine, scheduled preventative cleaning leads to system downtime. In less controlled environments the incremental contamination of an ion source may not be noticed until long past the point of compromised results or impacting the stability of the overall system.

Worse still, tuning routines will typically compensate for the loss in signal by increasing various voltages, not the least of which is at the detector. This decreases the detector's operational life, requiring additional maintenance time to resolve.

For these reasons, LECO has specifically designed the PEGASUS® BT systems with an ion source (**Figure 5**) that virtually eliminates the need for removal and cleaning.

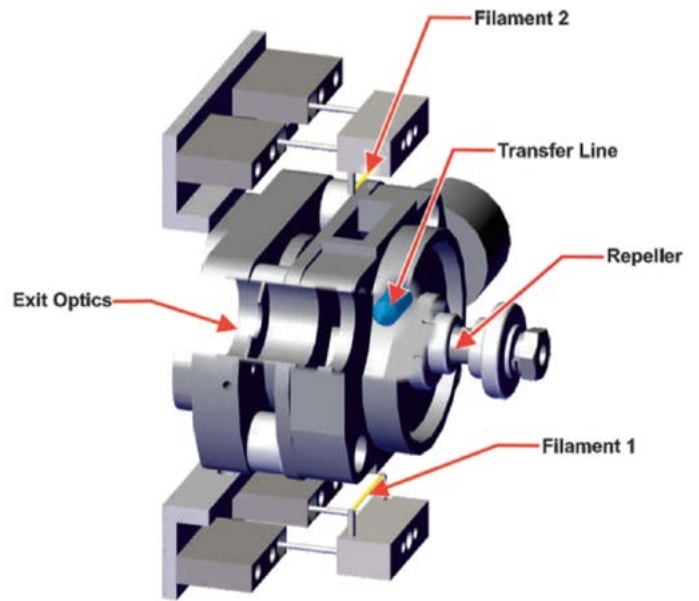


Figure 5: LECO StayClean® ion source



View the application note, which provides significant evidence that the LECO StayClean® ion source actually stays clean.

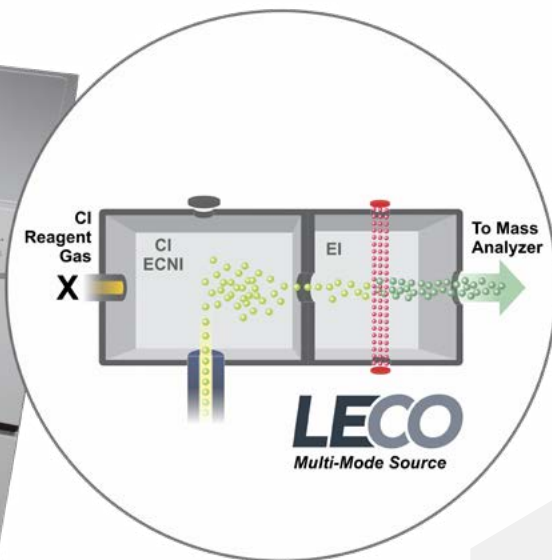
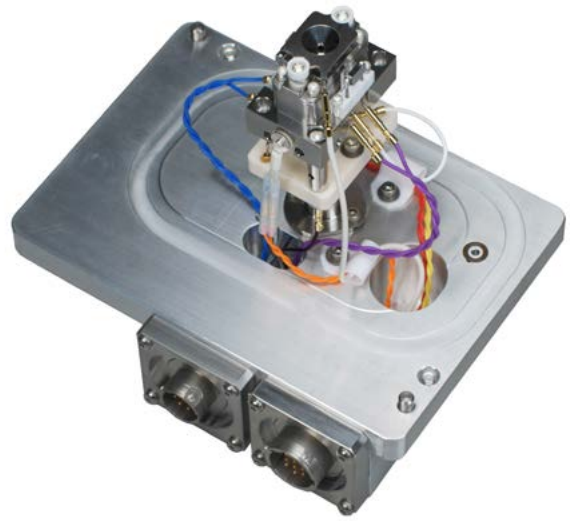


LECO MULTI-MODE SOURCE™ IONIZATION SOURCE FOR GAS CHROMATOGRAPHY MASS SPECTROMETRY

The innovative Multi-Mode Source™ (MMS™) takes all of the advantages of the three most common ionization modes – Electron Ionization (EI), Positive Chemical Ionization (PCI), and Negative Chemical Ionization (NCI/ECNI) – and combines them into one easy-to-use source. No more hardware switching, no more alignment issues: with the MMS, changing ionization modes is as easy as a click of a button.

The new MMS has great mass accuracy and high resolution on pseudo-molecular ions, which complements the traditional Electron Ionization Source (HR-EI) to provide the comprehensive characterization of unknowns. By not touching the hardware, peaks stay aligned between the ionization modes. Each of the three modes is available for GC-MS and GCxGC-MS analyses on both the PEGASUS® GC-HRT+ and the *Pegasus* GC-HRT+ 4D.

Don't limit yourself to just one approach. Ask about the new MMS to see what you've been missing!



LECO MODULATOR PORTFOLIO

GCxGC offers dramatic improvements over traditional GC for the analysis of complex mixtures. This is due to significantly increased chromatographic resolution. The modulator, considered the heart of the GCxGC system, is a device which injects the effluent from the primary column to the secondary column. There are two primary forms of modulators in GCxGC; thermal- and flow-based. These techniques are described in general terms, but with focus on flow modulation.

Thermal-based modulators (**Figure 6**) rely on a cooling mechanism to trap eluent from the first column, followed by heating to inject the eluent onto the second column for further separation. These modulators use of a cryogen such as liquid nitrogen for optimal cold-trapping performance.

Flow-based modulation (**Figure 7**) relies on either switching valves to inject on-column, or in some cases, combining valves with highly different flows to flush a sample loop onto the second column. Both types provide a GCxGC alternative that is virtually consumable-free. The choice of which GCxGC approach is most appropriate depends on the application that will be performed on a particular system. ^

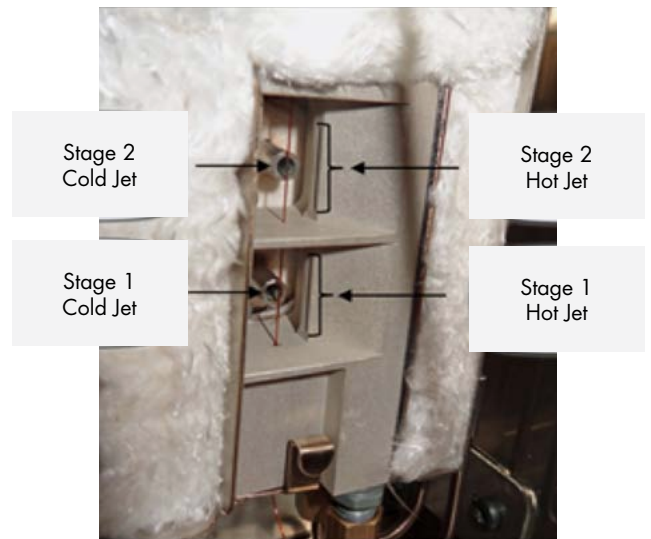


Figure 6: Thermal Modulator



Figure 7: Flow Modulator



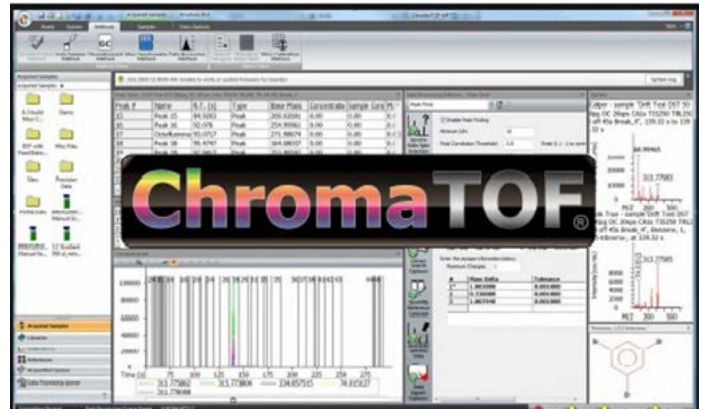
[View the full article FLUX™ GCxGC: The operation, use, and concepts behind a diverting flow technique](#)



LECO ChromaTOF® SOFTWARE

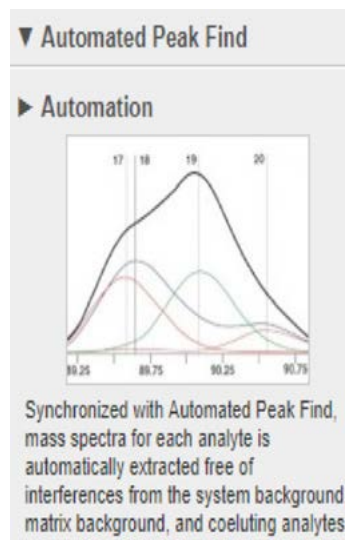
LECO's ChromaTOF software is uniquely designed to process and analyse the large amounts of data that are acquired with our time-of-flight instruments. ChromaTOF offers seamless control of both the instrument and its accessories, as well as an intuitive interface with highly integrated data processing.

ChromaTOF is the first mass spectrometry data system to fully accommodate multidimensional chromatographic data (GCxGC).



Benefits of LECO ChromaTOF

- Single software platform
- Automatic tuning within user-defined Quality Control methods
- Intuitive Acquisition Method Setup
- Automated Peak Find using Non-Target Deconvolution and Library Search
- Target Analyte Finding and Quantification
- Semi-Quantitative Analysis for the reporting of non-calibrated compounds
- Reference Compare tools for sample comparison
- GCxGC enhanced graphics and optimisation tools (Classifications, Filters)
- Automatically export data to PDF, CSV, ANDI MS, NETCDF, or Raw file formats



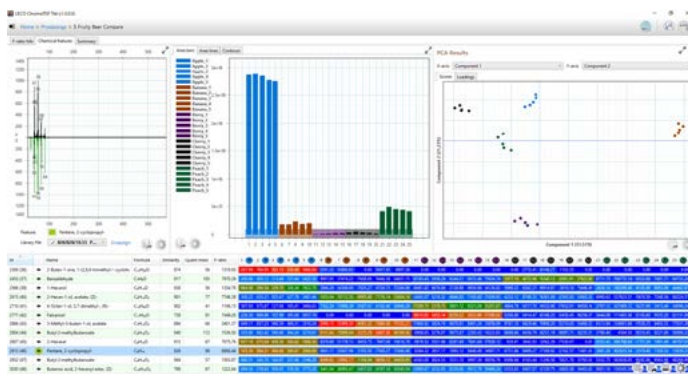
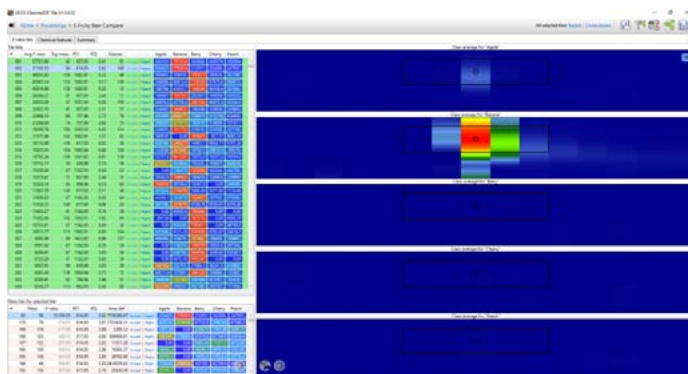
LECO ChromaTOF® TILE ANALYTICAL SOFTWARE

The volume of GCxGC data can quickly become overwhelming. Multiple tables of thousands of analytes can require months of data mining at a pixel level to find the minute differences between data sets, and even those results are plagued with false positives from normal chromatographic variation.

ChromaTOF Tile is an enabling technology that has reduced our peak picking time from 10 days to 10 minutes. We are now comparing groups of peak-rich samples from complex studies that would have previously required complicated, custom-built solutions.

Benefits of LECO ChromaTOF Tile

- ChromaTOF Tile is a separate, stand-alone product to be used in conjunction with ChromaTOF brand software
- All of the tables and plots throughout the interface are exportable for more efficient reporting and to allow you to do more with your data
- Clean library-searchable spectra is generated from the tiling process
- Areas of the tiles are used to approximately quantify trends across the samples



SEPARATION SCIENCE PRODUCT PORTFOLIO



LECO
EMPOWERING RESULTS

SEPARATION SCIENCE PRODUCTS



PEGASUS® BT GC-TOFMS

- Industry-leading sensitivity helps you find and quantify an unlimited number of analytes, while proprietary deconvolution algorithms yield clean, high quality spectra
- A complete historical record of all components for each sample is retained for future data mining
- The tried-and-tested reliability and durability of our Pegasus brand in a convenient benchtop unit

PEGASUS® BT 4D GCxGC-TOFMS

- Enhanced sensitivity by coupling our benchtop Pegasus BT with our high performance GCxGC thermal modulation system
- Ability to interrogate challenging samples where the best sensitivity is needed
- Unique and powerful ChromaTOF® brand software simplifies quantitation and analyte identification with features such as Non Target Deconvolution® (NTD®), Target Analyte Find, library searches, and more
- StayClean® ion source eliminates the need for source cleaning

QuadJet™ SD

- Enhanced separating power for complex sample analysis
- Easy-to-use ChromaTOF®-based software provides acquisition processing and reporting functionality within a single package
- Classification software feature simplifies component identification
- Available Cryogen-free modulator eliminates the need for LN2 dewars



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SEPARATION SCIENCE PRODUCTS



PEGASUS® GC-HRT+ GC-TOFMS

- The highest performance TOF mass spectrometer for the GCMS market
- Folded Flight Path® (FFP®) technology allows users to achieve resolutions of up to 50,000
- Employs ChromaTOF® software with automated High Resolution Deconvolution® (HRD®) and formula generation for seamless identification of unknowns, plus compatibility with standard GCMS libraries
- Spectral Analysis Toolkit harnesses the power of Mass Defect, Van Krevelen, and RDBE plots to take your unknown analysis to a new level
- 1 ppm mass accuracy identifies unique molecular formula
- Encoded Frequent Pushing® (EFP®) contributes to increased sensitivity, expanded dynamic range, and much more

PEGASUS® GC-HRT+ 4D GCxGC-TOFMS

- Combining the highest performance GCxGC and TOF on the market gives users an unprecedented ability to interrogate complex sample
- Find more analytes than ever before and identify components with the ultimate confidence
- With mass accuracies of 1 ppm and peak capacities at least two times greater than anywhere else in the marketplace
- The industry's most established GCxGC systems; thermal modulation with liquid nitrogen or cryogen-free versions
- Chemical Ionisation source (HR-CI) provides the same mass accuracy and high resolution on pseudo-molecular ions which complements the traditional Electron Ionisation source (HR-EI) to provide comprehensive characterisation of unknowns
- Integrated software platform acquires data, controls all hardware, and analyses and reports results with a high level of automation; tailored to get the most out of HR data



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FOOD TESTING APPLICATION COMPENDIUM

> Pesticides in Tomato

> Terpene Profiles in Cannabis

> Sensory of IPA Beer

> Volatiles in celery

> Fats in Food Products

> Pesticide Residue in Strawberries

> Non-target Detection of Pesticides

> Roast Level Differentiation of coffee

> Differentiation of honey aroma

> Yeast Metabolite Characterisation

> Differential Analysis of olive oils

> Pesticides in Tobacco

> PCBs in fish oil supplement

> Determining MOSH/MOAH



DETERMINATION OF PESTICIDES IN TOMATO BY GCxGC-TOFMS WITH PEGASUS® BT 4D



The tomato is one of the most consumed crops, globally. It's annual production is currently around 130 million tons. The top 5 largest tomato producing countries are: China, EU, India, USA, and Turkey. They account for 70% of global production.

Most freshly harvested tomatoes are immediately processed into products such as juice, puree and paste, ketchup/sauce or canned whole. The presence of pesticide residues in such products can cause a number of adverse health effects. Therefore, the identification and quantitation of pesticides in tomatoes is an important task for food control authorities. A GCxGC-TOFMS workflow, including a traditional QuEChERS extraction

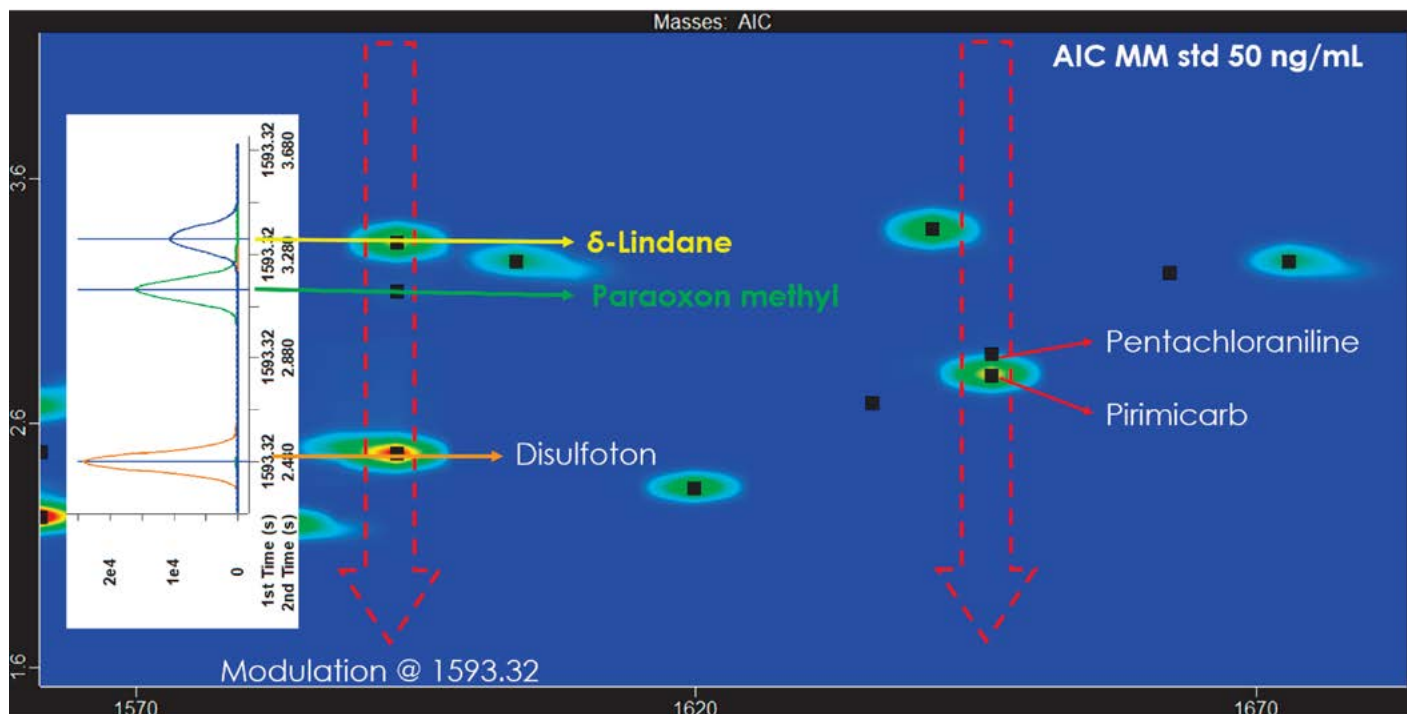
step, was developed for the detection and quantitation of targeted pesticides in peeled tomatoes. GCxGC technology significantly increases the separation efficiency, and ultimately allows a better separation of the target and non-target analytes from the matrix interferences. This, in combination with LECO's Pegasus BT 4D sensitivity, fast acquisition and deconvolution benefits, allowed the measurement of all the pesticides investigated, at required limits of detections to be performed easily and accurately.

Key Words

- # Pesticides
- # Food
- # GCxGC
- # TOFMS
- # Qualitative and Quantitative Analysis



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An example of the enhanced resolving power of the GCxGC technology, which highlights the chromatographic separation on the "y" axis of the contour plot.

Instrument: LECO PEGASUS® BT 4D



DETERMINING TERPENE PROFILES OF CANNABIS STRAINS USING GC AND GCxGC WITH HIGH PERFORMANCE TOFMS



Cannabis is a complex mixture of compounds (>500) including cannabinoids, terpenes, terpenoids, non-cannabinoid phenols, nitrogenous compounds, flavonoids, and contaminants such as residual solvents and pesticides. It is the total composition of cannabis that is important in determining its potency and medicinal effectiveness. This "entourage effect" is a synergistic relationship that exists between terpenes, cannabinoids, and potentially other cannabis components. Identification of cannabis components is critical for the "chemical categorization" of different cannabis strains. GC-TOFMS and GCxGC-TOFMS were used to analyze terpenes from different strains of cannabis

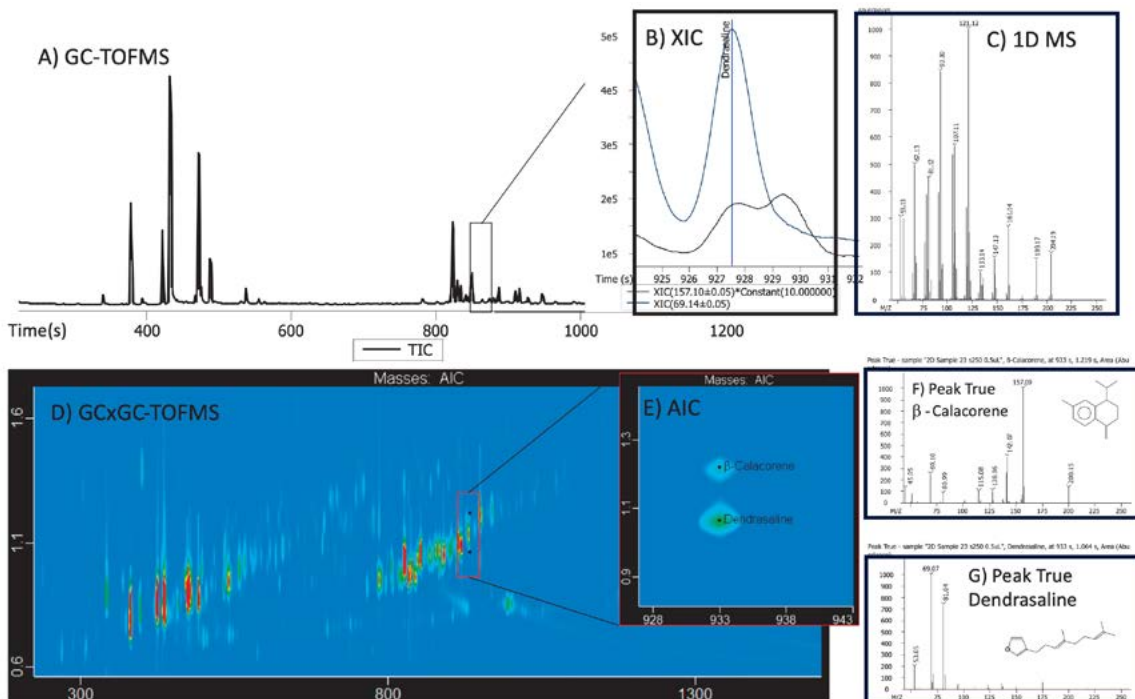
GCxGC-TOFMS analysis resulted in a >4x increase in peaks detected and >50% increase in terpenes identified over those found with single dimension GC-MS. This additional information was a direct result of coupling enhanced multi-dimensional chromatography with high performance TOFMS. Robust characterisation was achieved through spectral similarity searches of large, well-established databases, with the enhanced GCxGC separation and high quality deconvoluted mass spectral data therefore providing increased confidence in these determinations.

Key Words

- # GCxGC
- # PEGASUS® BT 4D
- # Cannabis
- # GC-TOFMS
- # High Matrix



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A) GC-TOFMS TIC for indica terpenes; B) Extracted ion expansion showing coelution in 1D GC-MS; C) Spectrum derived from 1D GC-MS coelution; D) GCxGC-TOFMS contour plot; E) Expansion showing GCxGC separated sesquiterpenes dendrasaline and β -calacorene which coeluted in 1D GC-TOFMS; F,G) Clean spectra for chromatographically separated β -calacorene and dendrasaline

Instrument: LECO PEGASUS® BT 4D



CORRELATION OF CHEMICAL AND SENSORY DATA TO TRACK AGING OF AN AMERICAN IPA BEER AT DIFFERENT STORAGE TEMPERATURE



Shelf stability and how products change with age and storage condition is an important topic to both manufacturers and consumers. Understanding changes in the aroma profile over time can help to understand the shelf life of that product and possibly how it can be extended.

Gas chromatography coupled to time-of-flight mass spectrometry (GC-TOFMS) is well-suited for investigating shelf stability applications because it provides non-targeted aroma profile characterisation. Sensory analysis is also common for shelf-stability and general product quality applications. These are complementary analytical techniques and using them together is beneficial.

The sensory analysis provided overall freshness and quality scores for each sample, while the non-targeted GC-MS analysis provided comprehensive aroma profile chemical data.

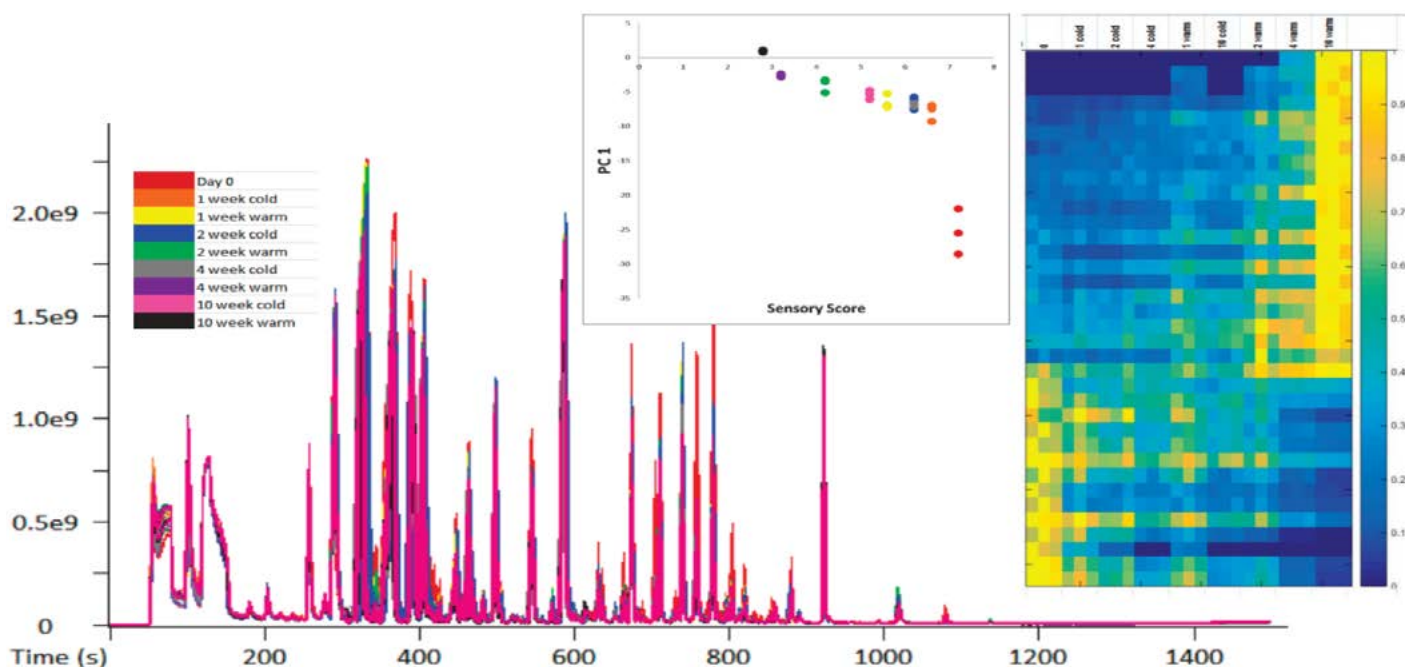
These data were mined for specific analytes of interest and were also reviewed to discover inherent trends and differences in the aroma profile that correlated with the sensory analysis results.

Key Words

- # Beer
- # Shelf-Stability
- # Aroma Profile
- # Sensory Analysis
- # HS-SPME
- # GC-TOFMS
- # Deconvolution
- # PCA



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Overlaid chromatograms from all samples are shown. A plot showing the correlation of the sensory scores with the PC1 scores from the chemical analysis shows good agreement. The heat map highlights peak areas of analytes that correlate with sensory score.

Instrument: LECO PEGASUS® BT



DISCOVERING THE SCENT OF CELERY HS-SPME, GC-TOFMS, AND RETENTION INDICES FOR THE CHARACTERISATION OF VOLATILES



Determining and identifying individual analytes within a complex sample can provide important characterisation information for better understanding of a sample, product, or process. This type of exploratory analysis is readily accomplished with GC-TOFMS, as it provides non-targeted data with every acquisition.

The PEGASUS® BT adds to the chromatographic separation by taking advantage of the full mass range data with mathematical deconvolution to further separate chromatographic coelutions.

The ChromaTOF® software contains tools to help streamline data analysis. For example, retention index methods can be created to calculate and compare retention index information for each peak in the table to support or improve library identifications.

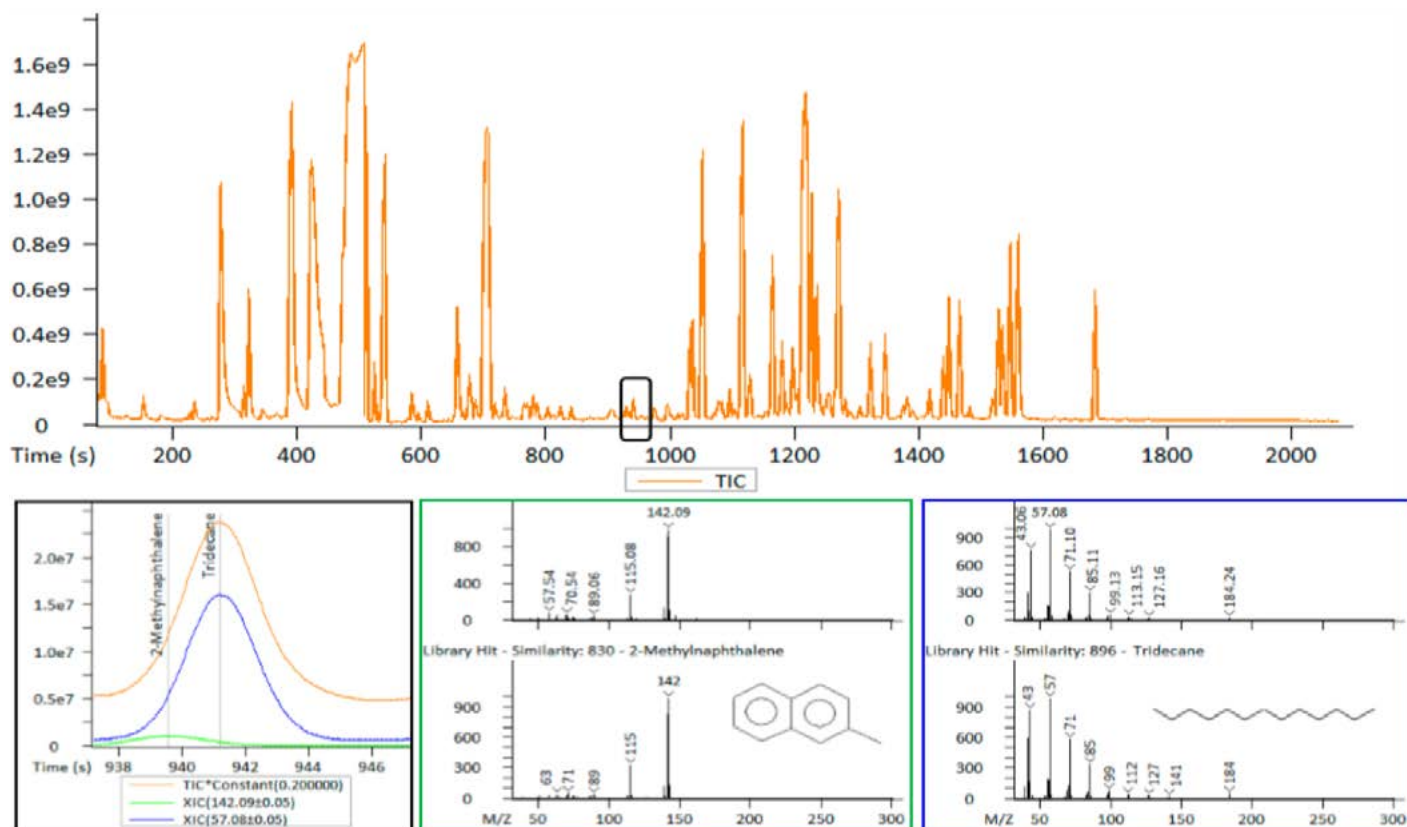
A celery sample was analysed with HS-SPME coupled to GC-TOFMS. The resulting data are reviewed, with retention index information providing valuable support to analyte identifications.

Key Words

- # GC-TOFMS
- # GC-MS
- # PEGASUS® BT
- # HS-SPME
- # Celery
- # Retention Index



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The Total ion chromatogram (TIC) for a celery sample is shown. One example of coelution is highlighted.

Instrument: LECO PEGASUS® BT



ANALYSIS OF FATS IN FOOD PRODUCTS WITH GC-TOFMS



Reporting the fat content of food on packaging material is required for many products. For this reason, the ability to detect and distinguish different types of fats is important.

Official methods for the detection of fats (total, saturated and unsaturated) uses GC paired with FID. As part of this method, the distinction of some cis and trans isomers is also accomplished, which is desirable information is trans related to the ban on fats. In this work GC with TOFMS was used

for fatty acids extracted from a variety of butter, margarine, and shortening samples. Applications that typically use FID can benefit from switching to MS, as demonstrated here.

Chromatographically coeluting analytes can sometimes be distinguished with deconvolution of the MS data, and analytes that are not present in the standard can be tentatively identified through searching of spectral databases.

Key Words

GC-TOFMS

GC-MS

PEGASUS® BT

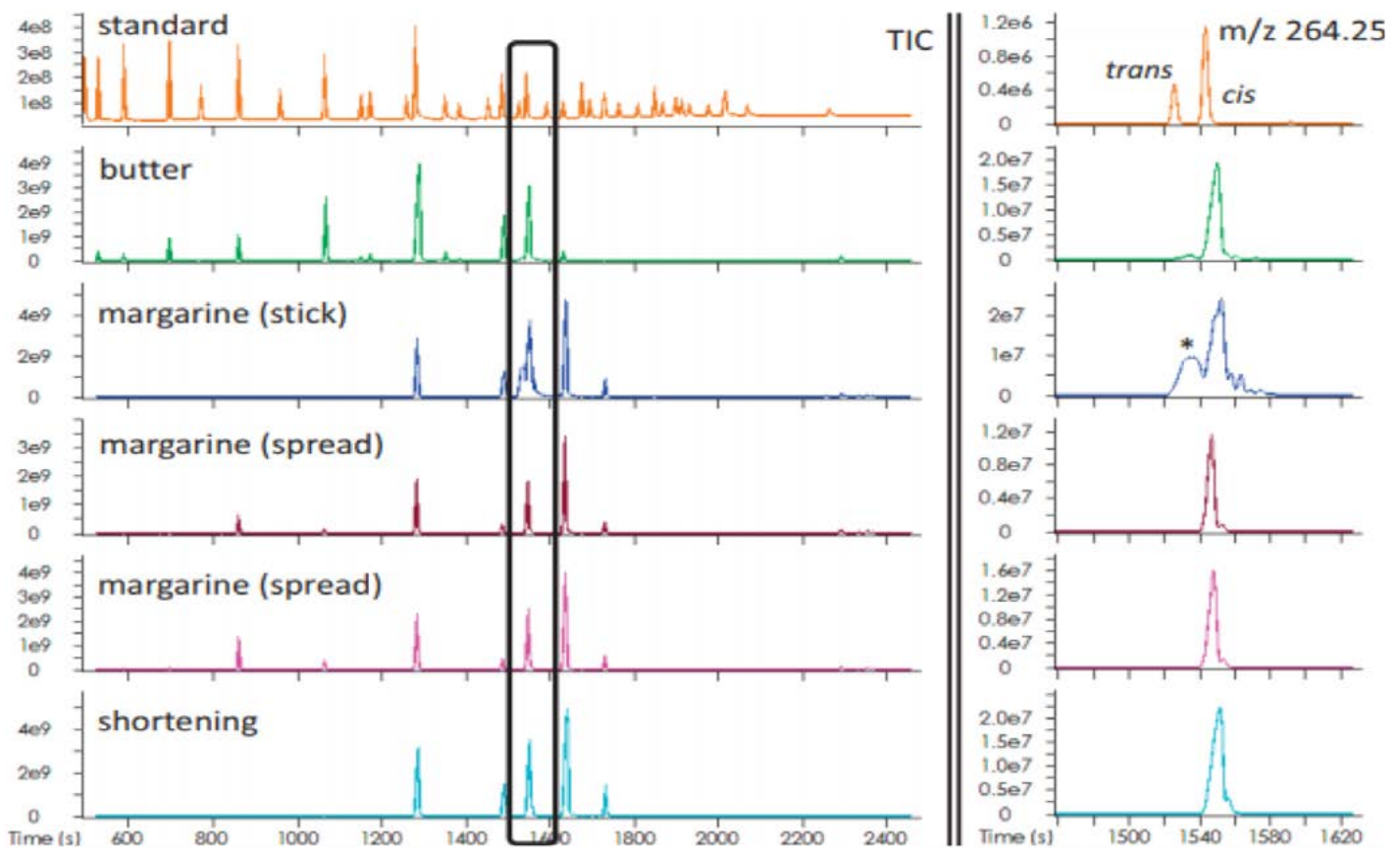
Deconvolution

Fatty Acids

FAMES



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TIC chromatograms for the standard and each of the screened samples. The cis and trans fatty acids are highlighted here with XIC 264.25 shown.

Instrument: LECO PEGASUS® BT



FAST PESTICIDE RESIDUE ANALYSIS IN FOOD WITH A BENCHTOP GC-TOFMS: PEGASUS® BT



Sample throughput including data processing is an important factor to consider when performing routine analyses. In this application note we used the speed and power of TOFMS to shorten the runtime of a standard pesticide residue analysis by using a 15 m column instead of a standard 30 m column without loss of analytical performance.

One objective was to maximise throughput without introducing a significant number of additional chromatographic coelutions not separable by deconvolution. The goal was for the same number of spiked pesticides to be detected under both analytical methods.

LECO's proprietary deconvolution algorithm, embodied as NonTarget Deconvolution™, was leveraged to maintain exceptional peak fidelity of the qualitative analysis, while the Target Analyte Find feature was utilised for robust quantitation and to establish method detection limits for organonitrogen pesticides spiked in QuEChERS strawberry extracts.

Key Words

Pesticide Residue Analysis

BT

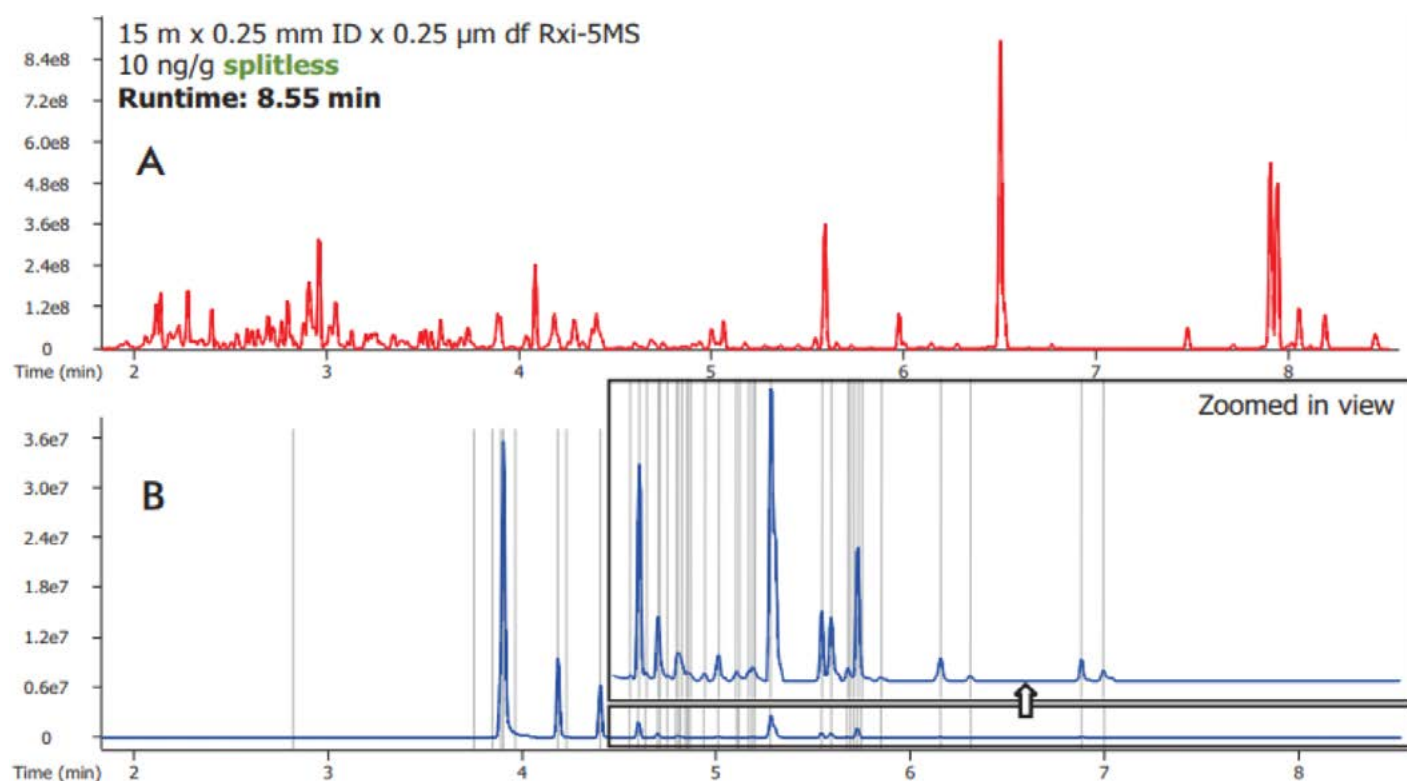
Quantitative Analysis

Qualitative Analysis

High Throughput



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Analytical ion chromatograms (AIC) of a fortified strawberry QuEChERS extract; (A) for analytes reported using Peak Find (non-target), and (B) analytes reported using Target Analyte Find.

Instrument: LECO PEGASUS® BT



QUANTITATION AND NON-TARGET DETECTION OF PESTICIDES IN SPINACH EXTRACT WITH PEGASUS® BT 4D



Matrix deleteriously affecting quantitation accuracy of pesticides in food commodities has been well documented and understood.

While significant improvements have been made in sample extraction strategies, cleanup of complex matrices continues to be an issue, especially as limits of detection (LOD) are decreased by various regulatory entities

Combined with the sensitivity available with LECO's Pegasus BT 4D, the ability to achieve required limits of detection, while minimising

matrix interferences to allow successful quantitation and effective identification of non-targeted pesticides, has been demonstrated.

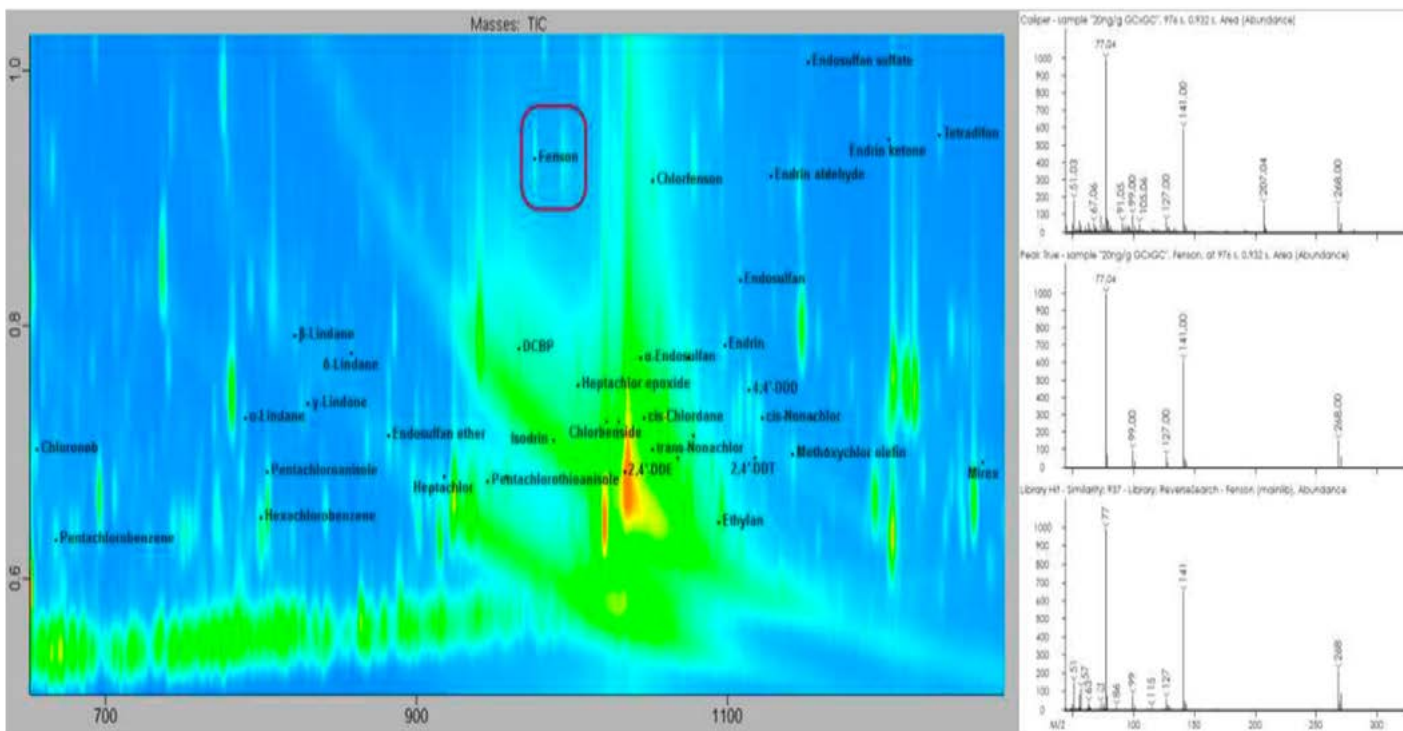
The GCxGC results easily met and exceeded the SANTE 2017 requirements.

Key Words

- # Pesticides
- # GCxGC
- # Quantitation
- # Non-Target Detection



[View Application Note](#)



Section of Contour Plot of the spinach QuEChERS extract spiked with pesticides at 20 ng/g
Instrument: LECO PEGASUS® BT 4D



GC, GCxGC, AND TOFMS FOR CHARACTERISATION AND ROAST LEVEL DIFFERENTIATION OF COFFEE



Coffee is one of the most consumed beverages in the world and the industry around it is an important part of the global economy. As expected with commodities, taste and flavor variation in coffee relate to differences in the variety and geographical origin of the beans, storage and processing conditions, roasting conditions, and brewing methods.

An understanding of these differences can be helpful for quality control, process optimisation, and also for providing information on flavors and characteristics that direct consumers to their preferred styles.

Non-targeted chemical analysis techniques like GC-MS and headspace solid phase micro-extraction (HS-SPME) are used to evaluate the aroma profile. GCxGC increases peak capacity and enhances S/N compared to GC, and also creates structured chromatograms.

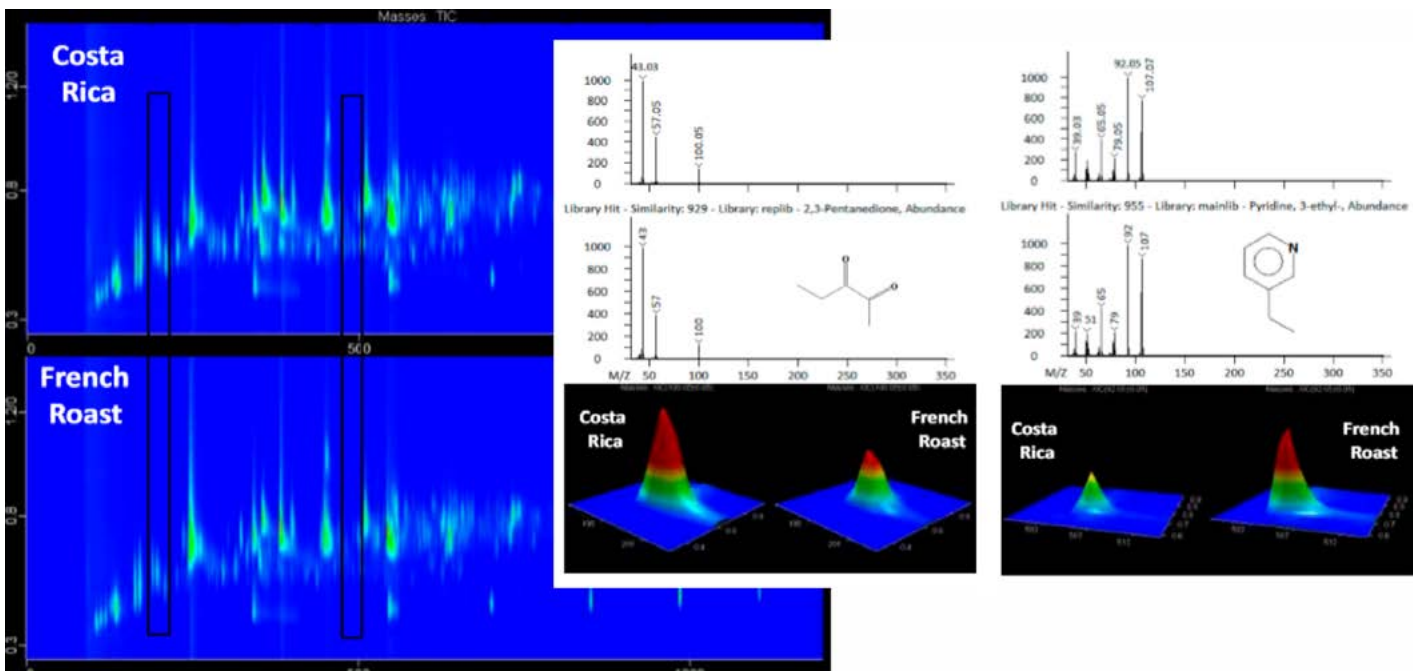
These additional analytical capabilities were explored and led to the detection of more analytes and an improved understanding of these complex samples

Key Words

- # GC-MS
- # GCxGC-TOFMS
- # PEGASUS® BT 4D
- # HS-SPME
- # coffee
- # sample differentiation



[View Application Note](#)



GCxGC chromatograms for coffee from medium and dark roasted coffee beans from Costa Rica are shown. Representative analytes that are present at different levels are shown.

Instrument: LECO PEGASUS® BT 4D



DIFFERENTIATION OF HONEY AROMA PROFILES WITH FLUX™ GCxGC-TOFMS



The aroma profile is the collection of volatile and semi-volatile analytes associated with an individual sample. In food and beverage applications, the aroma profile can be particularly interesting because many of the volatile and semi-volatile analytes are important contributors to the overall odor and flavor.

Gas chromatography (GC) is a useful tool for these types of chemical analyses as volatile and semi-volatile analytes are readily separated. For complex samples, however, the wide range of analytes contributing to the aroma profile can be difficult to separate with GC alone.

In these instances GCxGC can be very useful, adding a second column via a modulating device. The role of the modulator is to inject effluent from the primary column into the secondary column at frequent intervals throughout the primary separation, effectively separating the analytes in both dimensions.

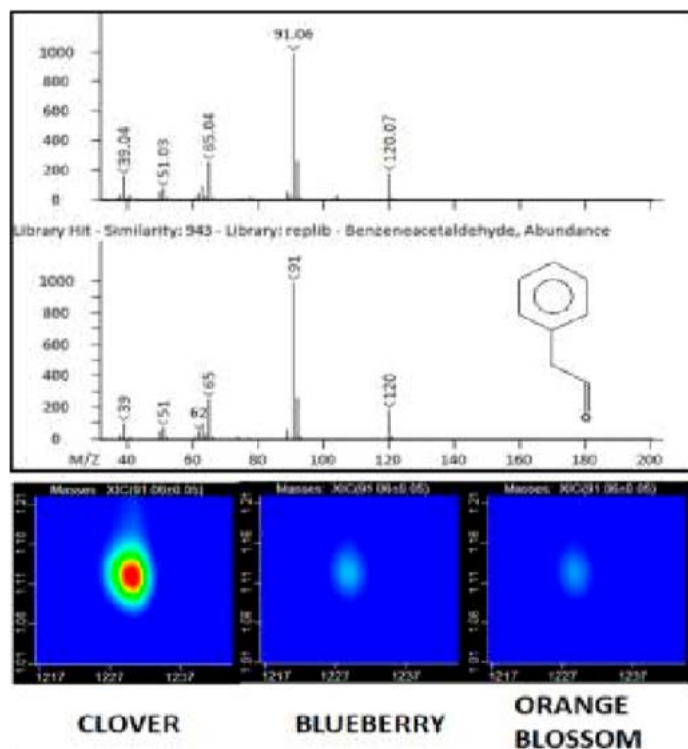
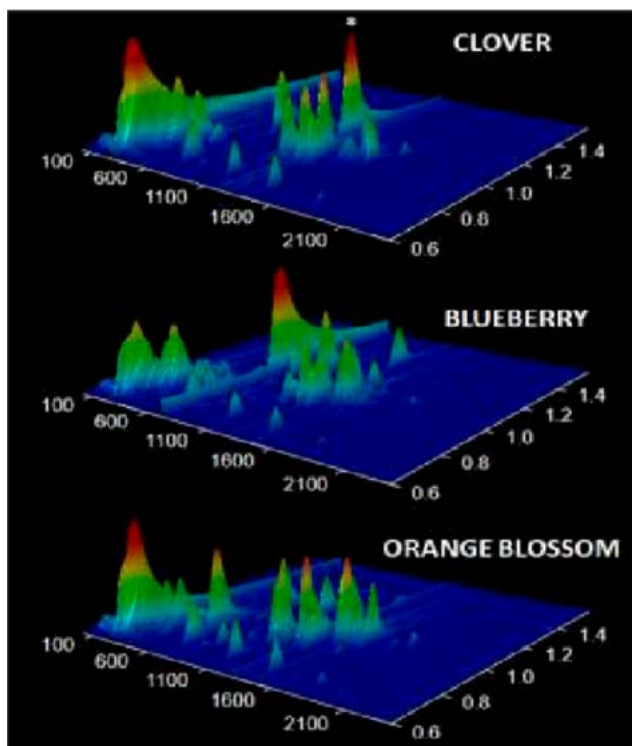
In this work, a robust and easy to use GCxGC system that incorporates a flow-based modulator is paired with a time-of-flight mass spectrometer (TOFMS) for honey aroma profiling.

Key Words

- # Aroma Profile
- # Sample Differentiation
- # HS-SPME
- # GCxGC-TOFMS
- # Flow Modulation



[View Application Note](#)



Three honey varieties (clover, blueberry, and orange blossom) were analysed by GCxGC-TOFMS and compared.

Instrument: LECO PEGASUS® BT 4D



UTILISING THE PEGASUS® GC-HRT 4D FOR IMPROVED YEAST METABOLITE CHARACTERISATION



Yeast has been used since ancient times for fermentation and production of wine. In modern times, the *S. cerevisiae* 2strain is the preferred cell workhorse for the production of bioethanol. Yeast also continues to serve as a model for systems biology and is being studied as a potential “cellular factory” for production of additional sustainable chemicals.

In order for this bioengineering to become realised, the metabolism of yeast must be clearly understood. The biggest bottleneck in metabolomics research and engineering is characterisation of the diverse classes of compounds found in living systems.

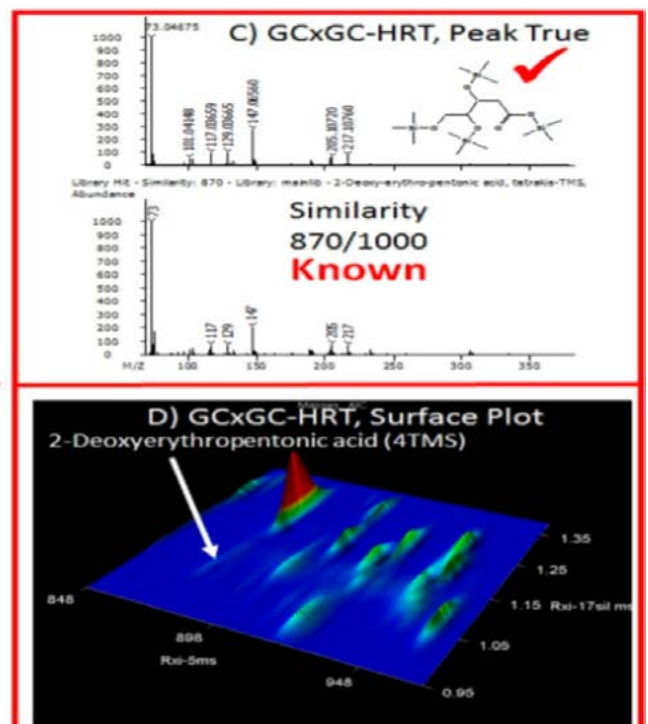
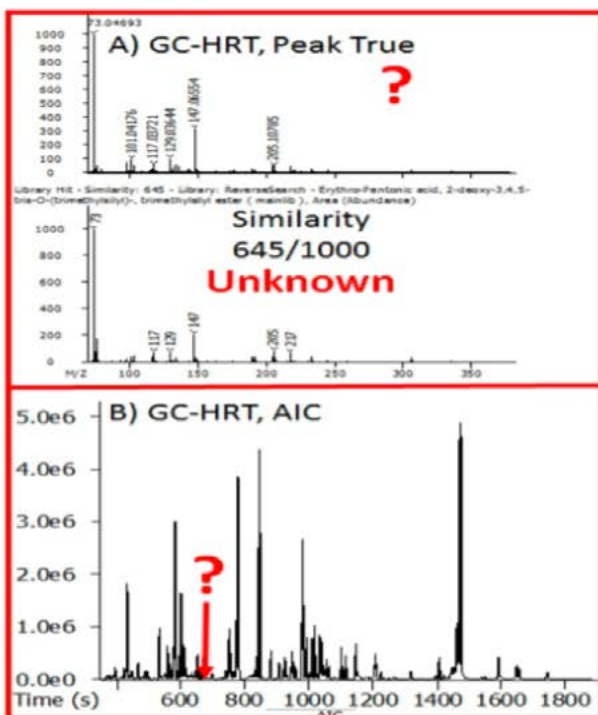
In this study, we explored the utilisation of GC-HRT and GCxGC-HRT for molecular profiling of yeast. Combining the strengths of GCxGC (increased peak capacity, chromatographic resolution, and the ability to provide cleaner spectra) with high resolution and accurate mass capabilities, the *Pegasus* GC-HRT 4D allows researchers to take their metabolomics discovery workflows to the next level.

Key Words

- # Yeast
- # Metabolomics
- # Gas Chromatography
- # High Resolution Mass Spectrometry



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GC-HRT Peak True Mass Spectrum and AIC (A, B) vs. GCxGC-HRT Mass Spectrum and Surface Plot (C, D) for Characterisation of 2-Deoxyerythropentonic Acid (4TMS)

Instrument: LECO PEGASUS® HRT 4D



DIFFERENTIAL ANALYSIS OF OLIVE OILS WITH PEGASUS® GC-HRT AND ChromaTOF-HRT® REFERENCE FEATURE



Characterisation of food products, including differential analysis, is important in the food industry for quality control, brand awareness, and authentication of materials and products. GC coupled with high resolution TOFMS isolates individual analytes within complex matrices through both chromatographic and mass spectral resolution and provides confident analyte identifications with industry-leading mass accuracy.

These analytical tools were employed for a nontargeted volatile analysis of aroma and flavor analytes in representative extra-virgin and light olive oil samples from a single manufacturer.

Automated Peak Finding and sample comparison tools, such as “Reference”, within the ChromaTOF-HRT software provide rapid sample characterisations and differentiation to help researchers reliably determine what else is in their sample and if it should be there.

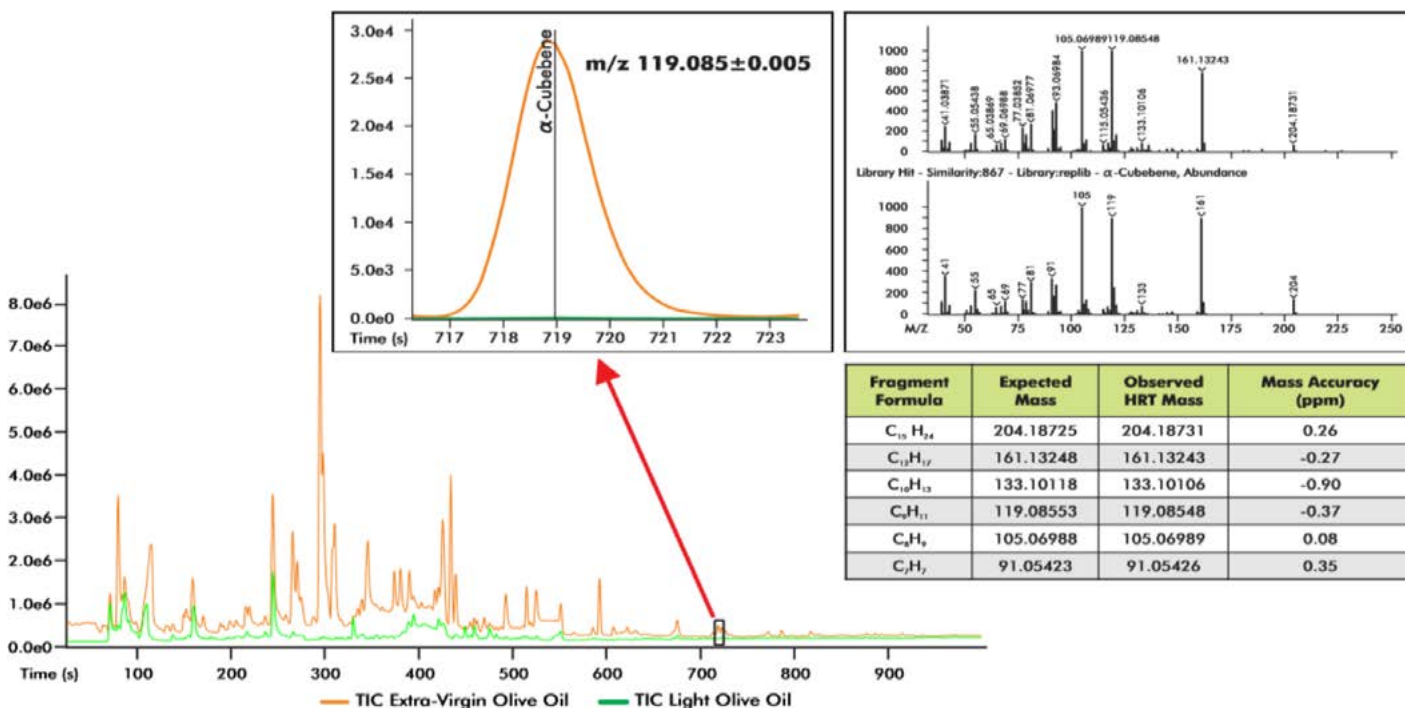
These analysis tools were used to confidently identify differences between the samples which are important in differentiating oil varieties and in determining the source of unanticipated analytes in the samples.

Key Words

- # Olive Oil
- # GC-HRT
- # HS-SPME
- # ChromaTOF Reference
- # Food Fraud
- # High Resolution
- # Accurate Mass



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Representative TIC chromatograms are overlaid for extra-virgin olive oil (orange trace) and light olive oil (green trace) from the same manufacturer. Many analyte differences are apparent and ChromaTOF's Reference feature was utilised to determine analytes unique to each sample with automated processing

Instrument: LECO PEGASUS® HRT 4D



UNAMBIGUOUS PESTICIDE IDENTIFICATION IN CIGARETTE TOBACCO



Tobacco is a complex matrix that can be challenging analytically, often requiring rigorous sample preparation before instrumental analysis which can be prone to false positives and false negatives. High resolution mass spectrometry (HRMS) is necessary to separate ions that have the same nominal mass from one another to ensure that only diagnostic (or characteristic) ions are assigned to any given analyte, thus minimising the risk of false positives and false. These accurate mass measurements are a requisite for accurate chemical formula determination and for detecting analytes in complex matrices so as to avoid isobaric interferences or to separate

coeluting analytes. The current objective was to confidently identify pesticide residues in cigarette tobacco with limited sample cleanup.

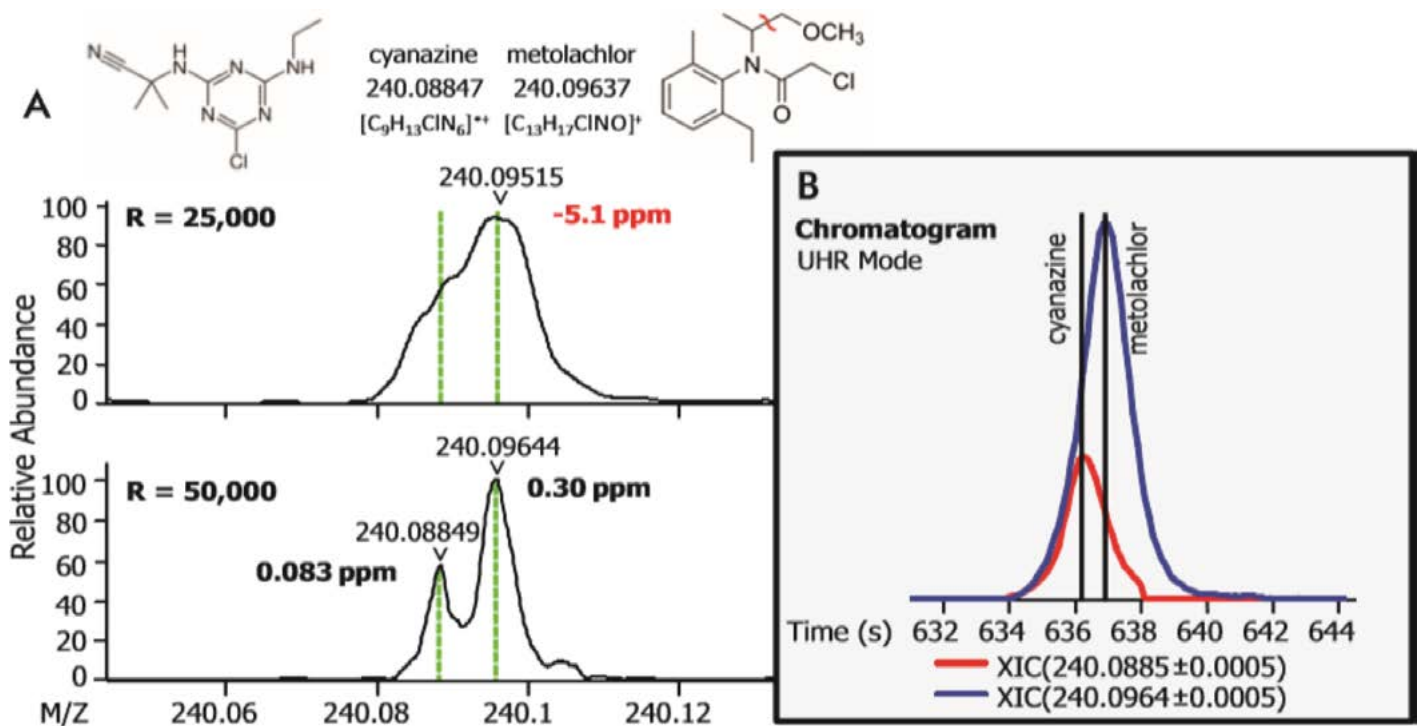
QuEChERS sample preparation was followed by gas chromatography high resolution time-of-flight mass spectrometry on a LECO PEGASUS® GC-HRT. The user can confidently identify compounds in this challenging matrix, while maintaining the ability to screen for other components such as additives and natural ingredients in tobacco.

Key Words

- # High Resolution Time-of-Flight Mass Spectrometry
- # Accurate Mass
- # Pesticides
- # Tobacco
- # Food Safety



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The pesticides cyanazine and metolachlor have isobarically convoluted masses at a 2:1 ratio that could only be resolved with a mass resolution greater than 40,000.

Instrument: LECO PEGASUS® HRT 4D



ANALYSIS OF POLY-CHLORINATED BIPHENYLS (PCBS) IN FISH OIL SUPPLEMENTS BY GAS CHROMATOGRAPHY WITH HIGH PERFORMANCE-TIME-OF-FLIGHT MASS SPECTROMETRY



The American Heart Association recommends eating two servings of fish per week, specifically fish with high fat content such as tuna and salmon.(1) This recommendation stems from the fact that they contain relatively high quantities of omega fatty acids.

Instead of eating fish, many people take fish oil supplements. But there are major concerns over the accumulation of fat-soluble, persistent organic pollutants (POPs) in the oil.

In this study, the advantages of using LECO's PEGASUS® GC-HRT to analyse complex matrices such as fish oil are highlighted.

The resolving power and sensitivity of the high resolution time of flight mass spectrometer with Folded Flight Path™ (FFP™) technology are critical for targeting specific analysis of trace components in complex mixtures.

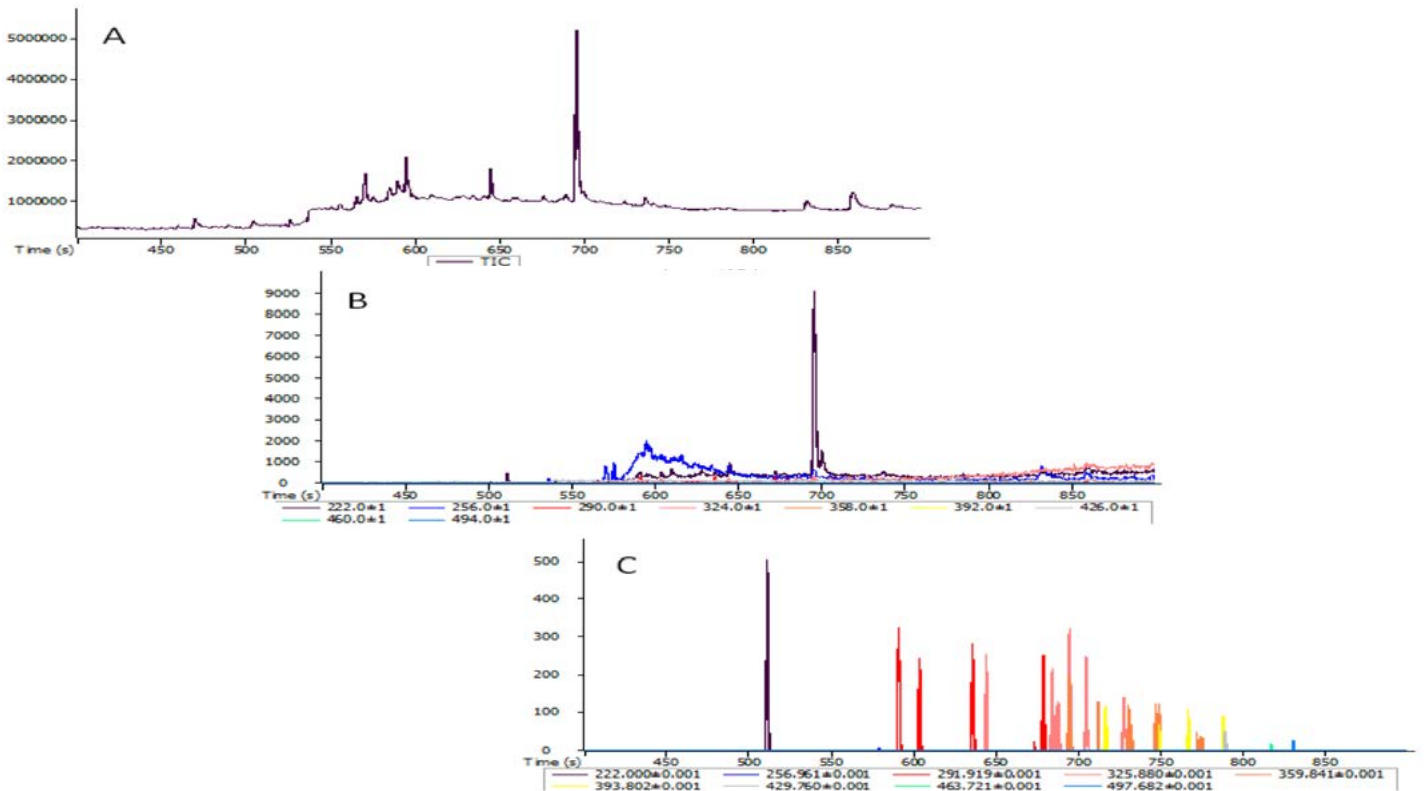
The instrument minimises background contamination and calibration problems typically associated with PCB congener analysis.

Key Words

- # High Resolution Time-of-Flight Mass Spectrometry
- # Persistent Organic Pollutants
- # Fish



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Fish Oil +10 ng/g PCB Standard – TIC (A), XIC at Unit Resolution (B), XIC at R = 25,000 (C).

Instrument: LECO PEGASUS® HRT



DETERMINING MOSH/MOAH WITH GC×GC-TOFMS



Food contamination with mineral oil hydrocarbons such as mineral oil saturated hydrocarbons (MOSH) and mineral oil aromatic hydrocarbons (MOAH) has been a growing concern since 2012, when the European Food Safety Authority flagged them as a potential health concern. With respect to the analytical methods, two choices have been proposed so far for the quantification of these substances: 1) an off-line method consisting of a solid phase extraction-SPE-, followed by a GC-FID analysis and 2) the most popular, on-line LC-GC-FID method. However, depending on the matrix, both methods sometimes result in inaccuracies and provide challenges from a qualitative/quantitative point of view, due to the lack of an associated confirmatory method (i.e. GC-MS, GC×GC-MS). In this respect, LECO's PEGASUS® BT 4D GC×GC-TOFMS system can help to unveil the complexity

of contaminated food samples, providing superior chromatographic resolution and identification capabilities. In fact, as also suggested by the EFSA opinion, the GC×GC-MS technology needs to be used as a confirmatory tool in case of uncertain results. In addition to the increased separation power and identification confidence, LECO ChromaTOF's "Classifications" feature can be routinely applied to quickly gather information from the samples about the presence of a specific chemical class such as hopanes or steranes, or the recently emphasized 3-7 rings from MOAH. This note describes a GC×GC-TOFMS workflow to separate and identify the MOSH/MOAH fractions from the biogenic substances normally occurring in a spice sample, namely Cumin.

Key Words

- # Food Safety
- # GC×GC-TOFMS
- # MOSH/MOAH



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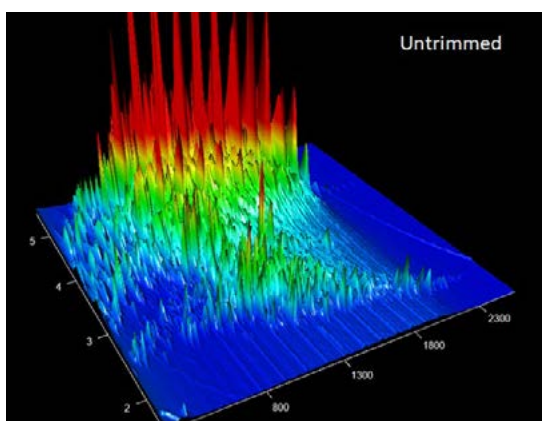


Figure 1

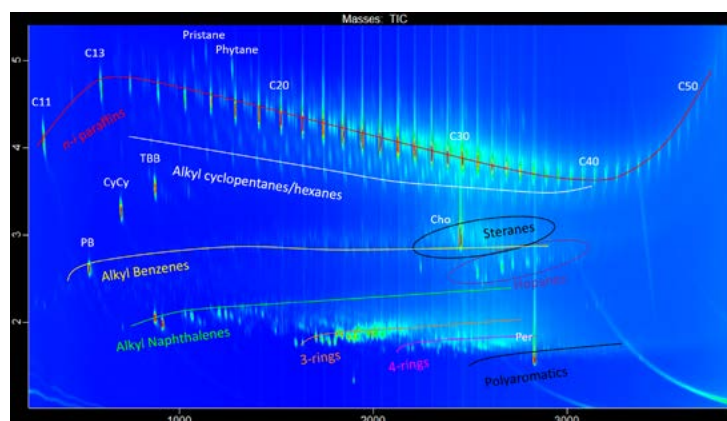


Figure 2

Figure 1: GC×GC Surface Plot of a contaminated food sample

Figure 2: GC×GC-TOFMS contour plot from the VGO sample + the MOSH/MOAH internal standards (VGO-IS)

Instrument: LECO PEGASUS® BT 4D



FOOD TESTING BIBLIOGRAPHY



FOOD TESTING BIBLIOGRAPHY

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FOOD TESTING BIBLIOGRAPHY

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Food-Lab International Interview with Dr. Ralf Löscher, Vice President Europe LECO B.V. <i>Authors: Thomas F. W. Kützemeier</i>	GCxGC	eFoodLab 02/2020
Food-Lab International Issue 01/2020 <i>Authors: Thomas F. W. Kützemeier</i>	GCxGC	eFoodLab 01/2020
Quantification of TCA to Detect Cork Taint Fault in Wine <i>Authors: LECO B.V.</i>	GC-TOF-MS	SepScience.com
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Volatile compounds associated with growth of <i>Asaia bogorensis</i> and <i>Asaia lannensis</i> -unusual spoilage bacteria of functional beverages <i>Authors: Hubert Antolak, Henryk Jeleń, Anna Otlewska, and Dorota Kręgiel</i>	GCxGC	Food Research International
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<p>Suspect Screening of Chemicals in Food Packaging Plastic Film by Comprehensive Two-Dimensional Gas Chromatography Coupled to Time-of-Flight Mass Spectrometry</p> <p><i>Authors: Maciej Jarzębski, Wojciech Smutek, Przemysław Siejak, Joanna Kobus-Cisowska, Danuta Pieczyrak, Hanna Maria Baranowska, Jarosław Jakubowicz, Mateusz Sopata, Tomasz Białopiotrowicz, and Ewa Kaczorek</i></p>	GCxGC	Food Hydrocolloids
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FOOD TESTING BIBLIOGRAPHY

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FOOD TESTING BIBLIOGRAPHY

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<p>Diversity and functionality of <i>Bacillus</i> species associated with alkaline fermentation of bambara groundnut (<i>Vigna subterranean</i> L. Verdc) into dawadawa-type African condiment</p> <p><i>Authors: Gabriel B Akanni, Yvette Naudé, Henriëtte L de Kock, and Elna M Buys</i></p>	GCxGC	European Food Research and Technology
<p>Essential oils (EOs), pressurised liquid extracts (PLE) and carbon dioxide supercritical fluid extracts (SFE-CO₂) from Algerian <i>Thymus munbyanus</i> as valuable sources of antioxidants to be used on an industrial level</p> <p><i>Authors: Hamdi Bendif, Khaoula Adouni, Mohamed Djamel Miara, Renata Baranauskienė, Paulius Kraujalis, Petras Rimantas Venskutonis, Seyed Mohammad Nabavi, and Filippo Maggi</i></p>	GCxGC	Food Chemistry
<p>Differentiation of Rums Produced from Sugar Cane Juice (Rhum Agricole) from Rums Manufactured from Sugar Cane Molasses by a Metabolomics Approach</p> <p><i>Authors: Laura Franitza, Luca Nicolotti, Michael Granvogel, and Peter Schieberle</i></p>	GCxGC	Journal of Agricultural and Food Chemistry
<p><i>Verbascum nigrum</i> L.(mullein) extract as a natural emulsifier</p> <p><i>Authors: Maciej Jarzębski, Wojciech Smutek, Mikołaj Kościński, Tomasz Białopiotrowicz, and Ewa Kaczorek</i></p>	GCxGC	Food Hydrocolloids
<p>Analysis of thermotolerance in <i>Brassica napus</i> L.</p> <p><i>Author: Chadwick Bruce Koscielny</i></p>	GC	
<p>The Key Aroma Compounds in Smoked Cooked Loin</p> <p><i>Authors: Monika Kosowska, Małgorzata Majcher, Henryk H Jelen, and Teresa Fortuna</i></p>	GCxGC	Journal of Agricultural and Food Chemistry
<p>NAC-NOR mutations in tomato Penjar accessions attenuate multiple metabolic processes and prolong the fruit shelf life</p> <p><i>Authors: Rakesh Kumar, Vajir Tamboli, Rameshwar Sharma, and Yellamaraju Sreelakshmi</i></p>	GCxGC	Food Chemistry



FOOD TESTING BIBLIOGRAPHY

LECO GCxGC Publications 2018

	Categories	Publication
<p>Metabolomics Reveal Optimal Grain Preprocessing (Milling) toward Rice Koji Fermentation</p> <p><i>Authors: Sunmin Lee, Da Eun Lee, Digar Singh, and Choong Hwan Lee</i></p>	GC	Journal of Agricultural and Food Chemistry
<p>Combined targeted and untargeted profiling of volatile aroma compounds with comprehensive two-dimensional gas chromatography for differentiation of virgin olive oils according to variety and geographical origin</p> <p><i>Authors: Igor Lukić, Silvia Carlin, Ivana Horvat, and Urska Vrhovsek</i></p>	GCxGC	Food Chemistry
<p>Untargeted GC-MS metabolomics reveals metabolic differences in the Chinese mitten-hand crab (<i>Eriocheir sinensis</i>) fed with dietary palm oil or olive oil</p> <p><i>Authors: Qian-Qian Ma, Xiao-Dan Wang, Yan-Yan Cui, Nan-Nan Zhang, Jian-Guang Qin, Zhen-Yu Du, and Li-Qiao Chen</i></p>	GC	Aquaculture Nutrition
<p>Complementary Use of Multi-dimensional Gas Chromatography and Proton Transfer Reaction Mass Spectrometry for Identification of Rapeseed Oil Quality Indicators</p> <p><i>Authors: Tomasz Majchrzak, Wojciech Wojnowski, Tomasz Dymerski, Jacek Gębicki, and Jacek Namieśnik</i></p>	GCxGC	Food Analytical Methods
<p>New Degradation Pathways of the Key Aroma Compound 1-Penten-3-one during Storage of NFC Orange Juice</p> <p><i>Authors: Veronika Mall, Ines Sellami, and Peter Schieberle</i></p>	GC	Journal of Agricultural and Food Chemistry
<p>Development of a SBSE-TD method coupled to GC-MS and chemometrics for the differentiation of variety and processing conditions in peach juices</p> <p><i>Authors: Alexis Marsol-Vall, Mercè Balcells, Jordi Eras, and Ramon Canela-Garayoa</i></p>	GC	Food Chemistry
<p>Unveiling the lager beer volatile terpenic compounds</p> <p><i>Authors: Cátia Martins, Tiago Brandão, Adelaide Almeida, and Sílvia M Rocha</i></p>	GCxGC	Food Research International
<p>Co-fermentation of red grapes and white pomace: A natural and economical process to modulate hybrid wine composition</p> <p><i>Authors: Paméla Nicolle, Charlene Marcotte, Paul Angers, and Karine Pedneault</i></p>	GC	Food Chemistry
<p>Reactive Carbonyl Species as Key Control Point for Optimisation of Reaction Flavors</p> <p><i>Authors: Laurianne Paravisini, and Devin G Peterson</i></p>	GC	Food Chemistry



FOOD TESTING BIBLIOGRAPHY

LECO GCxGC Publications 2018

	Categories	Publication
Microbiome-metabolomics Analysis of the Impacts of Long-term Dietary Advanced Glycation End Products Consumption on the C57BL/6 Mouse Fecal Microbiota and Metabolite <i>Authors: Wanting Qu, Chenxi Nie, Jinsong Zhao, Xiyang Ou, Yingxiao Zhang, Shanchun Yang, Xue Bai, Yong Wang, Jiawei Wang, and Juxiu Li</i>	GC	Journal of Agricultural and Food Chemistry
Reference samples guide variable selection for correlation of wine sensory and volatile profiling data <i>Authors: Emma Sherman, James F Harbertson, David R Greenwood, Silas G Villas-Bôas, Oliver Fiehn, and Hildegard Heymann</i>	GCxGC	Food Chemistry
Unravelling wine volatile evolution during Shiraz grape ripening by untargeted hs-spme-GCxGC-TOFMS <i>Authors: Katja Šuklje, Silvia Carlin, Jan Stanstrup, Guillaume Antalick, John W Blackman, Campbell Meeks, Alain Deloire, Leigh M Schmidke, and Urska Vrhovsek</i>	GCxGC	Food Chemistry
Micro-organisms growing on rapeseed during storage affect the profile of volatile compounds of virgin rapeseed oil <i>Authors: Claudia Wagner, Anja Bonte, Ludger Brühl, Karsten Niehaus, Hanna Bednarz, and Bertrand Matthäus</i>	GC	Journal of the Science of Food and Agriculture
Metabotypes Related to Meat and Vegetable Intake Reflect Microbial, Lipid and Amino Acid Metabolism in Healthy People <i>Authors: Runmin Wei, Alastair B Ross, MingMing Su, Jingye Wang, Seu-Ping Guiraud, Colleen Fogarty Draper, Maurice Beaumont, Wei Jia, and Francois-Pierre Martin</i>	GC	Molecular Nutrition & Food Research
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Spoilage Marker Metabolites and Pathway Analysis in Chilled Tan Sheep Meat Based on GC-MS <i>Authors: Liqin You, Yansheng Guo, Ruiming Luo, Yanli Fan, Tonggang Zhang, Qianqian Hu, and Shuang Bo</i>	GC	Food Science and Technology Research



FOOD TESTING BIBLIOGRAPHY

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	Categories	Publication
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Identification of key odorants responsible for chestnut-like aroma quality of green teas <i>Authors: Yin Zhu, Hai-Peng Lv, Chen-Yang Shao, Suyong Kang, Yue Zhang, Li Guo, Wei-Dong Dai, Jun-Feng Tan, Qun-Hua Peng, and Zhi Lin</i>	GCxGC	Food Research International



FOOD TESTING BIBLIOGRAPHY

LECO GCxGC Publications 2017

	Categories	Publication
<p>Compositional analyses of diverse phytochemicals and polar metabolites from different-colored potato (<i>Solanum tuberosum</i> L.) tubers</p> <p><i>Authors: W. Lee, Y. Yeo, S. Oh, K. S. Cho, Y. E. Park, S. K. Park, and S. Y. Park</i></p>	GC	Food Science and Biotechnology
<p>Microbial succession and metabolite changes during traditional serofluid dish fermentation</p> <p><i>Authors: Q. Li, J. Kang, Z. Ma, X. Li, L. Liu, and X Hu</i></p>	GC	LWT - Food Science and Technology
<p>Metabolomics approach to understand mechanisms of β-N-oxalyl-L-α,β-diaminopropionic acid (β-ODAP) biosynthesis in grass pea (<i>Lathyrus sativus</i> L.)</p> <p><i>Authors: F. Liu, C. Jiao, C. Bi, Q. Xu, P. Chen, A. L. Heuberger, and H. B. Krishnan</i></p>	GC	J. Agric. Food Chem.
<p>The metabolomics responses of chinese mitten-hand crab (<i>eriocheir sinensis</i>) to different dietary oils</p> <p><i>Authors: Q.-Q. Ma, Q. Chen, Z.-H. Shen, D.-L. Li, T. Han, J.-G. Qin, L.-Q. Chen, and Z.-Y. Du</i></p>	GC	Aquaculture
<p>Key odorants of lazur, a polish Mold-Ripened cheese</p> <p><i>Authors: M. A. Majcher, K. Myszk, A. Gracka, A. Grygier, and H. H. Jeleń</i></p>	GC	J. Agric. Food Chem.
<p>Development of a SBSE-TD method coupled to GC-MS and chemometrics for the differentiation of variety and processing conditions in peach juices</p> <p><i>Authors: A. Marsol-Vall, M. Balcells, J. Eras, and R. Canela-Garayoa</i></p>	GC	Food Chemistry
<p>Interactions of insoluble residue from enzymatic hydrolysis of brewer's spent grain with intestinal microbiota in mice</p> <p><i>Authors: J. Maukonen, A.-M. Aura, P. Niemi, G. S. Raza, K. Niemelä, J. Walkowiak, I. Mattila, K. Poutanen, J. Buchert, and K.-H. Herzig</i></p>	GCxGC	J. Agric. Food Chem.
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<p>Effects of pan cooking on micropollutants in meat</p> <p><i>Authors: C. Planche, J. Ratel, P. Blinet, F. Mercier, M. Angénieux, C. Chafey, J. Zinck, N. Marchond, S. Chevolleau, P. Marchand, G. Dervilly-Pinel, T. Guérin, L. Debrauwer, and E. Engel</i></p>	GCxGC	Food Chemistry



FOOD TESTING BIBLIOGRAPHY

LECO GCxGC Publications 2017

	Categories	Publication
<p>Unveiling elderflowers (<i>Sambucus nigra</i> L.) volatile terpenic and norisoprenoids profile: Effects of different postharvest conditions</p> <p><i>Authors: Â. C. Salvador, A. J. Silvestre, and S. M. Rocha</i></p>	GCxGC	Food Chemistry
<p>Characterisation of the key aroma compounds in white alba truffle (<i>tuber magnatum pico</i>) and burgundy truffle (<i>tuber uncinatum</i>) by means of the sensomics approach</p> <p><i>Authors: P. C. Schmidberger and P. Schieberle</i></p>	GCxGC	J. Agric. Food Chem.
<p>Quantitation of nine lactones in dairy cream by stable isotope dilution assays based on novel syntheses of Carbon-13-Labeled γ-Lactones and Deuterium-Labeled δ-Lactones in combination with comprehensive Two-Dimensional gas chromatography with Time-of-Flight mass spectrometry</p> <p><i>Authors: J. Schütt and P. Schieberle</i></p>	GCxGC	J. Agric. Food Chem.
<p>Interaction of human serum albumin with volatiles and polyphenols from some berries</p> <p><i>Authors: R. B. Shafreen, T. Dymerski, J. Namieśnik, Z. Jastrzębski, S. Veerasilp, and S. Gorinstein</i></p>	GCxGC	Food Hydrocolloids
<p>Reference samples guide variable selection for correlation of wine sensory and volatile profiling data</p> <p><i>Authors: E. Sherman, J. F. Harbertson, D. R. Greenwood, S. G. Villas-Bôas, O. Fiehn, and H. Heymann</i></p>	GCxGC	Food Chemistry
<p>Nutritional quality of maize-groundnut composite flours and resultant porridges</p> <p><i>Authors: M. C. Temba, P. Njobeh, D. Ndinteh, and E. Kayitesi</i></p>	GCxGC	Nutrition & Food Science
<p>Microorganisms growing on rapeseed during storage affect the profile of volatile compounds of virgin rapeseed oil</p> <p><i>Authors: C. Wagner, A. Bonte, L. Brühl, K. Niehaus, H. Bednarz, and B. Matthäus</i></p>	GC	J. Sci. Food Agric.
<p>Metabolite profiling of a Zinc-Accumulating rice mutant</p> <p><i>Authors: Y. Wang, S. Mei, Z. Wang, Z. Jiang, Z. Zhu, J. Ding, D. Wu, and X. Shu</i></p>	GC	J. Agric. Food Chem.
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